Simulations of Ultrashort-Pulse Laser Solid-Target Interactions

Ing. Ondřej Klimo


A dissertation thesis submitted to the CTU in Prague in partial fulfillment of the requirements for the degree of Doctor of Philosophy (PhD)

13th April 2007
Abstract

This thesis is based on a theoretical study of short-pulse laser interactions with solid targets and related phenomena. We utilize relativistic electromagnetic code based on the Particle-in-Cell method to describe laser interaction with target and subsequent transport of fast charged particles in plasma. Our code is one-dimensional in space and three dimensional in velocity and it evolved from the code LPIC++. In the frame of this work the code has been improved by incorporating ionization physics and revision of binary collisional algorithm. The theories of collisional ionization, electric field ionization and elastic collisions in plasma are reviewed and our computational algorithms based on these theories are described in details. Our code has been applied to study acceleration of electrons in the laser target interaction region, propagation of hot electron beam inside a cold dielectric target and acceleration of ions from the rear side of laser irradiated thin foils.

We demonstrate that electric field ionization decreases efficiency of electron acceleration due to resonance absorption in plasma with slowly decreasing undercritical density profile. Using this density profile our results show a good agreement with recent experiments of K-α emission from laser irradiated thin foils realized by the group of Dr. Zhavoronkov [1]. It is also found that electric field ionization has a significant effect on the angular distribution of electrons accelerated by high intensity laser pulses, namely it increases the divergence of the hot electron beam.

In the study of hot electron beam transport in cold dielectric target carried out with Prof. Tikhonchuk [2] we demonstrate that propagation of the beam is determined by self-induced quasistatic electric field. This field ionizes the target and provides seed population of free return current electrons. The shape and amplitude of the field depend on the hot electron beam density which results in relation between the beam density and its propagation velocity and energy losses.

In collaboration with Dr. Brantov [3] acceleration of ions from the rear side of laser irradiated thin foils composed of multiple species of ions is studied. It is demonstrated that the process of acceleration of lighter ions and in the presence of heavier ions results in formation quasi-monoenergetic peak in the distribution of lighter ions observed in recent experiments.
Declaration

This dissertation is the result of my own work, except where explicit reference is made to the work of others, and has not been submitted for another qualification to this or any other university.

Prague, 13th April 2007

Ondřej Klimo
Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisor, Doc. Ing. Jiří Limpouch, CSc. for his guidance, encouragement and his patience with me. I am very indebted to him for giving me many helpful suggestions regarding my work and especially this thesis. I appreciate his supervision very much. He has given me enough freedom to make my own mistakes and learn from them but at the same place he has gently pushed me forward in the right direction.

I am very grateful to Prof. Tikhonchuk, the supervisor during my stay in Bordeaux. It was pleasure for me to work under his leadership not only for his ever interesting ideas and suggestions but also for his inspiring enthusiasm for physics.

Further, I would like to thank very much to Dr. Zhavoronkov, Dr. Brantov and PhD student Debayle. I hope that our collaboration was beneficial not only for me.

I also take this opportunity to express my profound gratitude to my beloved parent.

Finally, support by the following projects is also thankfully acknowledged:

- Czech Ministry of Education, Youth and Sports, project No. LC528
- COST Office, project No. STSM-P14-01494
- Czech Science Foundation, project No. 202/06/0801
- Czech Ministry of Education, Youth and Sports, project No. FRVS 2471/G1

Many other people deserve my thanks but I must cut the list somewhere and I do it here. Excuse me and thank you.
## Contents

1 Introduction

1.1 Aims and new contributions of the work .................................. 3
   1.1.1 Modifications of the PIC code ........................................ 3
   1.1.2 Applications of the adapted code .................................. 4
1.2 Layout of the thesis ......................................................... 5

2 Short pulse laser interaction with solid target .......................... 7
   2.1 Chirped pulse amplification technique ................................ 7
   2.2 Laser prepulses ............................................................ 8
   2.3 Preplasma ................................................................. 9
   2.4 Laser absorption and charged particle acceleration ................. 12
      2.4.1 Basic parameters ..................................................... 12
      2.4.2 Laser absorption mechanisms .................................... 14
      2.4.3 Heating ............................................................... 16
      2.4.4 Acceleration of charged particles ............................... 18
   2.5 Hot electron population and its applications ....................... 24
      2.5.1 K-α radiation ....................................................... 25
      2.5.2 Ion acceleration .................................................... 27
      2.5.3 Fast ignition of inertial confinement fusion targets .......... 28

3 Theoretical models and computer simulations .......................... 30
   3.1 Kinetic description and its implementation .......................... 32
   3.2 Particle-In-Cell method .................................................. 33
3.2.1 Particle-mover .................................................. 35
3.2.2 Field-solver ..................................................... 35
3.2.3 LPIC++ code and its changes ............................... 36
3.3 Variable plasma ionization in the Particle-In-Cell model .... 38
  3.3.1 Electric field ionization ..................................... 39
  3.3.2 Implementation of electric field ionization ............... 48
  3.3.3 Collisional ionization ....................................... 52
  3.3.4 Implementation of collisional ionization ................. 60
  3.3.5 Recombination ................................................ 61
3.4 Elastic collisions .................................................. 62
  3.4.1 Distant encounters - Coulomb collisions ................ 63
  3.4.2 Close encounters - Elastic electron–atom scattering .... 72
  3.4.3 Implementation of elastic collisions ..................... 73
3.5 Short review of existing PIC codes ............................ 74
3.6 Monte Carlo electron transport calculations .................. 75

4 Results and discussions ............................................ 77
  4.1 Acceleration of electrons ...................................... 77
    4.1.1 Energy distribution of hot electrons ................... 80
    4.1.2 Angular distribution of hot electrons ................ 94
  4.2 Propagation of hot electrons inside the target ............ 112
    4.2.1 Hot electron beam propagation models ................ 114
    4.2.2 Hot electron beam studied in this work ............... 116
    4.2.3 Computational model of electron beam propagation .... 117
    4.2.4 Results of hot electron beam propagation and their discussions 123
    4.2.5 Summary and conclusions about hot electron beam propagation 136
  4.3 Acceleration of ions from the rear surface of thin foil target 137
4.3.1 Target Normal Sheath Acceleration - theory and simple estimates . . . 138
4.3.2 Energy distribution of accelerated ions . . . . . . . . . . . . . . . . . 140
4.3.3 Laser irradiated water droplet experiments . . . . . . . . . . . . . . . 141
4.3.4 PIC model of TNSA . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 141
4.3.5 Results and discussions of PIC simulations of TNSA . . . . . . . . . 143

5 Summary and conclusions 154

Bibliography 161

List of Figures 180

List of Tables 183
1 INTRODUCTION

In a few last decades techniques of generation and amplification of ultrashort laser pulses have been developed and put into practice. No doubt that this was one of the milestones in nowadays science. It afforded researchers opportunity to study both ultrafast and very high energy density phenomena in laboratories. Up to now the field of generation and amplification of ultrashort intense laser pulses is still undergoing very rapid progress. The scales of laser pulse parameters as well as processes taking place during the interaction with matter change every couple of years and bringing new questions to our attention again and again while leaving many others still unresolved. The following work attempts to address some of these questions theoretically and to shed more light on certain recently obtained experimental results.

Much of the interest in short laser pulses started after the technique of Chirped Pulse Amplification (CPA), originally developed for microwave (radar) applications, was adapted for laser radiation \([4]\). Thanks to this technique, it is now possible to increase energy of ultrashort laser pulses by many orders of magnitude without the risk of damage of the amplifier medium. State of the art laser systems producing intense ultrashort laser pulses are mostly based on self-mode-locked Ti:Sapphire oscillator. This oscillator has broad-bandwidth around the central wavelength of about 800 nm and through the use of mode-locking technique it can produce pulses only several tens of cycles long.

On one hand the CPA technique made it possible to further increase power of the most powerful short pulse laser systems, on the other hand it enabled construction of relatively cheap, powerful, and small laboratory table top lasers. Huge CPA laser systems with Nd:glass power amplifiers are able to deliver up to tenths of kJ in a single laser pulse with duration of order of tenths of ps thus giving the peak power in excess of PW \([5]\). These systems operate at a relatively low repetition rate of order of several shots per hour. Smaller CPA lasers produce less energetic, mostly mJ, pulses with somewhat shorter duration of tens of fs and the peak power exceeding TW. They have higher repetition rate up to kHz \([6]\) and they are installed in many laboratories around the world.

Ultrashort laser pulses of lower intensity find their applications in various fields of science and technology including chemistry, biology, medicine, communications etc.\([7]\). In the high and ultrahigh intensity regime interaction of ultrashort laser pulses with matter results in warm plasma formation and acceleration of charged particles up to very high energies. The most important applications than rely on these energetic particles and their transport in matter, e.g. generation of ultrashort pulse X and \(\gamma\)-ray radiation for ultrafast imaging of samples and processes in them \([8,9]\), heating of fusion fuel inside a precompressed pellet in the Fast...
Ignition (FI) concept of Inertial Confinement Fusion (ICF)\cite{10}, medical therapy using energetic protons\cite{11} etc.

This work is concerned with theoretical study of interaction of ultrashort intense laser pulses with solid density targets. At the very beginning of the interaction energy of the laser pulse absorbed in a thin surface layer of the target is sufficiently high to heat and ionize the matter. Target surface is thus converted into dense plasma and the interaction takes place essentially between the strong electromagnetic field of the laser wave and the plasma medium. Even if most of the physics of laser plasma interaction is described by four Maxwell’s equations and the Lorentz force equation, these equations are actually very difficult to solve for realistic problems. Laser plasma is often rapidly evolving, highly nonlinear, and even unstable. Thus theoretical models describing the interaction can often be solved only numerically.

Basically there are two principal types of theoretical models suitable to describe temporal evolution of plasma. Models of the first type are called kinetic and they treat plasma as an ensemble of charged particles. The governing equation of kinetic theory, Vlasov equation, states the temporal evolution of charged particle distribution functions in macroscopic electric and magnetic fields. Kinetic models are therefore very detailed. In the second type of theoretical models plasma is considered as fluid. Equations of the fluid model are derived from the kinetic plasma theory by taking the moments of Vlasov equation with the Boltzmann-Maxwell velocity distributions of particles assumed. In the fluid model plasma is in a local thermal (not thermodynamic) equilibrium or in other words the scales of spatial and temporal variations of intensive quantities are large compared to collisional mean free path and slow compared to the collisional frequency respectively. The models based on fluid theory are more macroscopic in the sense that they can be better applied to problems on larger spatial and longer temporal scales.

In ultrashort pulse laser target interactions the assumption of local Boltzmann-Maxwell velocity distributions of charged particles is often violated and kinetic plasma description must be applied. Numerical solution of the Vlasov-Maxwell system of equations is dominated by simulation codes based on the Particle-In-Cell method. So is also the simulation code used throughout the rest of this work. The code we use evolved from the code LPIC++\cite{12} originally developed in the Max-Planck Institute für Quantenoptik in Garching. This code is relativistic and electromagnetic and it describes distributions of charged particles in only one spatial but all three velocity dimensions. The code LPIC++ was previously modified in the frame of two master theses\cite{13,14} and enhanced to treat binary Coulomb collisions.
1.1 Aims and new contributions of the work

The aim of present work is to study ultrashort intense laser pulse interactions with solid targets. During these interactions laser energy coupling into hot electrons is often very efficient. It may even dominate over all other laser absorption processes. The phenomena related with acceleration of hot electrons and their transport inside the target are also of fundamental importance for various applications. For these reasons our investigation concentrates particularly on the population of hot electrons, parameters characterizing this population and processes leading to its formation. Transport of hot electron beam further inside the target and the related phenomena including target ionization, induction of self-consistent fields, rise of the neutralizing return current and ion acceleration at the rear surface of a foil target are studied as well.

1.1.1 Modifications of the PIC code

In the frame of this work the PIC code LPIC++ has been modified and its applicability has been extended by the addition of new physical processes and some functionality options. Namely, the code changed significantly in the following ways:

- **Variable plasma ionization has been implemented.**
  In the interactions of ultrashort intense laser pulses with targets the ionization process is often very fast. The average ion charge may increase even several times during the interaction and therefore incorporating variable plasma ionization into the theoretical description is indeed important. Both most frequent plasma ionization processes are substantial, the collisional as well as the one directly induced by the optical and the plasma electric fields. The former one operates efficiently in the dense matter inside the target while the later is dominant in the underdense plasma where the laser pulse propagates. Consequently, the algorithm of plasma ionization implemented into the code LPIC++ takes both these ionization processes into account. PIC codes suitable for simulations of short pulse laser target interaction with variable plasma ionization are computationally expensive. These codes are therefore relatively rare and currently they could probably be counted on the fingers of one hand. In this respect our code is a rather unique tool at this moment and it affords us opportunity to bring some new insights into the dynamics of short pulse laser plasma interaction.

- **Binary collisional algorithm has been revised.**
  The algorithm of binary collisions previously implemented into the code LPIC++ is based on a relatively obsolete method with limited applicability. To be applicable to certain simulations of hot electron transport in a cold solid density dielectric target
binary collisional algorithm had to be revised. The newly implemented computational procedure is valid over larger range of collisional frequencies and takes into account electron elastic scattering from neutral atoms as well.

- **Target may newly consist of multiple species of ions/atoms.**
  To make the code LPIC++ more realistic and produce results in a better agreement with experiments the code has been extended to treat targets composed of multiple elements. This enhancement is of particular importance for targets consisting of multiple layer from different materials or for the case when the target material is already a compound of several elements, e.g. water, polyethylene etc. Multiple ion species constitution of the target manifest itself especially in the calculations of ion acceleration where the ion charge to mass ratios of is very important. The multiple species extension of the code is however purely programming task and will not be discussed further.

### 1.1.2 Applications of the adapted code

In the frame of this work the adapted PIC code has been applied to study especially those issues where its new properties could be beneficially utilized. Namely these are the following ones:

- **Impact of variable plasma ionization on the energetic spectrum of accelerated electrons.**
  We have demonstrated that if the plasma density profile on the target surface formed during the interaction with the laser prepulse is slowly decreasing in the undercritical part, the optical laser field ionization may significantly lower the coupling efficiency of the main laser pulse energy into hot electrons. Hydrodynamic code Ehybrid has been utilized to calculate the density profile of plasma produced by the laser prepulse. This profile is used as an initial density profile in PIC simulations. Energy spectra of hot electrons accelerated during the main laser pulse interaction with target have been calculated by the PIC code and postprocessed by a Monte Carlo electron transport code specially tailored to calculate ionization in the K shells of atoms and the subsequent emission of K-\(\alpha\) photons. Due to collaboration with Dr. Zhavoronkov from Max-Born Institute in Berlin the calculated emission of K-\(\alpha\) photons from the short pulse laser irradiated foil targets has been successfully compared with experiments.

- **Impact of variable plasma ionization on the angular distribution of accelerated electrons.**
  It has been demonstrated that electrons released by the optical laser field ionization from inner ionic shells around the maximum of the short intense laser pulse often find themselves on a significantly distinct position in the momentum phase space than other
already free electrons. Upon acceleration these newborn electrons keep a high transverse velocity component in comparison with the bulk of other hot electrons and they increase the angular divergence of the laser accelerated hot electron beam. This divergence is very important parameter in many applications which rely to laser accelerated hot electron beams.

- **Propagation of dense hot electron beam in cold solid dielectric material.**
  In collaboration with Prof. Tikhonchuk and PhD student Debayle from the CELIA laboratory at the University of Bordeaux in France we have adapted the PIC code to simulate propagation of laser accelerated hot electron beam in a cold solid density dielectric target. During the hot electron beam propagation dielectric target is ionized by the self-induced electric field which rise in consequence of significant charge separation. To neutralize the parts of the target where the negative charge is missing newly released electrons are accelerated toward the beam and they form a return current. Our code has been used to study ionization of the target and its conversion into a plasma, heating of the plasma, formation of the return current, and the dynamics of the electron beam in the self-induced electric field. To our knowledge it is for the first time when a PIC code has been successfully applied to study the phenomena related to propagation of hot electron beam in a dielectric material.

- **Ion acceleration by the self-consistent electric field at the rear surface of a foil target.**
  Our PIC simulation code has also been applied to study acceleration of ions from the rear surface of laser irradiated foil target. In collaboration with Prof. Tikhonchuk and Dr. Brantov we have confirmed that in the presence of multiple species of ions at the target rear side a quasi-monoenergetic spectra of the lighter species of ions may be formed. The mechanism of quasi-monoenergetic spectra formation has been demonstrated on the simulations of acceleration of protons and deuterons from the water and heavy water targets respectively. Our results have been successfully compared with recent experiments.

### 1.2 Layout of the thesis

This thesis is divided into five chapters and organized in the following manner. At the beginning of Chapter 2 a short introduction into the generation and amplification of ultrashort laser pulses is given. Than the plasma formation process on the surface of a solid target is discussed and the main short pulse laser absorption processes are reviewed. Particular attention is paid to the processes resulting in acceleration of electrons and formation of the hot electron population. At the end of Chapter 2 the most relevant applications of hot electrons are mentioned.

Introduction into the theoretical description of plasma is given in the beginning of Chap-
ter 3. As the simulation code used throughout this work is based on the PIC method this method is discussed in more details. The code LPIC++ is described in details and put into the context of other simulation codes and methods. The processes of the optical and plasma electric field ionization and the collisional ionization are subsequently discussed and their implementation into the code is described. At the end of Chapter 3 binary collisions in plasma are analyzed and the modifications of collisional algorithm implemented into the code are stated.

In Chapter 4 applications of the adapted PIC code to study short pulse laser solid target interactions and related processes are presented in details. The results presented in this chapter have been briefly described in the previous Section 1.1.2. In Chapter 4 they follow in the same order as above.

In the last chapter, the main results of this work are summarized and our conclusions and prospects for the future work are presented. The list of publications in peer-reviewed journals and contributions at international conferences is given at the end.
CHAPTER 2. SHORT PULSE LASER INTERACTION WITH SOLID TARGET

2 ULTRASHORT HIGH INTENSITY LASER PULSE INTERACTION WITH SOLID TARGET

2.1 Chirped pulse amplification technique

The technique of chirped pulse amplification technique was originally developed for microwave devices (radars). In 1985 the team of Mourou proposed that similar technique can be applied to optical laser radiation [4] and in 1988 the first CPA laser was successfully demonstrated [15]. Since then the CPA technique was successfully applied to many conventional master-oscillator power-amplifier (MOPA) laser system, in which a tiny prototype laser pulse is passed through a chain of optical power amplifiers. A simplified diagram scheme of the CPA laser system is presented in Figure 2.1.

Figure 2.1: Schematic diagram of the CPA laser system.
2.2 LASER PREPULSES

In a CPA laser system, an ultrashort tiny laser pulse is first stretched to a much longer duration by means of a strongly dispersive element, the stretcher (e.g. a grating pair). In stretcher the gratings are arranged so that the low-frequency component of the laser pulse travels a shorter path than the high-frequency one. The laser pulse than becomes positively chirped and has longer duration than the original one by a factor of $10^3$ to $10^5$. Intensity of the stretched pulse is sufficiently low and safe for introducing the pulse into the gain medium and amplify it by a factor of $10^6$ or even more. After the gain medium, the amplified pulse passes through a dispersive compressor, an element with opposite dispersion to the stretcher, which removes the chirp and recompresses the pulse temporally to a duration similar to the input pulse. After passing through the compressor peak power of the again ultrashort laser pulse typically exceeds TW. CPA technique thus makes it possible to achieve very high peak power and on the other hand to miniaturize laser systems and build them on a tabletop. Detailed information about the development of ultrashort pulse high intensity laser systems as well as the state of the art techniques used for generation and amplification of these laser pulses can be found for example in the review papers [16, 17, 18].

2.2 Laser prepulses

Most of the energy of an intense ultrashort CPA laser pulse is concentrated in the main pulse with a very short temporal duration ranging from several up to hundreds of fs. The main laser pulse is however commonly preceded by femtosecond prepulses and Amplified Spontaneous Emission (ASE) [19]. The femtosecond prepulses originate from the imperfect isolation of the main pulse from its neighboring pulses in the master-oscillator or from the pulses leak from the early main pulse passes. The strength and structure of femtosecond prepulses depends on the quality of optical components and the laser configuration and generally these prepulses can be almost completely cleaned away e.g. using additional Pockles cells [20]. The ASE on the other hand is coming from the amplifier chain and it is a general feature found in all amplification systems operating based on population inversion process. ASE typically lasts for several ns and its intensity contrast ratio to the main pulse is a function exponentially growing with time up to about $10^{-6}$. There exist several special techniques to improve this intensity contrast ratio using plasma mirrors, saturable absorbers [21], etc. The third and also the last kind of the laser prepulse comes from imperfect recompression of the amplified pulse. The amplification process introduces some extra dispersion to the main laser pulse and it is difficult to correct it in the compressor. The imperfect recompression introduces to the main laser pulse a pedestal which starts about one picosecond prior to the main pulse and has an intensity contrast ratio of about $10^{-4}$. There exist some methods to compensate for the dispersion variation introduced by the amplifiers, for example adjustment of the angle of incidence between the stretcher and compressor. A typical temporal power profile of an
prepulse uncleaned laser pulse is shown in Figure 2.2. A number of techniques to clean away all three kinds of prepulses have been proposed in recent years, e.g. [22, 23]. However, most of these techniques are still in development and not yet well established.

### 2.3 Preplasma

In the early years of application of the CPA technique the peak intensity of ultrashort laser pulses even if they were tightly focused on the target rarely exceeded $10^{16}$ W/cm$^2$. The contrast ratio of prepulses preceding the main laser pulse was therefore usually sufficiently high to avoid creation of almost any preplasma. However, the peak intensity of the nowadays most powerful CPA laser systems reaches $10^{21}$ W/cm$^2$. The peak intensity of smaller lasers is several orders of magnitude lower but still usually well above $10^{17}$ W/cm$^2$. In the case of such high main laser pulse intensity, even if some prepulses are cleaned away and the contrast ratio is improved, the flux of radiation incident on the surface of the target before the main pulse arrival is sufficient to convert the surface layer of the target into a plasma. Even at radiation intensities as low as about $10^{10}$ W/cm$^2$ significant melting and evaporation of material from
the target surface into a background gas is observed in laser ablation experiments with several ns long Nd:YAG laser pulses [24]. When the prepulse radiation intensity is about two orders of magnitude higher (10^{12} \text{ W/cm}^2) ionization starts to be important and the matter subjected to this radiation is converted into a plasma.

The strength and the rate of melting, evaporation, ionization and plasma heating determine the temperature, the degree of ionization and the scale and shape of the density profile of the plasma formed prior to the main laser pulse arrival to the target. These parameters characterize the preplasma and they depend not only on the laser prepulses but also on the target material properties. It is reasonable to assume that the main laser pulse interacts with a layer of plasma on the target surface whose properties can be estimated from the particular knowledge of laser prepulses.

The temporal scale on which preplasma is created (the duration of ASE or the separation of higher intensity femtosecond prepulse from the main laser pulse) is usually longer than the thermalization time for electrons and ions. It is thus reasonable to assume that both electrons and ions are in some kind of equilibrium, namely that they acquire Boltzmann-Maxwell energy distributions. The temperature of preplasma generally ranges from several up to hundreds of eV. Knowing this temperature and the ion or atom density it is possible to approximately calculate the degree of ionization, for example the average atom model [25] can be used. When direct ionization by the optical field of laser prepulses (i.e. multiphoton, tunneling etc.) is negligible and only the collisional ionization by thermal electrons is to be taken into account, it is reasonable to expect that plasma temperature is not significantly higher than the lowest ionization potential of ions.

It is a rather complicated task to calculate the values of both the temperature and the plasma ionization degree accurately. Nevertheless, an approximate estimate can be obtained in particular cases. Let us give an example here. An aluminum target is being irradiated by ASE prepulse with the average intensity $I_{\text{avg}} = 10^{11} \text{ W/cm}^2$ and duration of $\tau = 1 \text{ ns}$. It is reasonable to assume that the target absorbs about $\eta = 30\%$ of the prepulse energy. Aluminum is an optically thick material for the Ti:Sapphire laser wavelength. Therefore, most of the prepulse energy is absorbed in a thin surface layer of the target where it is converted into thermal energy. This applies until the plasma formed on the target surface expands significantly. Aluminum is on the other hand a relatively good heat conductor with relatively high thermal diffusivity ($\alpha = 0.7 \text{ cm}^2/\text{s} \ [26]$). Heat conduction must therefore be taken into account and the energy density in the target surface layer is then calculated as [27]

$$U_{\text{surf}} = \frac{\eta I_{\text{avg}} \sqrt{\tau}}{\sqrt{\alpha}}. \quad (2.1)$$

For the above given example this energy density is approximately 1.14 MJ/cm$^3$. In the solid
density aluminum material there are three electrons in the valence band. There is no energy gap between valence and conduction band in aluminum and these electrons can move through the target almost like the free electrons in plasma. First of all the absorbed energy is thus distributed among these electrons. The number density of valence electrons in solid aluminum is about $1.8 \times 10^{23} \text{ cm}^{-3}$ and the resulting average thermal energy per valence electron of about 40 eV seems to be quite reasonable. Also the assumption that absorbed energy is distributed only among the valence band electrons is legitimate as the ionization potential for ionization of electrons in the next outermost shell is already 120 eV.

At temperature of more than several eV free electrons can propagate several millimeters on the time scale of the order of nanosecond. It is thus clear that preplasma is not confined to the target surface but it starts to expand toward vacuum and form a density profile. On the other hand, electrons must be followed by ions to maintain the quasineutrality. Preplasma expansion velocity is therefore a function of both electron temperature and ion charge to mass ratio. The simplest theory applied to describe this situation is the isothermal model for a freely expanding plasma [28, 29].

In this model it is assumed that energy spent by electrons to accelerate ions is supplied by the laser prepulse and thus the temperature is constant. The quasistatic electric field accelerating ions is determined from the electron pressure and the ion fluid is described by the continuity and mobility equations. With quasineutrality assumption a self-similar solution can be obtained. The isothermal expansion model results in an exponential plasma density profile on the target surface with the characteristic length

$$L = c_s t,$$

where $c_s = \sqrt{ZT_e/M}$ is the ion sound speed ($Z$, $M$ and $T_e$ are the ion charge and mass and electron temperature respectively) and $t$ is the expansion time. The exponential density profile is widely used as a starting point for numerical simulations and analytical models for its simplicity. However, its correctness is arguable for the following reasons. Firstly, the assumption of constant electron temperature and ion charge over the entire preplasma volume and the expansion time is not necessarily satisfied, secondly the quasineutrality condition is violated near the head of the ion expansion front [30], and thirdly the isothermal model does not account for the laser light pressure which can exceed the thermal pressure near the critical surface and thereby give rise to density profile steepening in this region. For these reasons it is better to calculate the density profile of preplasma on the target surface using a hydrodynamic code specially tailored for interaction of low intensity radiation with the target. Using the isothermal model for the example given above, i.e. assuming 0.5 ns long expansion of aluminum plasma with temperature of 20 eV and ion charge of 3, will result in preplasma density profile with the characteristic length of more than 7 \(\mu\text{m}\). For illustration, the preplasma density profile, temperature and average ion charge calculated by the atomic/hydrodynamic
2.4. LASER ABSORPTION AND CHARGED PARTICLE ACCELERATION

Figure 2.3: Plasma density profile, temperature and average ion charge calculated by the hydrodynamic code Ehybrid [31] for irradiation of Germanium target with a ns Ti:Sapphire laser pulse with intensity $10^{11}$ W/cm$^2$. The laser pulse is incident from the right and the spatial coordinate is defined with respect to the initial target surface.

Preplasma temperature and average ion charge do not significantly influence the subsequent interaction of the main laser pulse with the target. These parameters increase rapidly already at the rising edge of the main laser pulse and their initial values are thus washed away. On the other hand, the density profile of preplasma and particularly its shape and scale are indeed important as they determine the laser absorption process. Usually, the density profile does not change significantly during the interaction of the main short laser pulse so that it is defined by the prepulses. If the preplasma density gradient is long the main pulse interaction takes place in the underdense plasma and a substantial part of laser energy is absorbed in front and near the critical surface. On the contrary, in the case of step-like vacuum-plasma boundary the main laser pulse interacts directly with the overdense plasma in the regime of skin effect.

2.4 Laser absorption and charged particle acceleration

2.4.1 Basic parameters

Plasma can be described as a highly polarizable dielectric medium which supports collective oscillations due to self-consistent coupling between charged particles and electric and magnetic
fields. The ability of plasma to transmit (permit) electric field oscillating with high frequency is called dielectric constant (permittivity). In isotropic plasma this dielectric constant is a scalar function of the field frequency \( \omega \) (a second rank tensor in an anisotropic plasma) and thus plasma is also a dispersive medium. According to the generalized Drude model plasma dielectric constant can be defined in dimensionless units as

\[
\varepsilon_r = 1 - \frac{\omega_p}{\omega (\omega + i \nu_{ei})},
\]

where \( \omega_p \) is the plasma frequency and \( \nu_{ei} \) is the frequency of electron-ion Coulomb collisions. The plasma frequency in general includes contribution from both high frequency electron oscillations and low frequency ion oscillations. As the ion contribution is negligible on the very short time scale considered in this work, plasma frequency includes only the electron component here and it is defined as

\[
\omega_p = \sqrt{\frac{e^2 n_e}{\varepsilon_0 m_e}}.
\]

Here, \( n_e \) stands for the free electron density, \( e \) for the electron charge, \( \varepsilon_0 \) for the permittivity of free space and \( m_e \) for the electron mass. Plasma frequency characterizes the speed with which plasma electrons respond to the local electric field.

If electron-ion collisions are neglected plasma dielectric constant (relative permittivity) can be expressed as

\[
\varepsilon_r = 1 - \frac{n_e}{n_c},
\]

where the constant \( n_c \) denotes the critical density which is defined as

\[
n_c = \frac{\omega_p^2 \varepsilon_0 m_e}{e^2}.
\]

For laser wave with wavelength 800 nm (Ti:Sapphire laser) the critical density is about \( 1.75 \times 10^{21} \text{ cm}^{-3} \). At the point where local free electron density equals to the critical one, i.e. \( n_e = n_c \), plasma dielectric constant becomes zero and electromagnetic wave with frequency \( \omega \) cannot further propagate. In a more general case when an electromagnetic wave propagates through plasma at an arbitrary angle \( \theta \) with respect to the plasma density gradient, this wave can penetrate only to the point where the dielectric constant \( \varepsilon_r \) equals to \( \sin^2 \theta \). Behind this point the wave is exponentially damped and it vanishes on a distance of the order of skin depth \( l_s \) defined as

\[
l_s = \frac{c}{\omega_p} \left(1 - \frac{\omega^2}{\omega_p^2 \cos^2 \theta} \right)^{-1/2}.
\]
2.4. LASER ABSORPTION AND CHARGED PARTICLE ACCELERATION

Figure 2.4: Schematic view on the preplasma density profile with the critical density and the laser reflection point highlighted. Angle $\theta$ denotes the laser incidence angle with respect to the plasma density gradient.

At the point where $\varepsilon = \sin^2 \theta$ the wave is specularly reflected. Propagation and reflection of an obliquely incident laser wave is schematically demonstrated in Figure 2.4.

2.4.2 Laser absorption mechanisms

Depending on the preplasma density profile and target material, laser intensity and angle of incidence, laser wavelength and polarization and finally pulse shape and duration, the laser pulse is absorbed, reflected or eventually converted into different kind of radiation with variable efficiency. Generally, energy of the laser pulse absorbed in plasma is spend to increase temperature and the mean ion charge or to accelerate charged particles to very high energies. The most important laser absorption processes are collisional absorption (inverse bremsstrahlung),
2.4. LASER ABSORPTION AND CHARGED PARTICLE ACCELERATION

<table>
<thead>
<tr>
<th>Absorption mechanism</th>
<th>Heating × Acceleration</th>
<th>Type of process</th>
<th>Conditions for high efficiency</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collisional absorption</td>
<td>Heating</td>
<td>collisional</td>
<td>$L \gtrsim \lambda$ $\lambda_{mfp} = \nu_{ei} &lt; l_s$</td>
<td>[32,33,34]</td>
</tr>
<tr>
<td>Normal skin effect</td>
<td>Heating</td>
<td>collisional</td>
<td>$L \rightarrow 0$ $\lambda_{mfp} &lt; l_s$</td>
<td>[35]</td>
</tr>
<tr>
<td>Anomalous skin effect</td>
<td>Heating</td>
<td>collisionless</td>
<td>$\lambda_{mfp} \gtrsim l_s$, $v_{osc} &lt; v_t$, $\theta = 0^\circ$, $v_t/\omega &gt; l_s$</td>
<td>[36]</td>
</tr>
<tr>
<td>Sheath inverse bremsstrahlung</td>
<td>Heating</td>
<td>collisionless</td>
<td>$\lambda_{mfp} \gtrsim l_s$, $v_{osc} &lt; v_t$, $\theta = 0^\circ$, $v_t/\omega &lt; l_s$</td>
<td>[37]</td>
</tr>
<tr>
<td>Sheath transit absorption</td>
<td>Heating</td>
<td>collisionless</td>
<td>$\lambda_{mfp} \gtrsim l_s$, $v_{osc} &lt; v_t$, $\theta &gt; 0^\circ$</td>
<td>[38]</td>
</tr>
<tr>
<td>Vacuum heating</td>
<td>Acceleration</td>
<td>collisionless</td>
<td>$L &lt; v_{osc}/\omega$, $v_{osc} &gt; v_t$ $\theta &gt; 0^\circ$, p-polarization</td>
<td>[39]</td>
</tr>
<tr>
<td>Resonance absorption</td>
<td>Acceleration</td>
<td>collisionless</td>
<td>$\omega L/c \sim \sin \theta$ $\theta &gt; 0^\circ$, p-polarization</td>
<td>[34,40,41]</td>
</tr>
<tr>
<td>Ponderomotive acceleration</td>
<td>Acceleration</td>
<td>collisionless</td>
<td>relativistic intensity $a_0 &gt; 1$ linear polarization</td>
<td>[42,43,44,45]</td>
</tr>
<tr>
<td>Stochastic heating</td>
<td>Acceleration</td>
<td>collisionless</td>
<td>colliding waves, $a_1 * a_2 &gt; 1$ e.g. incident + scattered</td>
<td>[46,47,48]</td>
</tr>
<tr>
<td>Parametric instabilities</td>
<td>Acceleration</td>
<td>collisionless</td>
<td>$\Gamma(a_0, \omega_p) \lesssim \tau$, $L \gg \lambda$</td>
<td>[41,49,50,51]</td>
</tr>
</tbody>
</table>

Table 2.1: List of the most important laser absorption processes. The meaning of symbols used in the table is: $L$ - plasma density scale length, $\lambda$ - laser wavelength, $\nu_{ei}$ - electron-ion collision frequency, $\tau$ - laser pulse duration, $\lambda_{mfp}$ - electron mean free path, $v_t$ - electron thermal velocity, $l_s$ - skin depth, $v_{osc}$ - quiver velocity of electrons in the laser field, $\theta$ - angle of incidence, $a_i$ - dimensionless amplitude of the laser wave, $\Gamma$ - instability growth rate, $\omega_p$ - electron plasma frequency.

normal skin effect, anomalous skin effect, sheath inverse bremsstrahlung, sheath transit absorption, vacuum (Brunel) heating, resonance absorption, ponderomotive acceleration, stochastic heating and absorption due to parametric decay instabilities. In the following these processes are divided into two groups. Absorption processes in the first group increase kinetic energy of the bulk population of free electrons in the interaction region. As the result of these processes is primarily a rise in temperature of plasma on the target surface these processes are denoted as ‘heating’ in the following text. The second group of absorption processes includes processes that result in acceleration of free electrons to very high energies at least when some special conditions are met. These processes are thus denoted as ‘acceleration’. Yet the border line
between these two groups of laser absorption processes is not always obvious we find it usefull to provide this kind of classification. List of the most important laser absorption processes is presented in Table 2.1 together with their classification and the domain of parameters where efficiencies are high.

2.4.3 Heating

In the early years of CPA lasers, laser power was not very high (below TW) and the focused beam intensity on target did rarely reach $10^{16}$ W/cm$^2$. Moreover, the contrast ratio of ASE preceding the main laser pulse was usually sufficient to avoid generation of preplasma and hence the main laser pulse interacted directly with a step-like overdense plasma-vacuum interface. Electric field of the laser wave in the interaction region was lower than the atomic electric field (the field binding electron to the core of the hydrogen atom) and the magnetic field was not enough strong to significantly affect motion of nonrelativistic charged particles.

Collisional absorption and normal skin effect

In vacuum free electron does not gain energy from the plain electromagnetic laser wave due to energy and momentum conservation reasons. Electron oscillates in the electric field of the wave or if the field is strong enough circulates on a figure-8 or helical orbit and drifts along the laser propagation direction. However, after the laser beam passes by, free electron ends up with its initial energy again. In plasma the presence of ions makes the situation different. Free electrons can collide with ions and thereby gain some chaotic thermal energy from their organized oscillatory motion. This way electron-ion collisions transfer electromagnetic energy of the laser wave into kinetic energy of plasma.

In plasma the frequency of electron-ion Coulomb collisions with considerable momentum transfer is defined as [52]

$$\nu_{ei} = \frac{e^4 n_e Z \ln \Lambda}{4 \pi \varepsilon_0^2 m_e^2 v^3}, \quad (2.8)$$

where $Z$ is the ion charge and $\ln \Lambda$ is the Coulomb logarithm. This logarithm can usually be regarded as constant with the value of order of unity during the laser plasma interaction. Electron-ion collisional frequency thus depends on the density of free electrons $n_e$ and on the relative velocity of colliding particles $v$.

For efficient collisional absorption many electron-ion collisions must take place in the interaction region on the temporal scale of the laser pulse duration. This is usually fulfilled for relatively low laser intensities (below $10^{15}$ W/cm$^2$) and relatively long laser pulses (ns). In such case collisional absorption can be very efficient and result in transfer of more than 80%
laser pulse energy into plasma [53].

The first short pulse laser absorption models were based on the extension of the collisional absorption theory. However, with the advent of CPA technique laser intensity was increased while laser pulse duration was shortened. In such case the collisional absorption efficiency drops down. This is due to the strong dependence of collisional frequency (2.8) on the kinetic energy of colliding particles. The quiver velocity of free nonrelativistic electron in the electric field $E$ of the laser wave with frequency $\omega$ is

$$v_{osc} = \frac{eE}{m_e\omega}. \quad (2.9)$$

In the field of Ti:Sapphire laser wave with intensity $10^{16} \text{ W/cm}^2$ free electrons oscillate with kinetic energy in excess of 1 keV. The frequency of electron-ion collisions in the undercritical plasma consequently decreases down to several collisions per nanosecond and the collisional absorption becomes inefficient. In fact, collisional absorption starts to turn off already for laser irradiances $I\lambda^2 > 10^{15} \text{ Wcm}^{-2}\mu\text{m}^2$ [54].

A special case of collisional absorption called normal skin effect [35] takes place in plasma with very steep density profile ($L \to 0$). In this case absorption recovers the behavior of metal-optics expressed by Fresnel equations [55]. The field of the laser wave penetrates (with exponential damping) into overdense plasma region of the width of skin depth $l_s$. As the field in the skin layer is lower while the density of free electrons is very high, electron-ion collision frequency increase (2.8) and collisional absorption in the skin layer can be relatively efficient again. Nevertheless, neither collisional absorption nor normal skin effect can explain high absorption rates and electron temperatures observed in experiments with intense CPA laser pulses [56].

Anomalous skin effect, sheath inverse bremsstrahlung and sheath transit absorption

Similarly like normal skin effect, anomalous skin effect [36] as well as sheath inverse bremsstrahlung [37] and sheath transit absorption [38] presume steep plasma density profile. However, there is an important difference between these absorption process and the normal skin effect. Namely, anomalous skin effect and both sheath absorption processes are collisionless, meaning that the collisional mean free path ($\lambda_{mfp} = v_t/\nu_{ei}$) of electrons in the interaction region is longer than the skin depth. The situation can be regarded from another point of view. Plasma in the skin layer is heated by the laser pulse and both its temperature and mean ion charge increase with time. This implies that the collisional mean free path and the plasma frequency must increase as well. The former because of the strong dependence of collisional frequency on the velocity (temperature), the later because of higher free electron density in the skin layer. As a consequence, the skin depth decreases and becomes shorter than the collisional mean free
2.4. LASER ABSORPTION AND CHARGED PARTICLE ACCELERATION

Anomalous skin effect and both sheath inverse bremsstrahlung mechanisms assume that the quiver velocity of electrons in the field of the laser wave is lower than electron thermal velocity ($v_{\text{osc}} < v_t$). Consequently, these absorption processes turn off at high laser irradiances ($I\lambda^2 \gtrsim 10^{16} \text{ Wcm}^{-2}\mu\text{m}^2$) as well. Electrons in the interaction region oscillate in the electric field of the laser wave. However, at the same time they propagate with the thermal velocity and therefore they can transport some energy through the skin layer deeper inside the target where the laser wave cannot penetrate. This way the electric field is carried by thermal electrons deeper into the target where it is subsequently absorbed.

In the anomalous skin effect the mean thermal excursion length of electron $v_t/\omega$ is itself longer than the skin depth and electrons in the interaction region can traverse the skin layer in less than one laser period. In the sheath inverse bremsstrahlung, on the other hand, the electron transit time through the skin layer is longer than laser period so the energy transfer takes place in a series of successive steps. The sheath transit absorption mechanism is a generalization of the sheath inverse bremsstrahlung for the case of oblique laser incidence.

2.4.4 Acceleration of charged particles

All the absorption processes discussed in the previous section turn off at laser irradiances of about $10^{16} \text{ Wcm}^{-2}\mu\text{m}^2$. Moreover, they are efficient only in very steep plasma density profiles (with exception of the collisional absorption) and they can accelerate electrons to energies of usually less than keV. Energy of heated electrons is quickly thermalized in collisions with other electrons and ions in the overdense plasma and thus these electrons contribute to temperature and ion charge increase in a thin layer of plasma in the target behind the laser interaction region.

Many CPA laser systems which are in operation nowadays can produce beams with very high energy density. The peak intensity of CPA laser beams on target often approaches or even exceeds $10^{19} \text{ W/cm}^2$. If the pulse is not very carefully cleaned of prepulses one cannot assume steep plasma density profile on the target surface any more. With the exception of vacuum heating the main absorption mechanisms of high intensity laser pulse take place in the expanding plasma in front of the target. Because the interaction takes place in the undercritical plasma less electrons are involved in the absorption processes. On the other hand as the quiver velocity of electrons in the electric field of the laser wave approaches the speed of light, energy absorbed by a single electron can be much higher (up to tens of MeV). Because of high quiver electron velocity the influence of the magnetic component of the laser field on free electron trajectories becomes as important as the influence of electric field. The mechanisms of short high intensity laser pulse absorption generally result in acceleration of a smaller number of
electrons to very high velocities. Therefore the label ‘acceleration’ is used in this work.

**Vacuum heating**

Vacuum heating\cite{39} also known as Brunel’s heating (or ‘not-so-resonant, resonant absorption’) is a kind of complementary process to the processes of anomalous skin effect and sheath inverse bremsstrahlung. Vacuum heating takes place when a linearly p-polarized laser wave strikes a sharp-edged plasma density profile on the target surface obliquely. In this case electric field of the laser wave has also a component perpendicular to the target surface. This perpendicular field drags electrons from plasma into the vacuum in front of the target and pushes them subsequently back. Electrons thus undergo oscillations along the plasma density gradient with amplitude of \( v_{osc}/\omega \). If amplitude of these oscillations exceeds the density scale length, i.e. \( v_{osc}/\omega > L \) electrons penetrate into the overdense plasma behind the skin layer where the field is screened. Electron bunches are thus accelerated toward the target interior directly by the electric field of the laser wave every laser period. Contrary to anomalous skin effect and sheath absorption, higher quiver velocity of electrons is needed for vacuum heating to be efficient. Therefore, vacuum heating is also efficient for laser irradiances above \( 10^{16} \text{ Wcm}^{-2}\mu\text{m}^{2} \) and it can accelerate electrons to considerably high energies.

**Resonance absorption**

Likewise to the case of vacuum heating, resonance absorption takes place when a p-polarized laser pulse strikes surface of the target obliquely. As there is a component of the laser wave electric field perpendicular to the target surface laser wave drives electron oscillations also along the plasma density gradient. These oscillations can be resonantly enhanced in plasma and thus a part of energy of the incident laser wave is transferred into electrostatic energy of an electron plasma wave. In a very steep density profile which is the case of vacuum heating, excursion of free electrons can exceed the density scale length and electrons leave the interaction region before being pulled back by the field in the next half-period. Than the electron plasma wave is build and destroyed every laser cycle.

In the standard picture of resonance absorption the electric field component of the p-polarized laser wave directed along the plasma density gradient tunnels through the underdense plasma from the laser reflection point to the critical point \( (n_e = n_c) \). At this place the field is resonantly enhanced by the plasma and it excites electron plasma wave. This wave propagates into the underdense plasma and it is damped either by collisions and Landau damping at lower intensities or by particle trapping and wave breaking at higher intensities. The latter gives rise to population of very fast electrons propagating out of the target into vacuum. As the quasineutrality of plasma layer on the target surface is violated a large macroscopic quasistatic
electric field builds up in front of the target. This field is strong enough to stop most of accelerated electrons and turn them back.

Efficiency of resonance absorption depends on plasma density scale length \( L \) and angle of laser beam incidence \( \theta \). Based on theoretical works [34, 41] and confirmed by numerical simulations [38, 40] the maximum efficiency is achieved when the following relation between \( L \) and \( \theta \) is fulfilled

\[
(k_0 L)^{1/3} \sin \theta \approx 0.8 ,
\]

where \( k_0 \) is the laser wave number. Due to resonance absorption as much as 50% of the laser pulse energy or even more can be absorbed by fast electrons [57].

**Ponderomotive acceleration**

At high laser intensities (irradiances) the nonlinearity parameter of laser plasma interaction is the dimensionless amplitude of the vector potential \( A \) of the electromagnetic laser wave [58]. This dimensionless amplitude can be expressed using the electric field strength \( E \) and the wave frequency \( \omega \) or the intensity \( I \) and the wavelength \( \lambda \) as

\[
a_0 = \frac{eA}{m_e c^2} = \frac{eE}{m_e \omega c} = \sqrt{\frac{e^2}{2\pi^2 m_e^2 \varepsilon_0 c^5}} \sqrt{\frac{I}{\lambda^2}} .
\]

Comparing this expression with the relation (2.9) one can readily identify this parameter with the normalized (by the speed of light) quiver velocity (average oscillation velocity) of an electron oscillating in the electric field of the laser wave \( E \sin(\omega t) \). For Ti:Sapphire laser and intensity of about \( 2 \times 10^{18} \) W/cm\(^2\) the nonlinearity parameter \( a_0 \) approaches one and the electron quiver velocity becomes relativistic. In fact the expression for the quiver velocity given in (2.9) is valid only in the nonrelativistic case as the right hand side of (2.9) represents quiver momentum divided by the electron rest mass.

When \( a_0 \gtrsim 1 \) the laser pulse is called relativistic and the relativistic quiver velocity of free electron normalized to the speed of light is

\[
\frac{v_{osc}}{c} = a_0 \sqrt{\frac{1}{1 + a_0^2}} .
\]

The influence of the magnetic field component of the laser field on the free electron motion can no longer be neglected in the case of relativistic laser pulse. Whereas electron simply oscillates in the electric field of the laser wave perpendicularly to its propagation vector \( \mathbf{k} \) in the subrelativistic case \( (a_0 \ll 1) \), the \( \mathbf{v} \times \mathbf{B} \) term of the Lorentz force becomes as significant as the electric field term in the relativistic case. To demonstrate the effect of the \( \mathbf{v} \times \mathbf{B} \) term of
2.4. LASER ABSORPTION AND CHARGED PARTICLE ACCELERATION

Figure 2.5: Demonstration of free electron trajectory in the field of relativistic laser wave. In panels a) and b) the laser pulse duration is infinite, in panels c) and d) the laser pulse has $\sin^2$ temporal profile it is 10 periods long. The flow of time is illustrated by black arrows.

The travel of electron in the plane electromagnetic field of an infinite laser pulse is demonstrated in panel a). It can be divided into a drift motion of the center of electron oscillations in the direction of the laser wave propagation and into the oscillatory motion. In the drifting (ponderomotive) reference frame which propagates with the velocity

$$v_D = \frac{a_0^2}{4 + a_0^2}.$$ (2.13)
electron circulates on a figure-8 orbit. This can be seen in panel b) of Figure 2.5.

Electron excursion is demonstrated in panel c) for the case of a finite laser pulse. In the finite laser pulse electron travel cannot be divided into drift and oscillatory motion much like in the infinite pulse case. There is no inertial reference frame in which electron oscillations would be stationary every laser period. Instead electron is accelerated in the first half of the laser pulse and decelerated in the second half. This can be seen in panel d) where the trajectory of electron is plotted in the frame moving with average electron longitudinal velocity. Electron is at rest in the origin initially. Its velocity is lower than the average velocity during the laser pulse hence it moves in the negative direction in the chosen frame. As the field of the laser wave increases electron is accelerated along with the laser pulse, its velocity becomes higher than the average one and it moves in the positive direction. After the peak of the laser pulse electron is decelerated and at the end of the pulse it remains at rest as it was initially. For the circularly polarized laser wave the situation is three dimensional and the trajectory of electron is helical.

Ponderomotive force is the result of the Lorentz force that works on a charged particle in the electromagnetic wave\cite{59}. This force tends to push charged particles against the gradient of the laser electric field into regions of lower field amplitude. Ponderomotive force has two terms, a slowly varying DC term and a high-frequency one\cite{42}. The slowly varying term can be obtained by averaging the Lorentz force over a laser cycle. Electron subjected to electromagnetic field of an infinite laser pulse in vacuum does not feel the slowly varying term of the ponderomotive force and its laser cycle averaged propagation is a steady drift. On a time scale shorter than the laser period electron feels the high-frequency component of the ponderomotive force which force him to oscillate on the figure-8 trajectory. The high frequency term of the ponderomotive force oscillates with twice the laser frequency and it is significant in particular in the case of relativistic intensity\cite{45}.

The slowly varying part of the ponderomotive force shows up when the cycle-averaged electric field of the laser wave exhibits a spatial or temporal dependence. The gradient in the field may be for example due to radial laser intensity profile in the beam, due to a gradient in the density of plasma where the wave propagates, or simply due to the laser pulse temporal profile. As can be seen in Figure 2.5 panel c) the slowly varying ponderomotive force pushes electron ahead of the peak field, i.e. accelerates it toward the gradient of the maximum field. After the maximum passes by electron is again accelerated toward the gradient of the field maximum but this time the gradient is in the opposite direction and electron is in fact decelerated.

In the relativistic laser pulse solid target interactions acceleration of electrons by the high frequency ponderomotive force is regarded as a very important laser absorption process. This absorption process takes place in the vicinity of the critical surface and in fact it is very similar to the vacuum heating process. The main difference between these two processes is that in the
case of ponderomotive absorption the driving term of electron oscillations along the plasma density gradient is the high-frequency component of the $\mathbf{v} \times \mathbf{B}$ force.

Electrons accelerated by the high-frequency term of the ponderomotive force during the laser target interaction propagate in particular in the laser wave propagation direction and their energy distribution function is usually assumed to be the Boltzmann-Maxwell one with electron temperature equal to the ponderomotive potential $^{43, 44}$

$$T_e = m_e c^2 \left( \sqrt{1 + a_0^2} - 1 \right).$$ (2.14)

**Parametric instabilities and stochastic heating**

Parametric instability is generally a nonlinear phenomenon where a periodic variation in the medium induces growing oscillations at different frequency $^{41}$. The nonlinear effects in laser wave propagation in plasma, e.g. ponderomotive force, change of the mass due to relativistic velocity etc. may excite different wave modes which are otherwise present in plasma on the level of noise. In the absence of magnetic field three modes of waves are possible in plasma. These are an electromagnetic wave, an electron plasma wave and an acoustic ion plasma wave. In the short pulse laser plasma interactions motion of ions is mostly negligible on the time scale of the interaction. Thus the instabilities where ion acoustic waves are involved are not important. More important parametric instabilities are associated with electron plasma waves. Namely, these are stimulated Raman scattering and two-plasmon decay $^{49, 50, 51}$. In the case of stimulated Raman scattering the incident laser wave is decomposed into an electron plasma wave and a scattered electromagnetic wave (or two waves in the case of forward scattering) while in the case of two-plasmon decay laser wave is converted into two electron plasma waves.

Energy and momentum conservation laws imply following conditions for the frequencies and the wave vectors of the waves involved in the process

$$\omega_0 = \omega_1 + \omega_2, \quad \mathbf{k}_0 = \mathbf{k}_1 + \mathbf{k}_2.$$ (2.15)

The above condition for frequencies of the waves implies that the parametric decay of an electromagnetic wave ($\omega_0$) takes place in the plasma where $\omega \geq 2\omega_p$, i.e. where the density of plasma is less than quarter of critical density ($n_e < n_c/4$). Therefore, parametric instabilities are excited only in the undercritical plasma far from the target surface and their occurrence requires preplasma with gentle density gradient. The electron plasma wave resulting from the parametric decay propagates in the undercritical plasma and traps and accelerates electrons similarly like in the case of resonance absorption.

The last laser absorption and electron acceleration mechanism mentioned here is the recently proposed stochastic heating $^{46, 47, 48}$. In a multiwave system the motion of electron
becomes stochastic when certain thresholds of the laser wave amplitudes are exceeded. In the undercritical plasma the Raman backscattered or the specularly reflected laser wave may be intense enough and serve as the second counterpropagating wave which introduces the stochasticity in the electron motion. Stochastic heating may be also relatively efficient and in certain cases even the dominant laser absorption process in the underdense plasma. Energetic electrons produced by the stochastic acceleration scheme move predominantly in the direction of the pulse with higher intensity, i.e. in the direction of the incident laser wave propagation.

2.5 Hot electron population and its applications

In the previous section the most important mechanisms of laser pulse energy coupling into charged particles in plasma have been discussed. As one could have seen, there is quite a big zoo of absorption processes based on various physical mechanisms and efficient in different ranges of laser plasma interaction parameters. Most of the collisionless absorption processes result one way or another in preferential heating of a fraction of electrons to energies much higher than the bulk plasma temperature. Acceleration processes leading to formation of population of these energetic ‘hot’ electrons are of stochastic nature and there are strong cycle-to-cycle fluctuations in trajectories and energies acquired by hot electrons [60]. Moreover, several laser absorption processes may take place at once or smoothly transit from one to another. Therefore, averaging the velocities of many individual electrons that absorb energy of the laser or the plasma wave over time results very often in Maxwellian distribution.

In laser produced plasmas energy distribution of electrons has generally a shape close to the bi-Boltzmann-Maxwell distribution with one temperature $T_e$ characterizing the bulk of plasma electrons and another temperature $T_h$ characterizing the hot electron component, whereas $T_h \gg T_e$ [61,62]. As hot electrons leave the laser plasma interaction region very quickly and their mean free path is relatively long, they carry energy out of the surface plasma layer further into the target. Thus the temperature of plasma in the interaction region is more determined by the temperature $T_e$ characterizing the bulk population of electrons and these electrons are accordingly called ‘thermal’.

Whereas hot electrons are much less in number than the thermal ones their population often carries more energy. Acceleration and transport of hot electrons are therefore of particular interest in recent years and many newly proposed applications rely especially on these energetic electrons. Among the most important applications of hot electrons, short pulse K-α radiation emission from short-pulse laser irradiated solid targets, ion acceleration from foils or mass limited targets, and fast ignition of inertial confinement fusion targets are probably the most vital in recent years. These applications are briefly discussed in the following sections.
2.5. HOT ELECTRON POPULATION AND ITS APPLICATIONS

2.5.1 K-\(\alpha\) radiation

Hot electrons accelerated during the laser-target interaction mostly propagate further into the target where plasma is colder or even deeper where the majority of atoms are nonionized. On their travel hot electrons collide with ions and atoms and from time to time these collisions result in knock out of an inner shell electron. Ions with electron missing in the inner shell tend to relax to some less energetic state on a generally very short temporal scale of order of femtoseconds or even shorter. The relaxation occurs either via Auger process or via emission of characteristic photon.

In the Auger process an electron from more outer shell fills the vacancy in the inner shell and the redundant energy is given to another electron which becomes energetic enough to leave the ion. As through the Auger process the excess energy is emitted from ion in the form of another mostly not very energetic electron this process is in its consequence similar to an ionizing collision with well defined secondary electron energy. The Auger process dominates in the relaxation of ions with lower atomic number.

![Schematic illustration of K-\(\alpha\) radiation emission induced by hot electrons in short pulse laser irradiated solid target.](image)

In the other relaxation process the vacancy in the inner shell is filled by an electron from the more outer shell as well, however the redundant energy is emitted in the form of a photon. Only slightly depending on, from which shell electron that fills the inner shell comes, the energy of emitted photon is characteristic for a given ion species. The vacancies in innermost K shell are mostly filled by electron bound in the next L shell and the characteristic photon emitted during this relaxation process is called K-\(\alpha\) photon. K-\(\alpha\) emission is isotropic and the target is usually relatively transparent to this emission as the energy of K-\(\alpha\) photons is slightly below the threshold energy for inner shell photoionization. The process of K-\(\alpha\) photon generation in
short pulse laser irradiated solid target is schematically demonstrated in Figure 2.6.

K-α radiation emitted from the target irradiated by short laser pulse is very interesting as it has some unique properties. This radiation is almost monochromatic and mostly concentrated in a narrow X-ray spectral region. The pulses of K-α radiation emitted from the targets are very short, their duration ranges from hundreds of femtoseconds to picoseconds and thus it is comparable with the duration of the laser pulse itself [63]. In recent experiments K-α pulses only a few hundred femtosecond long have already been observed [64] and application of ultrashort laser pulses and specially designed targets may in principle result in even shorter K-α emission [65]. The spot size of K-α radiation emission from the target may be comparable to the size of the laser focal spot [66,67]. K-α emission spots of about 10 µm have been measured in [68]. Also the transformation of laser energy into energy of K-α radiation is sufficiently efficient. It can be almost of order of $10^{-4}$ [63,65,69].

Thus, short pulse laser irradiated solid targets may serve as very small sources of intense, temporally short and almost monoenergetic X-ray radiation. This radiation is very suitable for measurements of processes with very high spatial and temporal resolution [8,70,71,72]. In addition pulses of K-α radiation are well synchronized with the laser pulse itself and are therefore they are applicable as diagnostics of laser induced processes.

Foils with the thickness of only several tens of microns from various materials are often used in ultrashort pulse laser-target interaction experiments focused on generation of K-α radiation [73,74]. Emission from the rear side of these foils (opposite side to the laser irradiated one) is more advantageous in most applications. Soft X-ray radiation emitted from the coronal plasma on the laser irradiated side is significantly attenuated during the passage through the target and thus K-α radiation has better contrast on the rear side. For efficient source of K-α radiation very high electron energies are not always desirable. For elements with lower atomic number it is more advantageous when the population of hot electrons is bigger and their temperature is lower, of order of tens or hundreds of keV [65]. Therefore short pulse lasers with lower pulse energy but with very high repetition rate are mostly applied in recent years.

Whereas the spectrally resolved measurements of characteristic emission can provide some information about the laser produced plasma, measurement of efficiency of the laser energy transformation into K-α radiation can supply information about the population of hot electrons and their transport inside the target [75,76]. Measurements of K-α emission from so-called sandwich targets consisting of several (mostly four) layers of different materials are often used in experiments studying the population of hot electrons. Surface layer of these targets with which the laser pulse interacts and where acceleration of electrons takes place is often made of metal, e.g. aluminum. Behind the surface layer the next layer is called propagation layer and it consists of material in which transport of hot electrons is to be studied. The third
layer is called fluor layer. K-\(\alpha\) radiation produced in this layer is measured in dependence on the propagation layer thickness, density, resistivity etc. Finally, the last layer serves as an absorption layer for those hot electrons that penetrate through the fluor layer. The last layer is usually made of plastic. Comparison of K-\(\alpha\) emission measured in the experiment with the theoretical model makes it possible to estimate temperature of hot electrons. The measurements of K-\(\alpha\) emission used to characterize the population of hot electrons and its transport in solid material are of particular interest in recent years in connection with Fast ignition concept to Inertial confinement fusion.

### 2.5.2 Ion acceleration

Hot electrons accelerated during the laser target interaction may produce a quasistatic electric field which is strong enough to accelerate ions to very high energies. This strong electric field is produced when significant number of hot electrons leave the target and the target becomes positively charged. Electrostatic field inside the target is usually screened and the charge and current are neutralized by free electrons (return current). On the target vacuum interface however a very strong field can build up. This field tends to accelerate electrons towards and ions out of the target. This acceleration mechanism known as Target Normal Sheath Acceleration (TNSA) \[77,78,79,80\] is schematically demonstrated in Figure 2.7.

![Figure 2.7](image URL) **Figure 2.7:** Schematic illustration of target normal sheath acceleration of ions from the rear surface of thin foil target irradiated by intense short laser pulse.

Thin foil target are often used in TNSA experiments. Hot electrons accelerated in the laser target interaction region are energetic enough to fly through the foil with their energy and propagation direction almost unaltered. They leave the foil from the rear side and there the electrostatic field builds up. This field can be very strong with amplitude as high as several TV/m and it can easily ionize atoms and produce highly charged ions which are subsequently...
accelerated to very high velocities.

Accelerated protons are mostly observed in TNSA experiments even if the target material does not contain any hydrogen. These protons come from a contamination layer [81, 82] of water vapor or hydrocarbon compounds which settle on the target surface during evacuation of the target chamber. As the charge to mass ratio is the highest for protons, proton acceleration is the most rapid and thereby protons from the contamination layer inhibit acceleration of other species of ions. In recent experiments it has been demonstrated that if the target is heated before the main laser pulse strikes it the contamination layer can be evaporated and completely removed from the target surface. In this manner acceleration of more heavier ions is possible [83].

Interaction of short intense laser pulses with mass-limited targets is investigated to increase the efficiency and decrease the size of the source of accelerated ions [84]. A typical representative of mass-limited targets is a small water droplet. Even if electrons accelerated into the target travel preferentially in the target surface normal direction some fraction of hot electrons fly also in the lateral direction, for example due to self-generated magnetic field. Therefore, a part of laser energy absorbed in the target is deposited also in the material surrounding the laser target interaction region in foil targets and this portion of energy is effectively lost for ion acceleration. Here the case of mass-limited targets is advantages. Energy of the laser pulse absorbed in the target is confined in the small target volume by electrostatic forces and it can leave the target essentially only in the form of radiation. The repartition of energy between electrons and ions than results in a more numerous population of accelerated ions than in the case of foil targets [85].

2.5.3 Fast ignition of inertial confinement fusion targets

One of the main challenges facing the community of laser plasma scientists already for many years is the achievement of laser driven fusion [86, 87]. In the classical approach to Inertial confinement fusion (ICF) driven by laser a small pellet consisting of several shells, containing mostly half-and-half mixture of deuterium and tritium (DT) as the fuel for fusion, is irradiated by ns laser pulses of lower intensity. Shock waves produced by the thermal pressure propagate into the center of the pellet and compresses the fuel to very high density. In the center where the shock waves cross each other their energy is thermalized producing a hot spark where the fuel is ignited. The burn wave subsequently propagates outwards and ignites the rest of the compressed fuel before the pellet expands.

The key problem of this classical approach to Inertial confinement fusion is the necessity of very uniform spherical pellet compression. If there are irregularities in the flux of radiation compressing the pellet or the density of material in the pellet is not uniform, instabilities (e.g.
Rayleigh-Taylor instability [88]) may prevent uniform compression and cause fuel mixing which avoids an efficient burn [89]. In the classical scheme of ICF hot electrons are disadvantages as they preheat the fuel inside the pellet which makes its compression more difficult.

In recent years a new approach to Inertial confinement fusion where hot electrons are beneficial has been proposed. Just like in the classical approach the fuel pellet is compressed by the shock waves induced by long ns laser pulses. However, in the new scheme there is no need to compress the fuel so much uniformly as it is not necessary to produce the hot spark in the center where the shock waves thermalize. Instead a beam of hot electrons produced by a short petawatt laser pulse is supposed to heat and ignite the fuel in the right moment near the center of the pellet [10]. This new concept was given the name Fast ignition as ignition of the precompressed fuel is achieved in a very short time interval of order of ps. Fast Ignition scheme of ICF is schematically illustrated in Figure 2.8.

![Figure 2.8: Schematic illustration of Fast ignition of Inertial confinement fusion target. Fast ignition is achieved by a dense beam of hot energetic electrons which are accelerated by additional short petawatt laser pulse.](image)

However, just like the classical approach Fast ignition scheme has also its weak points and it is not clear yet if they will be resolved so that the Fast ignition scheme will be favorable. The biggest unknown of Fast ignition, of how such dense and energetic beam of hot electrons will be produced and transported through the dense fuel to the center of the pellet so that some kind of filamentation instability does not disturb it, still remains unresolved [90]. A golden cone embedded into the fuel pellet is supposed to help to resolve a part of the problem as hot electron beam produced near the tip of the cone will be closer to the center of the pellet. Finally, it should be noticed that alternative approaches to the hot electron beam driven Fast ignition have been proposed and are currently investigated. Presently one of the most promising of them makes use of beam of accelerated protons instead of electrons [91].
CHAPTER 3. THEORETICAL MODELS AND COMPUTER SIMULATIONS

3 THEORETICAL MODELS AND COMPUTER SIMULATIONS

Even if laser produced plasmas are investigated all around the world already for several decades there is not a single unified theoretical model capable to describe all physics involved in laser plasma interaction. This physics includes processes describing evolution of laser beam, coupling of laser energy into plasma and evolution of target itself. A complex model would thus have to describe laser pulse propagation, scattering, absorption and reflection, generation of plasma, its ionization, heating and expansion, self-consistent evolution of plasma fields and waves, propagation and acceleration of charged particles in these fields, particle collisions, shock waves, return currents, radiative process and many more.

Fortunately, not all of these processes take place at once or at least not on the same temporal and spatial scales. It is thus possible to simplify theoretical description of the interaction omitting or averaging the processes that take place on much larger or smaller spatial and temporal scales than the processes of particular interest. In an simplified instructive manner the main theoretical models of laser plasma interaction can be classified into categories according to the time scales characterizing the laser pulse and the plasma. The most important scales are the plasma period \( \tau_p = 2\pi/\omega_p \), the plasma Coulomb collision period \( \tau_c = 1/\nu_C \), the laser period \( \tau_l = 2\pi/\omega \) and the laser pulse duration \( \tau_d \).

Underdense plasma of a very low density can be usually regarded as more or less passive medium, meaning that the collective plasma dynamics takes place on temporal scale much longer than laser period \( \tau_p \gg \tau_l \). The underdense plasma affects the laser pulse passing through it mostly via local changes in the refractive index and causes e.g. its self-focusing. Trajectories of charged particles can be often considered as mutually independent in this case and a test-particle model can be applied to calculate them. In the test-particle model a single charged particle with appropriately chosen initial conditions is traveling in the fields of the laser wave while the plasma fields and particle-particle interactions are neglected.

If the density of plasma is higher electric and magnetic fields self-consistently induced in the plasma due to the motion of charged particles in the laser wave become important. Trajectories of charged particles are no longer mutually independent. Instead, they are interconnected with each other via the fields induced in plasma. If the plasma period becomes comparable with the laser wave period, \( \tau_p \sim \tau_l \), then the self-induced fields are of similar amplitude as the field of the laser wave itself. Than plasma is no longer transparent to the laser pulse, the pulse is reflected and its further propagation into plasma is screened. On the temporal scale where \( \tau_p \) is
comparable to $\tau_l$ plasma can be treated as an ensemble of charged particles moving in the laser wave and the self-induced electric and magnetic fields. This ensemble is usually represented by the velocity distribution function. The most of physics involved in laser plasma interaction can be described by the four Maxwell equations and the Lorentz force equation applied to distributions of charged particles in plasma. This model is called kinetic and it usually seeks to determine the distribution function of charged particles self-consistently. It is well suited for the description of plasma where wave-particle interactions occurring on the temporal scale comparable with the laser and plasma period have to be treated.

The kinetic description is usually unnecessarily detailed and too lengthy to resolve when one wants to describe plasma which is overdense to the laser pulse $\tau_l \gg \tau_p$ and the laser pulse is long enough so that $\tau_d \gg \tau_l$. Moreover, when plasma is not too hot so that collision period is relatively short in comparison with the laser pulse duration $\tau_d \gg \tau_c$, short range particle-particle interactions, screened Coulomb collisions play an important role. In the collisionally dominated plasma, collisions quickly turn the distributions of charged particles into local Maxwellsians and establish local thermal equilibrium (not thermodynamic). Therefore, it is no longer needed to describe the plasma through the distribution functions of charged particles. Instead, parameters characterizing the Maxwellian distributions locally (temperature, drift velocity and density) are sufficient. These parameters are already macroscopic quantities and knowing them it is possible to calculate higher moments of the Maxwellian distribution, i.e. the stress tensor, the energy flux density etc.

This description of plasma is called hydrodynamic as the governing equations are the same as in the fluid dynamics. If the magnetic field generation is incorporated the model is called magnetohydrodynamic. The equations of the hydrodynamic model are obtained taking moments of the equation describing the temporal evolution of the distribution function. Usually, the first three moments are taken into account and the resulting equations are the laws of conservation of physical quantities, namely mass, momentum and energy. The set of these equations is usually closed by the equation of state which expresses pressure and internal energy as a function of density and temperature. In the hydrodynamic model laser is treated only as an external source of energy. With this plasma dynamics model it is possible to handle much bigger regions on much longer time scale than with the kinetic description. However, the price paid for this potency is the loss of detailed plasma dynamics in the laser target interaction region, mainly in the vicinity of the critical surface.

In short high intensity laser pulse interactions with solid targets the field of the laser wave is usually very strong while the Coulomb collision period is much longer than laser and plasma periods. The appropriate model handling the main physical aspects is consequently the kinetic one. This model is discussed in the next section in more details.
3.1 Kinetic description and its implementation

Kinetic description follows temporal evolution of plasma in the 6-dimensional phase space where the coordinates are the position and the velocity vectors. In this theory charged particles are represented by their distribution functions. Generally, there are two approaches to the kinetic theory. The microscopic approach is based on the Klimontovich distribution function which is a sum of Dirac delta functions representing the positions of particles in the phase space. This distribution function satisfies the continuity equation which means that the distribution of particles can change in an infinitesimally small volume around some phase space coordinate only due to particle flow through the boundaries surrounding this volume, i.e. particles are neither created nor destroyed. The continuity equation for the Klimontovich distribution function yields Klimontovich equation \[92\] which is an exact description of plasma including exact trajectories of all particles. Due to its complexity Klimontovich equation is however practically unresolvable for systems consisting of many particles. Instead it is a good starting point for derivation of less complex plasma models.

The starting point of the second macroscopic approach is the Liouville distribution function. This distribution function is \(6 \times N\)-dimensional as it is a product of distribution functions for \(N\) individual particles. Just like in the microscopic approach the distribution function satisfies the continuity equation which yields the Liouville theorem \([93, 94]\). The complexity of the problem described by the \(6 \times N\)-dimensional distribution function is however further reduced integrating the distribution function over unnecessary dimensions and neglecting some multiparticle correlations. This procedure is called BBGKY hierarchy \([95]\).

Using either of these approaches it is possible to arrive to the governing equation of collisionless kinetic theory for the temporal evolution of the distribution function \(f(x, v, t)\), the Vlasov equation \([96]\)

\[
\partial_t f(x, v, t) + \frac{p}{m\gamma} \nabla_x f(x, v, t) + q \left( E + \frac{p}{m\gamma} \times B \right) \nabla_p f(x, v, t) = 0 \ . \tag{3.1}
\]

If the influence of collisions on the particle distribution function cannot be neglected a collisional term is added on the right hand side of Vlasov equation and the new equation is called Vlasov-Boltzmann. The collisional term can be derived using in the BBGKY hierarchy. For example, taking into account two-particle correlations (Coulomb collisions) Fokker-Planck-Landau collisional term can be derived.

Vlasov equation is very complicated partial differential equation, an advection equation. When the Vlasov equation is coupled with Maxwell’s equations the resulting system of equations cannot be solved analytically in most cases due to its complicated non-linear structure. Often the system must be discretized and than its solution can be found numerically. A careful choice of the discretization scheme is however necessary to avoid the development and temporal
increase of non-physical oscillations and numerical instabilities. Several approaches to solve the Vlasov-Maxwell system of equations numerically have been developed. Among the most successful of them belong [97] Euler methods, solvers of the Vlasov equation in its conservative form, semi-Lagrangian methods with time-splitting and methods utilizing the functional expansion of the distribution function. Most of these methods have been effectively applied to physical problems which can be treated in less dimensions due to their symmetry, for example the problems concerning electrostatic waves and instabilities [98] in one spatial and one velocity dimension (1D1V). In multiple dimensions however the direct numerical solution of the Vlasov-Maxwell system of equations becomes too demanding and time consuming. Fortunately, there exist another method for solution of the Vlasov-Maxwell system of equations which is relatively efficient also in more spatial and velocity dimensions. It is the Particle-In-Cell (PIC) method.

### 3.2 Particle-In-Cell method

For many decades numerical solution of the processes in plasma that are described by kinetic theory is dominated by the Particle-In-Cell (PIC) method. The PIC method is a very intuitive approach to the treatment of kinetic plasma theory. Plasma is in fact a huge ensemble of charged particles, electrons and ions that interact with each other due to self-consistently induced electric and magnetic fields. PIC methods treat plasma right this way with two exceptions. The number of charged particles is cut down by many orders of magnitude and the self-induced fields are discretized on a grid.

Instead of real charged particles PIC methods utilize virtual macroparticles which behave like a cloud of real particles with the same velocity and a given fixed spatial distribution. Thus PIC method assumes that real charged particles are locked together in clouds and the number of particles is reduced to the number of clouds, macroparticles. For example, in PIC simulations presented in this work the number of charged particles represented by a single macroparticle is usually about \(10^{13}\). The charge to mass ratio of the macroparticle is independent of the number of real particles it represents. Macroparticles therefore behave in electric and magnetic fields exactly like real particles. This ‘Particle’ aspects of the Particle-In-Cell method is connected with the representation of the particle distribution function contained in the Vlasov equation.

The second, ‘In-Cell’ aspect of the method is connected with Maxwell equations, i.e. electric and magnetic fields and charge and current densities. Yet, there exist some pure particle numerical models they cannot be applied to a large number of macroparticles without any special treatment. Each of \(N\) macroparticles interacts with all other ones which gives almost \(N^2\) interactions in total. This is too lengthy to solve when \(N\) is a large number. In PIC method this problem is solved by not considering all the binary interactions one by one but only the collective ones. Thus instead of calculating the fields on the particles directly they
are calculated on a spatial grid and interpolated on particle positions.

In plasma the non-collective interactions are screened on some distance. When plasma is not very cold and dense this distance can be found from the Debye-Hückel theory \[99,100\] and it is called the Debye length. It is usually reasonable to consider the screening to be particularly due to electron motion and than the Debye length is used in the form

\[
\lambda_D = \sqrt{\frac{\varepsilon_0 T_e}{n_e e^2}}.\tag{3.2}
\]

In the definition of Debye length \(T_e\) is the thermal velocity of electrons. The cells in the PIC method are often chosen so that their size is about the Debye length. A similar constraint on the choice of the cell size, i.e. the cell size should be of the order of the Debye length, can be deduced from the point of view of numerical stability of the PIC method \[101\].

The PIC model can be separated into two parts, the particle-mover and field-solver. The particle-mover part uses the known fields discretized on the grid to calculate charged particle acceleration according to the Lorentz force and to advance particle positions according to their new velocities. Afterwards charge and current densities are deposited back onto the grid and the field-solver part advances the electric and magnetic field according to the Maxwell’s equations. If additional physical processes like elastic binary collisions or ionization are included in the PIC method they are usually calculated at the end of the particle-mover part. The workflow of PIC algorithm is demonstrated in Figure 3.1.

![Figure 3.1: Illustration of the PIC algorithm workflow.](image)

PIC method is in fact Lagrange-Euler approach to the solution of Vlasov-Maxwell system of equations. The distribution in the Vlasov equation is discretized using the Lagrangian approach while the Maxwell equations are discretized using the Eulerian approach. Lagrangian discretization of the distribution function in the Vlasov equation make PIC method much more efficient than Eulerian discretization in many cases as the distribution function is represented in the phase space only where some particles and hence some plasma are present. Thus the significant advantage of the PIC method over other discretizations of the distribution in the Vlasov equation is that it is not needed to maintain a grid in the full phase space. On the other hand plasma physics is full of non-linear effects like instabilities and resonances where a small
3.2. PARTICLE-IN-CELL METHOD

population of charged particles might be indeed more important than the bulk. Therefore, in some cases sufficiently accurate representation of the distribution function in the PIC model requires very high number of macroparticles. Although this difficulty can be resolved via introducing different numerical weights for individual macroparticles other treatments of the Vlasov equation might be more successful.

3.2.1 Particle-mover

In the PIC method the macroparticles are assumed to have some internal charge distribution often called form factor. The density in the phase space, the distribution function, is than a sum of individual macroparticle distributions, form factors, in the spatial part of the phase space and delta functions in the velocity part. According to the form factors the fields are assigned to the position of each macroparticle from several neighboring grid cells. Macroparticles then advance in the phase space along the characteristics of the Vlasov equation which are the equation for particle displacement

\[ \frac{dx}{dt} = \frac{p}{m\gamma} \] (3.3)

and the equation of motion with the Lorentz force

\[ \frac{dp}{dt} = q \left( E + \frac{p}{m\gamma} \times B \right). \] (3.4)

Advancing the macroparticles in time along the characteristics of Vlasov equation, exact conservation of the phase space density is guaranteed if the fields applied to the macroparticle can be regarded as constant within the particles volume. This means that macroparticles do not evolve internally and keep their initial form factor. Solution of the Vlasov equation which is an advection type of partial differential equation is thus reduced to the solution of two ordinary differential equations of particle motion.

3.2.2 Field-solver

After macroparticles are advanced in time, the charge and current densities can be assigned to the grid cells using the same form factors as in the field interpolation to macroparticles. With the new charge and current densities electric and magnetic field can be advanced in time according to Maxwell’s equations. On the microscopic scale which is mostly the case in the kinetic plasma description vacuum Maxwell’s equations are applicable. These are the
\[ \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \quad (3.5) \]

Gauss’s law for magnetism
\[ \nabla \cdot \mathbf{B} = 0 \quad (3.6) \]

Faraday’s law
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (3.7) \]

Ampere’s law
\[ \nabla \times \mathbf{B} = \frac{j}{\varepsilon_0 c^2} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} \quad (3.8) \]

In the Maxwell’s equations there is a partial differential equation of the elliptic type, the Gauss’s law along with the equations for electromagnetic wave propagation, the Faraday’s and the Ampere’s laws which are equations of the hyperbolic type. Using the electric potential Gauss’s law can be expressed as Poisson equation and in practice it is used to describe the scalar ‘potential’ part of the electric field. Taking the divergence of the Ampere’s law and substituting the Gauss’s law gives the continuity equation
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (3.9) \]

If the Gauss’s law is satisfied initially and the self-consistent electric field is calculated from the Ampere’s law with the continuity equation always fulfilled, the Gauss’s law remain satisfied all the time. Similarly if the Gauss’s law for magnetism is satisfied initially and the magnetic field is calculated from the Faraday’s law, the Gauss’s law for magnetism remains satisfied as well. PIC methods utilizing these properties of Maxwell’s equations are called local and they use special definition of the current density to guarantee that the discrete version of the continuity equation is always fulfilled \[102\]. The advantage of this approach is that only the Ampere’s and Faraday’s law are advanced in time from the local electric and magnetic fields and current density, which is the initial value problem, and the Poisson equation, which is the boundary value problem, does not need to be solved.

In the PIC method the electromagnetic wave incident upon the plasma, i.e. the laser pulse is specified as a temporally varying boundary condition for the electric and magnetic fields at the boundaries of the region which is considered in the calculations.

### 3.2.3 Particle-In-Cell simulation code LPIC++ and its changes

The PIC simulation code used throughout the rest of this work has evolved from the code LPIC++ \[12\] which was developed in Max-Planck Institute für Quantenoptik in Berlin for modeling of laser interactions with overdense plasma surfaces accompanied by generation of high harmonics. To handle the laser wave the code is obviously electromagnetic. In this code both, particle velocities and electric and magnetic fields have components along all three
spatial dimensions and thus not only linear but also elliptic polarization of the laser wave can be treated.

On the other hand only a single spatial dimension along the direction of the laser wave propagation is considered. PIC codes that cut the dimensions of the phase space under consideration this way are referred to as 1D3V. The laser wave is supposed to be a plain wave and particles are treated as slabs with one finite and two infinite dimensions. In fact this approach is applicable to the situation in which the transverse dimensions of the laser pulse are relatively big so that intensity of laser radiation can be assumed homogeneous in a relatively big area, i.e., the pulse is not too tightly focused. The single spatial dimensional approach is used for its relatively low demands on computational resources even if it poses some constraints on the kinds of physical processes that can be simulated. Oblique incidence of the laser wave onto the target is enabled using a moving frame transformation\cite{103}. When the Lorentz transformation is performed from the laboratory frame to the frame moving with a certain velocity $v_m$ in the plane of laser incidence parallel to the target surface, the laser pulse is incident normally in the moving frame. This is schematically demonstrated in Figure 3.2. The speed of the moving frame is determined from the angle $\theta$ of laser wave incidence as

\[ v_m = c \sin \theta. \] (3.10)

As the velocity of moving frame in which the laser pulse propagated perpendicularly to the target surface is often comparable to the speed of light LPIC++ simulation code is of course relativistic. In the case of p-polarized laser wave the work of the electric field component

\[ \text{Figure 3.2: Relativistic boost frame transformation enables to treat oblique incidence in one spatial dimension. In the moving frame the laser wave is incident normally.} \]
pointing perpendicularly to the target surface in laboratory frame, is replaced by the $v \times B$ force in the moving frame. Being relativistic the code enables also to simulate the processes where very energetic particles are produced.

Finally, it should be pointed out that the code LPIC++ was written in the C++ programming language, it is object oriented, and the particles are stored in dynamic array. The choice of programming language and object oriented concept is found to be rather helpful as the code is quite intelligible and can be relatively easily modified to include additional physical processes. Particularly, the dynamic array of particles is advantageous for the ionization algorithm where new particles are injected into the simulation box.

The code LPIC++ was previously modified in the frame of two master theses [13, 14]. Binary Coulomb collisions were implemented into the code using the Takizuka-Abe Monte Carlo approach [104] and the collisional algorithm was corrected to treat collisions of electrons with relativistic velocities correctly. The option of exponential plasma density profile on the target surface was also added to enable to the start of calculations with more realistic initial conditions given by the isothermal model of free expanding plasma. Option of absorbing boundary condition for fast electrons was also added. When these electrons reach the rear boundary of the simulation box they are absorbed and substituted by thermal ones. This option is necessary for simulations in which acceleration of electrons during the laser plasma interaction is efficient and it guarantees charge and current neutralization at the rear boundary of the target.

The main objective of this work has been to modify the code LPIC++ to treat some additional physical processes and to utilize the adapted code for laser solid target interaction studies. Of our particular interest is the influence of variable plasma ionization on the dynamics of laser plasma interaction and charged particle acceleration but the code has also been modified to treat several different species of ions and the collisional algorithm has been revised. The most important changes made to the code LPIC++ are discussed in the following sections.

3.3 Variable plasma ionization in the Particle-In-Cell model

The vast majority of PIC simulation codes applied to study short pulse laser solid target interactions assume that the ion charge is constant in both space and time during the interaction. This assumption is generally taken into account while simulation parameters are selected and the mean ion charge is chosen so that it approximately corresponds to the ion charge, one can expect around the peak of the laser pulse. In many cases the assumption of constant ion charge during the short pulse laser solid target interaction is sustainable. In general, ionization by the optical field of the laser pulse proceeds very quickly at the beginning of the pulse when ions are only lowly ionized and the ionization potentials of the outermost shell electrons bound to
them are relatively low (of order of tens of eV). The outermost shells are thus quickly depleted and later during the interaction average ionization varies more slowly. At the rising edge of a short intense laser pulse the density of free electrons in the laser plasma interaction region increases several times while around and after the peak of the pulse it stays approximately constant.

Nevertheless, under certain conditions it is indeed necessary to take variable plasma ionization into account. This applies in particular to situations when the target should be considered as initially neutral or only lowly ionized or when the density profile of plasma changes very significantly due to the increasing number of free electrons. Plasma ionization influences optical properties and thereby further propagation and interaction of the incident laser light. Moreover, electrons released from ions do often not appear at the same place in the phase space where the initially free electrons find themselves. Therefore, ionization does not only increase the magnitude of the electron distribution function but it changes its shape as well. Variable plasma ionization should be taken into account in simulations of ion acceleration too, as the spatially and temporally dependent charge to mass ratio is important to involve the interplay between different ion charge states.

### 3.3.1 Electric field ionization

Three energy scales and the corresponding temporal scales are of particular importance in the theory of ionization by the optical electric field [105]. These are the photon energy $\hbar \omega$, ionization potential $U_i$, and the ponderomotive potential $U_p = e^2 |E|^2/(4m_e \omega^2)$ which is the average energy of electron oscillating in the field of an electromagnetic wave with frequency $\omega$ and electric field amplitude $E$. Additional timescales may be introduced by the laser pulse duration and by the energy spectrum of atom through typical transitions.

#### Single photon ionization - $\hbar \omega > U_i$

In the UV and X-ray or even $\gamma$ range of the electromagnetic radiation spectrum energy of photons can be higher than energy binding an electron to the atom, i.e. $\hbar \omega > U_i$. Then a bound electron can be released from atom upon absorption of a single photon. The process of single photon ionization (SPI) was introduced already by Albert Einstein to explain the photoelectric effect in 1905 [106,107]. However, in general such ionization process cannot be induced directly by the laser light because most lasers are operating in the visible or infrared spectral range where the individual photon energy is always insufficient for SPI of even the most weakly bound electrons. Photon with wavelength lower than 320 nm is required to release an electron bound in the 6s shell of cesium atom which has probably the lowest ever ionization potential of 3.89 eV (excluding unstable chemical elements and chemical compounds).
Multiphoton ionization - $U_i > U_p$, $(U_i > \hbar \omega)$

In the case when the ponderomotive potential is very small compared to the ionization potential, i.e. $U_i \gg U_p$, the perturbative theory of Multiphoton Ionization (MPI) in the lowest nonvanishing order can be applied. This theory assumes that before being released bound electron absorbs exactly $N$ photons, where $N$ is the minimal number of photons required to reach the ionization threshold (i.e. $N\hbar \omega > U_i$, but $(N-1)\hbar \omega < U_i$). The atomic binding potential is usually considered as unperturbed by the laser field during the ionization process. Under these conditions the ionization rate of the multiphoton ionization process is proportional to the $N$-photon ionization cross section and the $N$th power of the laser radiation intensity \[108, 109].

When the radiation intensity is increased (but still $U_i > U_p$) absorption of more than $N$ photons by a single bound electron becomes more and more often. The energy spectra of ejected electrons reveals distinct peaks separated by photon energy. This regime is often referred to as non-perturbative MPI or Above-Threshold Ionization (ATI) \[110, 111\]. Upon being released free electrons start to oscillate in the electric field of the laser wave. Influence of the magnetic field component on the ejected electron trajectory is negligible for the radiation intensities in the range of applicability of the MPI theory. Furthermore the quiver amplitude of the freed electron in the field of the laser wave $(eE/m_e \omega^2)$ is comparable to the dimension of the atom. Therefore, the newly released electron often returns back to the parent ion after approximately half laser cycle and interacts with this ion via either radiative decay or some collisional process.

\[ a \quad b \quad c \]

(a) ATI  (b) NSI  (c) HHG

**Figure 3.3:** Illustration of three common processes (Above threshold ionization - ATI, Nonsequential ionization - NSI, high harmonic generation - HHG) that take place when electron released by multiphoton ionization in a strong laser field returns back to the parent ion.
The radiative decay results in High-Harmonic Generation (HHG), the inelastic collision may result in Non-Sequential Ionization (NSI) and the elastic collision leads to extension of the ATI electron spectra, e.g. [112]. These processes are schematically illustrated in Figure 3.3.

The range of applicability of the MPI theory, \( U_i > U_p \), can be expressed in the units of laser irradiance as

\[
\frac{8\pi^2\varepsilon_0^2c^3m_e}{e^2} U_i \geq I\lambda^2, \tag{3.11}
\]

where SI units are assumed. In practical units for the Ti:Sapphire laser wavelength of approximately 800 nm this condition reads

\[
1.677 \times 10^{13} U_i \text{ [eV]} \geq I \text{ [W/cm}^2\text{]} . \tag{3.12}
\]

**Tunneling ionization - \( U_p > U_i \), \( (U_i > \hbar\omega) \)**

When the radiation intensity is further increased (or the frequency decreased) the binding potential of ion is perturbed significantly by the potential of the external electric field. The outermost bound electron feels an effective potential which is sum of the Coulomb potential of the ionic core screened by other bound electrons and the instantaneous electric potential of the laser wave. The shape of the effective potential shows a barrier through which electron may escape, tunnel. The ionization process in which electron tunnels through the effective potential barrier is schematically illustrated in figure Figure 3.4 panel b) and compared with the MPI process, panel a), and the Barrier Suppression Ionization (BSI) process which will be

![Image of Figure 3.4 showing the difference between MPI, tunneling, and BSI processes.](image)

**Figure 3.4:** Illustration of the difference between multiphoton ionization (MPI), tunneling ionization and barrier suppression ionization processes (BSI).
considered later, panel c). In fact the MPI process can be thought of as an 'vertical' ionization channel. Electron, while being scattered by the shaking walls of the potential well absorbs photons and climbs up the vertical energy axis until it escapes from the potential well. On the other hand tunneling ionization can be thought of as a 'horizontal' ionization channel in which the electron wavepacket penetrates the potential barrier of a finite thickness.

Tunneling of the electron wavepacket through the potential barrier is a quantum mechanical problem which was first considered by Oppenheimer\footnote{113} in the limit of constant electric field, i.e. \( \omega = 0 \). The probably first ionization rate (or frequency) formula which is asymptotically correct in the limit of weak and constant external electric field and which is applicable for the tunneling of electron from the 1s state of an atom was derived by Landau and Lifshitz\footnote{114}:

\[
w_L \left[ s^{-1} \right] = 4\omega_a \left( \frac{U_i}{U_H} \right)^{5/2} \frac{E_a}{E} \exp \left[ -2 \frac{E_a}{3} \left( \frac{U_i}{U_H} \right)^{3/2} \right], \tag{3.13}
\]

where \( E_a \) is the atomic unit of electric field strength (\( E_a = e/(4\pi\varepsilon_0 a_B^2) = 5.14 \times 10^{11} \) V/m), \( \omega_a \) is the atomic unit of frequency (\( \omega_a = eE_a a_B/\hbar = 41.3 \) fs\(^{-1} \)), \( a_B \) is the Bohr radius (\( a_B = 4\pi\varepsilon_0 \hbar^2/(m_e e^2) = 0.053 \) nm) and \( U_H \) is the ionization potential of hydrogen atom in the ground state (\( U_H = eE_a a_B/2 = 13.6 \) eV). The original formula presented by Landau and Lifshitz in was derived for the 1s state of hydrogen atom. However, it can be easily extended to 1s state of any H-like ion (like the one presented in equation (3.13)) if the dependence on the ionization potential is explicitly included.

Soon after the work of Landau and Lifshitz, Keldysh\footnote{115} published his theory of ionization of atoms in the strong external oscillating electric field (laser field with magnetic component neglected). In his work Keldysh introduced a parameter \( \gamma \) as the ratio of the approximate tunneling time \( \tau \) (the time it takes electron to make it through the potential barrier) and the laser period

\[
\gamma = \omega \tau, \quad \tag{3.14}
\]

with the tunneling time approximated as

\[
\tau = \frac{\sqrt{2m_e |U_i|}}{eE}. \quad \tag{3.15}
\]

The tunneling time defined by Keldysh is the time it would take a classical particle to traverse the barrier pretending that its motion is classically allowed. Upon substitution of this time into the definition of the Keldysh parameter \( \gamma \) and rewriting the laser frequency using the
ponderomotive potential, parameter $\gamma$ becomes

$$
\gamma = \sqrt{\frac{|U_i|}{2U_p}}. \tag{3.16}
$$

Using the parameter $\gamma$ Keldysh showed for the first time that the tunnel and the MPI processes are two limiting cases of the nonlinear photoionization process. Namely, the MPI theoretical approach is applicable in the region where $\gamma \gg 1$ while the tunneling approach is valid in the region $\gamma \ll 1$. In the region where $\gamma$ is close to unity both MPI and tunneling ionization coexist and the ionization theory must account for both of them. The theory proposed by Keldysh is supposed to be more accurate in the tunneling limit where $\gamma \ll 1$ but it is applicable in the MPI region with $\gamma \approx 1$ as well. In the case of tunneling ionization the potential barrier can be assumed static while electron penetrates it and therefore $\gamma$ is often called adiabaticity parameter.

In the theory of Keldysh electron starts in its ground bound state described by the ionization potential $U_i$ and at some instant it is kicked by the laser field into the continuum. From this time on it is assumed that the motion of electron is governed by the laser field while before the laser field is neglected. In the continuum electron is described by the Volkov wave function which is an exact solution for the motion of free electron in the laser field [116,117]. The influence of the binding Coulomb potential is neglected from the instant of ionization. This is the essence of Strong Field Approximation (SFA), e.g. [118], which is applied to make the time-dependent Schrödinger equation analytically solvable. The solution presented by Keldysh was found using the saddle-point technique with an exponential accuracy. The full Keldysh formula for the tunneling ionization rate of an electron in the 1s state of atom or ion subjected to the electric field of the linearly polarized laser wave is

$$
w_K [s^{-1}] = A \omega \left( \frac{U_i}{\hbar \omega} \right)^{3/2} \left[ \frac{\gamma}{\sqrt{1 + \gamma^2}} \right]^{5/2} S \left[ \gamma, \frac{U_i}{\hbar \omega} \left( \frac{1}{1 + \frac{1}{2\gamma^2}} \right) \right]
\times \exp \left\{ -2\frac{U_i}{\hbar \omega} \left( \frac{1}{1 + \frac{1}{2\gamma^2}} \right) \arcsinh \gamma - \gamma \sqrt{\frac{1 + \gamma^2}{1 + 2\gamma^2}} \right\}, \tag{3.17}
$$

where $A$ is a numerical factor of order unity which accounts for the weak dependence on the
3.3. VARIABLE PLASMA IONIZATION IN THE PARTICLE-IN-CELL MODEL

details of atom and the function $S$ is defined as

$$S[\gamma, x] = \sum_{n=0}^{\infty} \exp \left( -[2(x + 1) - x + n] \left[ \arcsinh \gamma - \frac{\gamma}{\sqrt{1 + \gamma^2}} \right] \right) \times \Phi \left( \left\{ \frac{2\gamma}{\sqrt{1 + \gamma^2}} [(x + 1) - x + n] \right\}^{1/2} \right),$$  

(3.18)

Here, $\Phi(x)$ is the so called Dawson’s integral and the symbol $\langle x \rangle$ denotes the integer part of the number $x$, i.e. the term $\langle 1 + 1/2 \gamma^2 \rangle U_i/(h\omega) + 1$ is the minimal number of photons required for ionization. In the tunneling limit ($\gamma \ll 1$) and for static electric field this rather complicated formula reduces to a more simple expression

$$w_{Kt} [s^{-1}] = \frac{\sqrt{6\pi\omega}}{2^9/4 \omega_a U_i U_H} \left[ \frac{E}{E_a} \left( \frac{U_H}{U_i} \right)^{3/2} \right]^{1/2} \exp \left[ -\frac{2 E_a}{3 E} \left( \frac{U_i}{U_H} \right)^{3/2} \left( 1 - \frac{1}{10 \gamma^2} \right) \right],$$  

(3.19)

which is considered as exponentially accurate because the preexponential factor does not match with the one derived by Landau and Lifshitz. This discrepancy originates from the SFA in which the Coulomb interaction with the resultant ion is neglected in the final state electron wave function [119]. To get the correct preexponential coefficient a quasi-classical correction, which accounts for the Coulomb field effects on the electron final state, must be included.

Very soon after it appeared the work of Keldysh was extended by Perelomov, Popov and Terentev [120, 121, 122, 123] and their theoretical approach is called the PPT theory. To avoid problems arising from the application of the saddle-point technique in the Keldysh approach the PPT theory utilized the Imaginary Time Method (ITM) in which the sub-barrier electron motion is described by the classical equations of motion with imaginary time. The PPT theory is derived with the approximation of the short range Coulomb potential by a $\delta$-function and the effect of Coulomb interaction on the electron final state is included through a first order correction. The ionization rate resulting from the PPT theory is valid for arbitrary laser wave polarization and accounts for the atomic shell dependence. For linearly polarized laser wave and in the tunneling limit it reads

$$w_{Pl} [s^{-1}] = 2\omega_a U_i U_H \sqrt{\frac{3}{\pi \omega_a E_a} \left( \frac{U_H}{U_i} \right)^{3/2}} f(l, m) \left| C_{kl} \right|^2 \left[ 2 \frac{E_a}{E} \left( \frac{U_i}{U_H} \right)^{3/2} \right]^{2n^* - |m| - 1} \exp \left[ -\frac{2 E_a}{3 E} \left( \frac{U_i}{U_H} \right)^{3/2} \left( 1 - \frac{1}{10 \gamma^2} \right) \right].$$  

(3.20)

In this expression $n^*$ is the effective principal quantum number and $l$ and $m$ are the orbital angular and magnetic quantum numbers. In a purely Coulombic field, the ionization potential
is uniquely dependent on the ion charge $Z$ and the principal quantum number $n$. Here $Z$ is the charge of the ionic core seen by the electron under consideration, i.e. the ion charge upon ionization. In complex atoms, the effective quantum number $n^*$ accounts for the quantum defect due to shielding of the ionic core by other electrons. This quantum number is obtained from the independently determined (experimentally measured or calculated using sophisticated atomic structure calculations) ionization potential $U_i$ as

$$n^* = \frac{Z}{\sqrt{U_i/U_H}}. \quad (3.21)$$

In the tunneling ionization rate (3.20) the term

$$\sqrt{\frac{3}{\pi} E_a \left( \frac{U_H}{U_i} \right)^{3/2}}$$

comes from averaging of the ionization rate over one laser cycle and therefore $E$ is not the instantaneous value of the electric field strength but its amplitude. The ionization rate formula applicable for the instantaneous electric field is obtained easily by removing this term.

The atomic structure dependence is introduced in the PPT rate (3.20) through the factors $f(l,m)$ and $C_{kl}$. The factor $f(l,m)$ takes the form

$$f(l,m) = \frac{(2l + 1)(l + |m|)!}{2|m|!l!(l - |m|)!}. \quad (3.22)$$

The factor $C_{kl}$ is a dimensionless asymptotic coefficient which is used as normalization of the electron wave function away from the nucleus. Its form for a pure Coulomb potential was proposed by Hartree, e.g. [124], and it can be generalized to other atoms using the effective principal quantum number $n^*$ and the effective orbital quantum number $l^*$ as

$$|C_{kl}|^2 = \frac{2^{2n^* - 2}}{n^* \Gamma(n^* + l^* + 1) \Gamma(n^* - l^*)}, \quad (3.23)$$

where $\Gamma$-function is the generalization of the factorial function to complex and non-integer numbers. Perelomov, Popov and Terentev did not give an explicit expression for $C_{kl}$ in their work and their ionization rate formula was not widely accepted.

About 20 years after the publication of PPT theory Ammosov, Delone and Krainov[125, 126] have extended the PPT tunneling ionization rate by making an approximation for the factor $|C_{kl}|^2$. Using the Stirling formula for the $\Gamma$-function ($\Gamma(n^* + 1) \approx \sqrt{2\pi n^*}(n^*/e)^{n^*}$, $e$ is the Euler number) and assuming $l^* \ll n^*$ they proposed the factor $|C_{kl}|^2$ to be of the form

$$|C_{kl}|^2 \approx \frac{1}{8\pi n^*} \left( \frac{2e}{n^*} \right)^{2n^*}. \quad (3.24)$$
3.3. VARIABLE PLASMA IONIZATION IN THE PARTICLE-IN-CELL MODEL

Their ionization rate formula is often referred to in the form which is valid for s shell (i.e. \( l = 0, m = 0 \))

\[
w_A [s^{-1}] = \omega_a \frac{1}{8\pi Z E_a} \sqrt{\frac{3n^*}{\pi Z^3 \bar{E}}} \left( \frac{4e Z^2}{n^*^4 \bar{E}} \right)^{2n^*} \exp \left[ -\frac{2}{3} \frac{E_a}{\bar{E}} \left( \frac{U_i}{U_H} \right)^{3/2} \right]. \tag{3.25}
\]

The term

\[
\sqrt{\frac{3n^*}{\pi Z^3 \bar{E}}}
\]

comes again from averaging of the ionization rate over one laser cycle and should be removed to get the instantaneous rate. The tunneling ionization rate formula proposed by Ammosov, Delone and Krainov (ADK) is often used in theory for its relative simplicity and reasonable accuracy which was approved in comparison with many experimental measurements, e.g. [127, 128].

The Keldysh theory was also extended by Faisal and Reiss [129, 130]. Their calculations are performed in radiation gauge instead of the former electric field gauge. This makes it easier to solve for the ionization rate analytically without making a low-frequency field approximation as in the work of Keldysh. Their ionization rate formula is enough accurate when the actual initial state wave function is used. In this case however the formula takes a rather complicated structure.

In recent years many works appeared which try to improve the ionization rate formulas or extend their applicability for example to molecules [119] or higher charge states where the subbarrier electron motion may become relativistic [131]. These corrections however seem not be important in the frame of this work.

Comparison of the instantaneous tunneling ionization rates calculated using the Landau & Lifshitz (3.13), Keldysh (3.19) and ADK (3.25) formulas is presented in Figure 3.5 for hydrogen atom and for triply ionized aluminum ion for comparison. The rates are plotted only in the range of their approximate applicability, i.e. in the tunneling ionization regime. For hydrogen atom Landau & Lifshitz and ADK formulas are in a good agreement. This is not surprising as for hydrogen atom apart from a small numerical constant of order unity the instantaneous ADK formula reduces to the Landau & Lifshitz DC tunneling ionization rate. For aluminum ion the rate calculated using the ADK formula which takes into account the atomic shell structure approximately, is supposed to be more accurate. Nevertheless, the results calculated using the Landau & Lifshitz formula are still of the same order as the ADK ones. The Keldysh formula in the form (3.19) seems to fail in predicting the correct tunneling ionization rates in both cases because the Coulomb potential is not taken into account in the final state wave function. This results in a different power dependence of the preexponential part of the formula on the
3.3. VARIABLE PLASMA IONIZATION IN THE PARTICLE-IN-CELL MODEL

Figure 3.5: Comparison of the tunneling ionization rates by the instantaneous electric field of the laser wave calculated using the Landau & Lifshitz (3.13), Keldysh (3.19) and ADK (3.25) formulas. The electric field amplitude of the wave with the wavelength 800 nm (Ti:Sapphire) is assumed in the ionization rate formulas. The ionization potentials of are set to 13.6 eV and 120 eV for hydrogen and Al$^{3+}$ ions respectively.

electric field. The inaccuracy of the Keldysh tunneling ionization rate is in agreement with [127] where the rate calculated using the Keldysh expression had to be shifted significantly along the laser intensity axis to fit the results of experimental ion production measurements. Nevertheless, the work of Keldysh deserves consideration as it was an important milestone in the theory of electric field ionization and it served as a starting point of most subsequent works dealing with tunneling ionization.

Barrier suppression ionization - $E > E_{crit}$

All the above mentioned theories use the quasi-classical approach in which the wave function is expressed in a WKB approximation. This approximation is valid only if ionization occurs slowly in comparison with the atomic time, which hold provided that the external electric field is much less than the intra-atomic field. On the other hand if the electric field amplitude of the laser wave approaches a certain threshold which is called critical field ($E_{crit}$) electron may escape from the atomic core classically without the necessity of tunneling through the barrier [132]. This ionization process is often called Barrier Suppression Ionization (BSI) [127] and it is schematically demonstrated in Figure 3.4 panel c).

The total potential of a hydrogen-like ion with the nuclear charge $Z$ and the quasi-static electric field of the laser wave can be written in a single spatial dimension as

$$V(x) = -\frac{Ze}{4\pi\varepsilon_0} - Ex.$$  \hspace{1cm} (3.26)
This potential has a relative maximum which can be easily found from the zero point of the derivation with respect to $x$. Setting this maximum equal to the ionization potential the following expression for the critical field is found

$$E_{\text{crit}} = \frac{E_a}{4Z} \left( \frac{U_i}{2U_H} \right)^2. \quad (3.27)$$

This formula can be applied to many-electron atoms as well and than $Z$ is the ion charge upon ionization. For hydrogen-like ion however this one-dimensional analysis along the laser polarization direction is too simplified due to the symmetry of the potential. Using a more proper calculation in the parabolic coordinates [133] yields the critical field

$$E_{\text{crit}} = (\sqrt{2} - 1)E_a \left( \frac{U_i}{2U_H} \right)^{3/2}. \quad (3.28)$$

In the units of laser intensity which is often called the appearance intensity the critical field for barrier suppression ionization of a many-electron atom to the charge state $Z$ can be expressed as

$$I_{\text{app}} \, [\text{W/cm}^2] = 4 \times 10^9 \frac{U_i^4 \, [\text{eV}]}{Z^2}. \quad (3.29)$$

### 3.3.2 Implementation of electric field ionization

Approximate range of applicability of the individual electric field ionization models is demonstrated in Figure 3.6 for Ti:Sapphire laser pulse. The curve which separates MPI and tunneling ionization results from equation (3.12), which is just the expression for $\gamma = 1$. The curve separating tunneling ionization and BSI is calculated from equation (3.28) which is valid for hydrogen-like ions but can serve as approximation for other ions as well.

In the frame of this work only tunneling ionization by the electric field is taken into account. MPI is more important during interactions of longer, lower intensity, and higher frequency laser pulses with targets. Concerning femtosecond laser pulses with high intensity ($> 10^{16} \, \text{W/cm}^2$) MPI takes place only during the laser prepulse interaction with the target and can be neglected during the interaction of the main laser pulse as can be seen from (3.12).

On the other hand tunneling ionization model fails when the regime of BSI is approached. The critical field for BSI of atomic shells with a mid range ionization potential ($< 400 \, \text{eV}$) can be easily surpassed by nowadays short pulse high intensity lasers. Nevertheless, concerning Ti:Sapphire lasers the ionization process can be still described by the tunneling theory. Even if the laser pulse is only several cycles long atomic shells with mid range ionization potentials are most likely depleted due to tunneling ionization before the critical field for BSI is approached. For example, the ADK rate of tunneling ionization of most atomic shells with mid range
ionization potential is very high (of the order of 10 fs$^{-1}$ or even higher) already below the critical field. In comparison with time dependent Schröedinger equation calculations most tunneling ionization models overestimate the ionization rate already before the BSI regime is approached [134]. In future, if our calculations will advance to higher laser intensities ($> 10^{19}$ W/cm$^2$), we will implement some tunneling ionization rate with applicability extended up to BSI like the one proposed in [135].

In our PIC code electric field ionization has been implemented using a Monte Carlo approach similarly like in [136]. We currently use the simplified instantaneous version of the ADK tunneling ionization rate (3.25) to calculate ionization due to the local electric field which is a sum of the field of the laser wave and the plasma field. Previously, the ionization rate formula implemented in our PIC code was the same like the one used in [136]. However, in this ionization rate the electric field is laser cycle averaged and the formula is valid for the special case when $l = 1$ and $m = 0$, where $l$ and $m$ are the orbital angular and magnetic quantum numbers of electron to be ionized. In our point of view application of such ionization rate might be moot and therefore it has been replaced in our code by the instantaneous version of the ADK rate given in (3.25). This ionization rate is valid for s shell electrons.

The ionization rate implemented in our code takes a relatively simple form. It depends only on the electric field, ionization potential and the ion charge state. Its evaluation is therefore not too computationally expensive. The probability that electron remains bound decays exponentially with the product of time and the ionization rate (frequency). Thus the probability of electric field ionization of an ion with charge $Z$ and ionization potential $U_i$ in the instantaneous local electric field with amplitude $E$ to occur during the time interval $\Delta t$
can be calculated as

\[ \Gamma = 1 - \exp \left( \int_0^{\Delta t} w_A(Z, U_i, E(t')) dt' \right) . \] (3.30)

The time interval \( \Delta t \) is given by the time step in our calculations. During this time step ionization probability is assumed constant. Thus the integration is reduced to the product \( w_A \Delta t \). As the time step in our simulation is always very small, of order of \( 10^{-17} \) s or even smaller, the product \( w_A \Delta t \) is much smaller than one and it is possible to approximate the exponential function by the first two terms of its Taylor series expansion. The ionization probability can be expressed as

\[ \Gamma = w_A(Z, U_i, E(t)) \Delta t , \] (3.31)

with a small error of order \( (w_A \Delta t)^2 \). This probability is calculated every time step and in each cell for every ion or atom whereas the electric field amplitude is linearly interpolated to ion or atom position from the borders of the corresponding cell. The ionization potentials used in our calculations are taken from the database [137] which can be found at http://spectr-w3.snz.ru.

Using a random number \( RND \) with uniform distribution between 0 and 1 it is decided if the ionization event takes place. Namely, ionization takes place if \( RND < \Gamma \). If this is the case new electron is injected into the simulation box on the same place as his parent ion and it is initiated with the same velocity as is the velocity of ion. Electric field ionization is known to produce cold electron distributions with most electron energies in the range of several eV [138, 139]. Therefore the assumption of zero relative velocity of newly released electron with respect to the parent ion is justifiable. However, in the case when elastic collisions are accounted for in the simulation, it is advantageous to initiate newly released electrons with nonzero velocity. Therefore, if the parent ion is at rest (or almost at rest) newly released electron is initiated with velocity sampled from Maxwellian distribution with a low temperature of order of eV. This may result in a very mild increase of total energy inside the simulation box. Such energy increase is however negligible and it does not have any important influence on our results. Elastic collisions are discussed in more details further.

During the next simulation step upon ionization the newborn electron and its parent ion start to separate from each other by electric and magnetic fields due to different charge to mass ratio. Charge and mass of the parent ion are adjusted after the ionization event and the ionization potential is changed to account for the new ion charge state. We remark that ionization is assumed to be a sequential process and a Single Active Electron (SAE) approximation is used in which ionization is possible only for the most weakly bound electron. This approximation is used in the derivation of most of ionization rates as well.

To guarantee energy conservation energy spent for ionization must be subtracted from the
field [140]. This is done introducing an artificial ionization current $j_{\text{ion}}$ locally. This current is directed along the electric field and it is given as

$$j_{\text{ion}} = E \frac{W_{\text{ion}}}{\Delta t \Delta x |E|^2},$$

(3.32)

where $W_{\text{ion}}$ is the total energy spent on electric field ionization in a given simulation cell per time step of $\Delta t$, and $\Delta x$ is the simulation cell volume (or length in a single dimension). Before the ionization takes place it is checked that the field still has enough energy to ionize another atom or ion. Namely, the condition

$$W_{\text{ion}} \Delta x \leq \frac{1}{2} \varepsilon_0 |E|^2,$$

(3.33)

must be fulfilled where $\Delta x$ is again the simulation cell volume. If this is not the case the ionization process is suppressed until the next step. This check must be done in order to guarantee that the rapid ionization process in a dense material does not change the sign of the electric field through the ionization current.

In PIC algorithms numerical weights of individual particles can be different. Using different particle weights might be advantageous e.g. if the distribution function of some sort of particles is to be represented with better resolution. In such case it is possible to lower their numerical weight so that each of these particles represents less real particles in comparison with other particles in the simulation, and contrary raise their number in the simulation box. However, using a different numerical weight in simulation with variable ionization is not so trivial task.

If the ionization probability is much lower than one it is possible to assume a higher numerical weight for ions than for electrons. This approach is especially useful in simulation where ion motion is unimportant and can be neglected. In such case ions can serve only as static ionization centers.

When one simulation ion represents more real particles than simulation electron the ion can be ionized several times with the same ionization potential. Strictly speaking, if the number density of real electrons represented by a single simulation electron (i.e. the electron numerical weight) is denoted as $n_e$ and the corresponding weight for ions is denoted $n_i$ than the simulation ion has $n_e/n_i$ equivalent electrons in each subshell. The ion must ‘remember’ the number of electrons ($n$) released from individual subshells and the ionization rate must be correspondingly adjusted to account for different numerical weights

$$w = w_0 \left( \frac{n_i}{n_e} - n \right),$$

(3.34)

where $w_0$ is the ionization rate in the case of same numerical weights. Care must be taken not to make the difference in the numerical weights too big to comply with the condition $w \Delta t < 1$. 
Using the above stated approach the resolution of ionization algorithm based on a Monte Carlo method becomes worse but the computational time can be reduced significantly.

The situation when electrons should have a higher numerical weight than ions is even more complicated. In such case more ions would have to be ionized at once to give rise to a single free electron or a single ion would have to be ionized in several subshells at once. Nevertheless, the case when electrons have higher numerical weight than ions is rather rare.

Finally, we would like to point out that there are two different approaches used to treat variable plasma ionization in PIC codes. In the first approach, which is used in [141], the number of simulation particles is kept constant and the increasing free electron density is taken into account by adjusting the numerical weights of simulation electrons in the same cell where the ionization event takes place. However, this way only the density of electrons is changed but the energy (momentum) distribution is conserved. In the second approach, applied in [136], new simulation electrons are injected into the simulation box. Due to increasing number of simulation particles the calculation becomes more time consuming as ionization proceeds. However, not only the free electron density increase due to ionization but also the energy distribution of electrons are described correctly in this case. As will be seen later energy distribution of free electrons may change significantly due to ionization in particular cases and therefore the second approach is utilized in our code as well.

### 3.3.3 Collisional ionization

Tunneling ionization is efficient when electric field is high. However, macroscopic electric field is usually screened in plasma on a distance of order of Debye length (3.2) and time scale of order of plasma frequency (2.4). Therefore, one can expect that with increasing plasma density the electric field ionization rate will drop down and ionization will become less efficient. It has been demonstrated e.g. in [142] that the presence of plasma decreases the tunneling ionization rate due to screening by free electrons. Tunneling ionization is thus expected not to be important in the dense plasma deeper inside the target. Of course, there is an exception. Plasma itself supports collective oscillations and the electric field associated with these oscillations might be strong enough for tunneling ionization. Nevertheless, in the dense plasma another ionization mechanism is usually much more important. This mechanism is associated with inelastic collisions of free electrons with ions and it is consequently called collisional ionization.

It is common to describe collisions in terms of cross sections in particle physics. Cross sections express the likelihood of interaction between particles in units of area and thus they are the measure of the effective surface area of the collision center which must the impinging particle strike for the collisional process under consideration to take place. Cross sections of particle interactions are usually described either by theoretically derived formulas or by empirical
3.3. VARIABLE PLASMA IONIZATION IN THE PARTICLE-IN-CELL MODEL

formulas with several free parameters which are fitted to match experimental measurements.

When electron passes through the matter it undergoes many collisions with atoms or ions. These collisions can be divided into elastic, inelastic and radiative ones. There is no energy transfer between the incident electron and the massive scattering center, atom, (up to the order of electron and atom mass ratio) in elastic collision. This kind of collisions results in the deflection of the incident electron while the atom is not influenced. On the other hand if the collision is inelastic there is a certain energy and momentum transfer from the incident electron to an electron bound to the atom and the collision results in either excitation or ionization. The last kind of collisions mentioned above occurs when there is an energy loss of the incident electron during the collision but the atom is left intact. Energy lost by the incident electron is than emitted in the form of braking radiation–bremsstrahlung and these collisions are consequently referred to as radiative in the following. Further in this section we concentrate only on the collision with a significant energy loss of the incident electron and more specifically on those collisions which result in a release of a bound electron into continuum.

Inelastic collisions can be further classified according to the impact parameter $b$ which is the distance of the closest approach of the incident electron to the scattering center if the incident electron would not be deflected. The definition of impact parameter is in fact correct only if the de Broglie wavelength associated with the relative motion of colliding particles is small compared to the size of the electron and atom interaction region e.g. [143]. In this case the trajectory of electron is well defined and the classical mechanics treatment of the interaction is possible.

Figure 3.7: Classification of electron-atom collisions according to the impact parameter $b$. Large impact parameter results in distant collision while smaller impact parameter results in close collision. If the impact parameter is significantly smaller than atomic radius the collision is usually radiative.
If the impact parameter is large compared to the size of atom the incident electron interacts with the atom as a whole and the inelastic collision is called soft or distant. If the impact parameter is of the order of atomic dimension the inelastic collision occurs between the incident electron and an electron bound to the atom. This collision is called hard or close. Finally, when the impact parameter is even smaller, significantly smaller than the atomic radius, deflection of the incident electron in the electric field of the nucleus is the most important and the bremsstrahlung radiation is emitted. Classification of collisions according to the impact parameter $b$ is illustrated in Figure 3.7.

In the case of close collisions there is a significant energy transfer from the incident electron to one of the electrons bound in the target atom. Than the binding potential can be neglected during the interaction and the close inelastic collision can be approximately described in the classical sense as a collision between an incident particle and a free electron which is initially at rest. Cross section for such kind of collision was first derived on the basis of classical mechanics and using the Rutherford cross section by Thomson in 1912 [144,145]. This cross section was later extended and employed in the theory of stopping power proposed by Bohr [146,147].

The energy transfer in close collision of two electrons can be very high and the incident electron may lose more than 50% of its initial energy in the collision. Then after the collision the two electrons become indistinguishable which is called the exchange effect in the theory. The correction due to this effect was introduced into the Rutherford cross section by Mott in 1930 [148,149,150,151]. The Mott cross section was further extended in the so called binary-encounter theory [152,153] by assigning some kind of momentum or velocity distribution to the target electron. This momentum distribution should approximate the orbital motion of a bound electron.

In the concept of stopping power the contribution from close collisions dominates at lower incident electron energies. However, when kinetic energy of the incident electron is much higher than the binding potentials of target electrons, the contribution from distant collisions to the stopping power becomes more important. As binary-encounter theory describes particularly close collisions it is not possible to recover the correct stopping power behavior in the high energy limit using the cross sections derived using the binary-encounter approach. Asymptotically correct behavior for the stopping power at high energies of the incident electron is well described by the quantum mechanical theory of inelastic collisions established by Bethe in 1930 [154,143]. This theory was derived using the first Born approximation in which the incident particle is treated as plain wave and the energy transfer in the collision is supposed to be sudden, i.e. the impulse approximation is utilized. Bethe recognized that distant collisions take place essentially through the dipole interaction between the incident and the target electron. In these collisions the cross section consists of two distinct factors, one dealing with the incident electron only and the other dealing with target only. The second factor is called generalized oscillator strength and it can be approximately derived using quantum mechanical
A theory which successfully combines close and distant inelastic collisions together to find a single and relatively simple cross section for electron impact ionization of atoms or molecules has recently been proposed by Kim and Rudd\[155\]. Their cross section interconnects modified Mott cross section which account for close collisions with the cross section of Bethe to account for distant collisions. The resulting theory is free of adjustable parameters and the authors call it the ‘Binary-Encounter-Dipole’ (BED) model. In the simplified version the generalized oscillator strength valid for hydrogen is assumed in the cross section formula and this model is called ‘Binary-Encounter-Bethe’ (BEB). The total BEB cross section for electron impact ionization of the i-th atomic subshell takes the form

\[
\sigma_{i \text{ BEB}} = 4\pi \xi_i a_B^2 \left( \frac{U_H}{B_i} \right)^2 \frac{1}{t + u_i + 1} \left[ \frac{Q_i}{2} \left( \frac{1}{t^2} \right) \ln t + (2 - Q_i) \left( \frac{1}{t} - \frac{\ln t}{t+1} \right) \right] 
\]

In the above equation \(\xi_i\) is the electron occupation number of the i-th subshell (number of electrons in the shell with the same binding energy) and \(B_i\) is the binding energy (not to be confused with the ionization potential which is the binding energy of the most tightly bound electron here). Extensive tables of energy levels (and binding energies) determined theoretically or experimentally can be found e.g.\[156\],\[157\]. Kinetic energy of the incident electron \(t\) as well as the orbital kinetic energy \(u_i\) are both normalized to the binding energy. The orbital kinetic energy was introduced to the binary-encounter collisional model by Burgess\[158\]. It accounts for the fact that the kinetic energy of the incident electron as seen by the bound electron should include also the kinetic and the potential energy of the latter. The orbital kinetic energy or average kinetic energy of electron on a given atomic orbit can be calculated using quantum mechanical atomic codes or taken from\[159\],\[156\]. For the elements listed in\[159\] (He, Ne, Ar, Kr, Xe) the value of \(u_i\) ranges from 1 to approximately 7 depending on the element and the atomic shell under consideration. The dipole constant \(Q_i\) is defined in terms of the continuum dipole oscillator strength \(df/dW\), where \(W\) is the kinetic energy of the ejected electron. When the dipole oscillator strength is not known \(Q\) can be set equal to one as a further approximation\[155\].

The BED (BEB) electron impact ionization model proved its reliability in comparison with many experimental measurement\[155\],\[160\],\[161\] and was extended to account for relativistic effect\[162\] as well as for ionization of molecular orbitals\[163\],\[164\]. The relativistically extended BED (BEB) formula is suitable not only for ionization of outer shells but the inner shell ionization cross sections is reproduced with similarly good accuracy. BED (BEB) model is applicable also for ions with a minor correction\[165\]. Another theoretical model of electron impact ionization proposed recently by Deutsch and Märk\[166\] is based on the binary-encounter approach of Gryzinski\[152\] and it is similarly successful in reproducing the experimentally
3.3. VARIABLE PLASMA IONIZATION IN THE PARTICLE-IN-CELL MODEL

Determined ionization cross sections accurately.

In the limit of high incident electron energies \( t \gg 1 \) and with the assumption of \( Q_i = 1 \) the BEB cross section approximately becomes

\[
\sigma_{i, BEB} \approx 4\pi \xi_i a_B^2 \left( \frac{U_H}{B_i} \right)^2 \frac{\ln t}{t} = 3.25 \times 10^{-14} \text{ [cm}^2 \text{ (eV)}^2 \text{]} \frac{\ln t}{tB_i^2} \quad (3.36)
\]

Therefore, this cross section recovers the correct \( \ln t/t \) dependence on the incident electron energy derived by Bethe\[143, 154]\]. Another empirical formula for the electron impact ionization cross section with the same asymptotic dependence was proposed by Lotz\[167\]. The Lotz cross section is probably the most widely used because it takes a very simple form and a reasonable accuracy of about \( \pm 40\% \)[168]. This cross section was originaly given by Lotz in the following form

\[
\sigma_{i, L} = a_i \xi_i \ln t \frac{tB_i^2}{tB_i^2 \left\{ 1 - b_i \exp \left[-c_i(t - 1)\right] \right\}} . \quad (3.37)
\]

The constants \( a_i, b_i \) and \( c_i \) are to be determined from the best fit to the experimental data. For most atomic shells the constant \( a_i \) is about \( 4 \times 10^{-14} \text{ cm}^2 \text{ (eV)}^2 \) and very often this formula is used in the high energy limit where the other constants become unimportant. In the high energy limit Lotz formula takes the form

\[
\sigma_{i, L} = 4 \times 10^{-14} \text{ [cm}^2 \text{ (eV)}^2 \text{]} \xi_i \ln t \frac{tB_i^2}{tB_i^2} , \quad (3.38)
\]

and as can be seen it corresponds very well with high energy limit of the BEB formula given in equation \( (3.36) \).

For demonstration the BEB cross section for individual shells of aluminum atom is plotted in Figure 3.8 panel a). Input data\[156\] of the BEB model for individual orbitals of the aluminum atom (including fine structure splitting of the 2P shell) are summarized in the Table 3.1.

From Figure 3.8 panel a) it can be seen that the cross sections for electron impact ionization of individual aluminum atomic subshells with the same principal quantum number are similar (of the same order). With decreasing principal quantum number the binding energy increases significantly and the magnitude of the cross sections decrease strongly because of the inverse square dependence on the binding energy given by equation \( (3.36) \). Similar behavior applies for other atoms as well.

In panel b) of Figure 3.8 the ionization frequency for electron impact ionization of individual atomic shells of solid density \( (6 \times 10^{22} \text{ cm}^{-3}) \) aluminum is plotted versus electron energy. The
collisional ionization frequency is obtained as

$$\nu = n \sigma v,$$

(3.39)

where \(n\) is the number density of aluminum atoms and \(v\) is the velocity of ionizing electron.

For collisional ionization to significantly increase the free electron density and the mean ion charge in the target on the subpicosecond time scale, it is necessary to have a huge population of ionizing electrons. Hence, the collisional ionization is in particular due to thermal electrons which are heated someway. In our case the heating can be provided either by the laser pulse

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
Orbital & \(B_i\) [eV] & \(u_i\) & \(\xi_i\) \\
\hline
1\(S_{1/2}\) & 1595.5 & 1.36 & 2 \\
2\(S_{1/2}\) & 134.1 & 2.22 & 2 \\
2\(P_{1/2}\) & 87.8 & 3.07 & 2 \\
2\(P_{3/2}\) & 87.4 & 3.07 & 4 \\
3\(S_{1/2}\) & 10.7 & 2.39 & 2 \\
3\(P_{1/2}\) & 5.98 & 2.61 & 1 \\
\hline
\end{tabular}
\end{table}

\textbf{Table 3.1:} Table of constants used in the BEB model (3.35) to calculate electron impact ionization cross sections for aluminum plotted in Figure 3.8.

\begin{figure}
\centering
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{collisional_cross_sections}
\caption{(a) Collisional ionization cross sections}
\end{subfigure}
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{ionization_frequencies}
\caption{(b) Ionization frequencies}
\end{subfigure}
\caption{Cross sections and ionization frequencies for electron impact ionization of individual aluminum atom subshells. The cross sections are calculated from equation (3.35) with the constants given in Table 3.1 and \(Q_i = 1\). The ionization frequencies are calculated according to (3.39) with solid density aluminum target assumed.}
\end{figure}
or by some strong field induced in plasma (e.g. Ohmic heating). In the target such heating violates the initial equilibrium between ionization and recombination processes on behalf of the ionization.

Although, heating increases total energy stored in plasma it should be noted that collisional ionization results in a kind of plasma cooling. The ionizing electrons are losing kinetic energy to knock bound electrons out of ions and their remaining energy is collisionally partitioned between them and the newly released electrons. In a dense heated plasma the collisional ionization process can be fast enough so that a kind of equilibrium between heating and cooling is established and the average electron kinetic energy is maintained below the ionization potential. Of course, this applies only until their are enough ions to be ionized with the lowest energetic shell still occupied. When this shell is significantly depleted average electron kinetic energy (electron temperature) increases.

For the above stated reasons and from the cross sections and collisional frequencies plotted in Figure 3.8 it is possible to conclude that the collisional ionization process can be regarded in a dense matter as advancing shell by shell starting from the shell with the lowest binding energy. The cross sections are relatively low for the shells closer to the atomic nucleus and significant ionization of these shells is improbable on a subpicosecond time scale. The outermost shells are depleted first and it is sufficient to consider collisional ionization of only these shells as a first approximation.

As the population of fast electron in plasma is often much less numerous than the population of thermal electrons and as cross section for collisional ionization (as well as collisional ionization frequencies) decreases with increasing electron energy, collisional ionization by fast electrons can often be neglected. On the other hand in particular cases it is interesting to calculate also hard X-ray (e.g. K-α) radiation originating from the relaxation process of higher Z atoms ionized in their innermost shells. This radiation is not strongly attenuated while propagating through the target. As noted in Section 2.5.1 K-α radiation can be further utilized for other measurements or as a diagnostic of the experiment. Collisional ionization of inner shells is particularly due to fast electrons. Binding energy of K shell electrons in higher Z elements is very high and the relaxation process in which the vacancy in the K shell is filled is very fast. Considering target composed of higher Z element the K shell is never depleted due to collisional ionization by the less numerous population of fast electrons and the density can be assumed constant in the equation for ionization frequency (3.39).

The cross sections given in equations (3.35) and (3.37) are derived assuming nonrelativistic energies. These cross sections should be corrected to account for the relativistic effects to describe collisional ionization of the innermost K shell by fast electrons correctly. The binary-
encounter-Bethe cross section with relativistic correction takes the form [162]

\[
\sigma_{i \text{ BEBr}} = \frac{4\pi \xi a_Z^2 \alpha^4}{2b'_i (\beta^2_i + \beta^2_{ai} + \beta^2_{bi})} \left\{ \frac{Q_i}{2} \left[ \ln \left( \frac{\beta^2_i}{1 - \beta^2_i} \right) - \beta^2_i - \ln(2b'_i) \right] \left( 1 - \frac{1}{t^2} \right) \right. \\
+ \left. (2 - Q_i) \left[ 1 - \frac{1}{t} - \frac{\ln t}{t + 1} \frac{1 + 2t'}{(1 + t'/2)^2} + \frac{b'_i^2}{(1 + t'/2)^2} t - 1 \right] \right\}, \tag{3.40}
\]

with

\[
\beta^2_i = 1 - \frac{1}{(1 + t')^2}, \quad t' = \frac{T}{mc^2}, \\
\beta^2_{bi} = 1 - \frac{1}{(1 + b'_i)^2}, \quad b'_i = \frac{B_i}{mc^2}, \\
\beta^2_{ai} = 1 - \frac{1}{(1 + u'_i)^2}, \quad u'_i = \frac{U_i}{mc^2}.
\]

In the above equations \( \alpha \) is the fine structure constant \( \alpha = \sqrt{2U_H/(mc^2)} = 1/137 \) and \( T, B_i \) and \( U_i \) are the incident electron kinetic energy, the binding energy and the orbital kinetic energy respectively. The approximation of \( Q_i = 1 \) can be applied in this cross section as well. The relativistic effects on the collisional ionization cross section are particularly significant in targets composed of higher \( Z \) elements [162, 169] and at energies higher than \( mc^2 \). They result in relativistic rise of the cross section and this rise may eventually overcome the peak in the cross section at lower energies [169]. Such relativistic rise of the cross section for K shell ionization of silver atom can be seen in Figure 3.9 where the relativistic (3.40), and nonrelativistic (3.35), BEB models are compared.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3.9.png}
\caption{Comparison of the nonrelativistic (3.35) and the relativistic (3.40) binary-encounter-Bethe ionization cross sections for ionization of the K shell of silver atom. The constants used in equations are taken from [162] and \( Q_i = 1 \) is assumed.}
\end{figure}
3.3.4 Implementation of collisional ionization

Collisional ionization is implemented into our PIC code using a Monte Carlo approach. The algorithm is local and energy conserving and it is simplified for computational reasons. We assume the collisional ionization process as advancing shell by shell from the outermost shell as discussed in previous section. If desired, the algorithm can be extended in future to take into account collisional ionization of all shells at once however this would be at the expense of making the computation more demanding. Moreover, if inner shell ionization is to be considered the inner atomic relaxation should be taken into account which is currently impossible in our code. Consequently, neither excitation is taken into account and ground state configuration is assumed for all shells.

According to the locality of the algorithm only ionizing collisions between electrons and ions in the same cell are considered. First of all, densities \( n_i \) of ions in individual charge states are calculated where \( i \) ranges from 1 to \( Z \) (the atomic number). Subsequently for all the charge states \( i \) for which \( n_i > 0 \) the cross sections \( \sigma_i \) for collisional ionization are calculated for the electron under consideration at the moment. Of course, only those shells are taken into account for which electron energy is higher than the binding energy. Currently, we use either the Lotz formula as given by equation (3.38) or the BEB formula as given by equation (3.35) to calculate the cross sections. The choice of cross section formula in individual simulation comes out from the competition between the desired accuracy and the available computational resources. Using the cross sections \( \sigma_i \) and ion densities \( n_i \) the total collisional ionization frequency for a given electron can be calculated as

\[
\nu = \sum_i n_i \sigma_i v ,
\]

where \( v \) is the electron velocity. The probability that the electron ionizes some ion (atom) during a timestep of \( \Delta t \) is given similarly like in the case of electric field ionization as \( \Gamma = \nu \Delta t \) (the approximation of \( \nu \Delta t \ll 1 \) is applied). This probability is sampled using a number \( RND \) which ranges between 0 and 1 and is randomly chosen from uniform distribution. Namely, if \( RND < \Gamma \) collisional ionization takes place.

Particular shell which should be ionized can be chosen in a Monte Carlo way again. Let \( RND \) be a newly chosen random number with the same properties as previously. Than the \( i \)-th shell should be ionized for which the condition

\[
\frac{1}{3} \sum_{k=1}^{i-1} n_k \sigma_k \leq RND < \frac{1}{3} \sum_{k=1}^{i} n_k \sigma_k
\]
holds true where $S$ is the normalization constant

$$S = \sum_{k=1}^{Z} n_k \sigma_k = \frac{\nu}{v}. \quad (3.43)$$

Fortunately, the products $n_k \sigma_k$ are readily available from the calculation of collisional frequency (3.41). Another approach is possible in which the probabilities for electron impact ionization are calculated and sampled for all individual shells directly. This approach is however more computationally expensive as more random numbers have to be chosen.

When the shell which is to be ionized is known from the above described technique, an ion for which this shell is the outermost occupied one is randomly selected in current cell and its charge and mass are correspondingly adjusted. The densities of ions in individual charge states are modified as well. A new electron is then injected into the simulation box on the corresponding place and initialized with the same velocity as its parent ion. Once again if ions are at rest and elastic collisions are taken into account a small initial velocity is assigned to the newborn electron. This energy is randomly sampled from the Maxwellian distribution with temperature of order of eV. The energy spent on ionization and the small thermal energy with which the newly released electron is initialized are both subtracted from energy of the ionizing electron so that its propagation direction does not change. Care is taken not to initialize the newly released electron with too high velocity so that energy can be conserved. The same procedure is applied to all free electrons in all cells.

The collisional ionization algorithm described in this section is quite general but also computationally very expensive as the number of electrons in the simulation box is usually very high. Therefore, collisional ionization is taken into account only when necessary to handle important physical processes correctly and if possible additional simplifying assumptions are applied. Finally, it should be noted that the rate at which collisional ionization takes place depends not only on the ion density but also on the number or density of ionizing electrons and if the heating of plasma is sufficiently high this may give rise to a kind of avalanche effect.

### 3.3.5 Recombination

Radiative and three-body recombination are the inverse processes to single photon ionization and collisional ionization respectively. In radiative recombination process ion binds an imminent free electron from the electron sea to produce a lower charge state with subsequent radiation of photon. The radiative recombination rate is usually obtained from the photoionization cross section applying the detailed balance principle and averaging over Maxwellian velocity distribution of electrons with temperature $T_e$. Using this procedure a simple radiative recombination rate was proposed by Kramers [99, 170] and later improved by Seaton [99, 171].
The Seaton’s rate \([172]\) per ion reads

\[
\alpha_r = 5.2 \times 10^{-14} Z n_e \sqrt{\frac{B_Z}{T_e}} \left[ 0.43 + \frac{1}{2} \ln \left( \frac{B_Z}{T_e} \right) + 0.47 \left( \frac{B_Z}{T_e} \right)^{-1/3} \right] \text{[s}^{-1} \text{]}, \tag{3.44}
\]

where \(Z\) is the ion charge state, \(n_e\) is electron density in \(\text{cm}^{-3}\) and \(B_Z\) is the binding energy of the respective ionic state. For the reasonable values of \(Z < 20\), \(B_Z/T_e \in (10^{-2}, 10^2)\), and even relatively high electron density of \(10^{23}\) \(\text{cm}^{-3}\) this rate is below 3 ps\(^{-1}\) and hence it is negligible on the femtosecond time scale.

In the three-body recombination process two free electrons collide in the vicinity of ion and they exchange their kinetic energy so that one of them remains bound after the collision. As it is a three-body process its rate depends strongly on plasma density. In the three-body recombination process electron is captured most probably in an excited state and the ion may be eventually re-ionized on a short temporal scale. The rate for three-body recombination is usually obtained from the collisional ionization rate applying the detailed balance principle. The ratio of rates of collisional ionization \(\beta\) and three-body recombination \(\alpha_{3b}\) processes can be expressed as \([99, 173]\)

\[
\frac{\alpha_{3b}}{\beta} = 3.3 \times 10^{-24} n_e n_T^2 \exp \left( \frac{B_Z}{T_e} \right), \tag{3.45}
\]

where \(n\) is the principal quantum number of level to which electron recombines. Unless the temperature is significantly lower than the binding energy of the state to which electron should be captured and unless the density of electrons is very high \((10^{23}\ \text{cm}^{-3})\) the collisional ionization process is more important and three-body recombination can be considered as small correction or even neglected. It is possible to incorporate three-body recombination process in an approximate manner by lowering the collisional ionization rate.

Both the above mentioned recombination processes do not have important effect on the results of simulations presented in this work and therefore neither of them is taken into account here.

### 3.4 Elastic collisions

Strongly heated plasma just like those produced during short-pulse laser irradiation of target are far from thermal (kinetic) equilibrium. In kinetic equilibrium particles obey the Boltzmann-Maxwell velocity distribution which is characterized by a single parameter, temperature. If this is not the case the system is gradually driven until kinetic equilibrium is established. The driving force responsible for this thermalization process is due to elastic collisions. Unlike in the case of inelastic collisions discussed in the previous section there is no conversion of kinetic
energy into other forms in elastic collisions. Hence these collisions conserve total kinetic energy of colliding particles and their impact is associated with redistribution of total kinetic energy within the system so that the kinetic equilibrium is reached.

Essential part of the kinetic theory describing collisions between particles was established by Boltzmann [174, 93]. In order to explain the properties of dilute gases by analyzing elementary collision processes between pairs of molecules he derived an expression for temporal evolution of test particle described by the distribution function $f_t(x, v, t)$ which interact through elastic collisions with a system of field particles described by distribution $f_f(x, v, t)$. In the following the subscripts $t$ and $f$ denote quantities related with the test and field particles respectively (e.g. $q_t, m_t$ are the test particle charge and mass). Boltzmann expression takes the form

$$\frac{df_t(x, v_t, t)}{dt} = \left[ \frac{\partial f_t(x, v_t, t)}{\partial t} \right]_c + \int \int d\mathbf{v}_f d\Omega \left| \mathbf{v}_t - \mathbf{v}_f \right| \sigma \left[ f_t(x, v'_t, t)f_f(x, v'_f, t) - f_t(x, v_t, t)f_f(x, v_f, t) \right].$$

In the Boltzmann equation (3.46) $v_t$ and $v_f$ denote the velocities of interacting particles of both species before and $v'_t$ and $v'_f$ after collision, $\sigma$ is the scattering cross section depending on the scattering angle and the relative velocity of colliding particles and the integration is carried over the solid scattering angle $\Omega$ and the velocity of field particles. The total derivative $d/dt$ of the distribution function of test particles is taken along the trajectory in the phase space. In the derivation of Boltzmann equation (3.46) some simplifying assumptions are made (e.g. molecular chaos, Markovian character, binary collisions). Nevertheless this equation is still very general and in particular cases also difficult to solve in this form.

In the classical sense elastic collisions just like the inelastic ones can be described using the impact parameter $b$ and categorized into two groups close and distant. Usually the impact parameter $b_0$ separating these two groups is chosen so that the angular deflection in a single collision with impact parameter $b_0$ is equal to $\pi/2$. For the Coulomb interaction between two particles with charges $q_1$ and $q_2$, relative velocity $g$ and reduced mass $\mu$ such situation occurs when

$$b_0 = \frac{q_1 q_2}{4\pi\varepsilon_0 \mu g^2}.$$  

3.4.1 Distant encounters - Coulomb collisions

Close encounters with $b < b_0$ cause serious deflections of colliding particles. However, the cross section for close encounter to take place is relatively small ($\pi b_0^2$). It was demonstrated for example by Jeans [175, 176] that in the case of inverse square force law (i.e. Coulomb or gravitational force) between interacting particles the distant encounters usually outweigh the
3.4. ELASTIC COLLISIONS

Effect of the close ones. For example, if the maximum impact parameter taken into account is \( b_1 \) than for collisions of electrons with heavy ions the mean square deflection per unit time interval is proportional to [176]

\[
\langle \sum_{b < b_1} \sin^2 \chi \rangle \propto \left[ \ln \left( 1 + \frac{b_1^2}{b_0^2} \right) - \frac{1}{1 + b_1^2/b_0^2} \right].
\] (3.48)

The mean square deflection angle calculated using equation (3.48) is plotted in Figure 3.10. As can be seen in the figure the cumulative effect of many distant collisions \( (b_1 \gg b_0) \) produces much larger deflection than close collisions \( (b_1 = b_0) \). Close collisions with impact parameter \( b < b_0 \) are therefore often of minor importance. The classical approach which utilizes concept of impact parameter is again applicable only if the de Broglie wavelength \( \lambda_B (= h/p, p \) is the momentum) associated with the colliding particle is smaller than the distance of closest approach which is approximately the impact parameter. If \( b < \lambda_B \) dispersion of the particle wave packet can be significant and a proper calculation should be done quantum mechanically. For the above reasons collisions with impact parameter \( b < \max\{b_0, \lambda_B\} \) are usually disregarded in the theory of elastic collisions in systems with long range interaction potentials.

With the assumption that many distant small angle encounters dominate transition of the distribution due to elastic collisions, the distributions of test and field particles after collision can be expanded into Taylor series around small \( \Delta v \) (velocity change during the collision). This way the postcollision distribution functions are removed from the Boltzmann equation and if higher order terms (of order \( \Delta v^3 \) or higher) are neglected Fokker-Planck equation is derived [177,178].

**Figure 3.10:** Mean square deflection of electron due to elastic collisions with heavy ions per unit time interval. The deflection is calculated according to (3.48) and it is normalized to the value obtained for \( b_1/b_0 = 1 \).
3.4. ELASTIC COLLISIONS

Fokker–Planck equation takes the form

\[
\frac{df_t}{dt} = -\frac{\partial}{\partial v_t} (f_t(\Delta v_t)) + \frac{1}{2} \frac{\partial^2}{\partial v_t^2} (f_t(\Delta v_t^2)) , \quad f_t = f_t(x, v_t, t) \tag{3.49}
\]

\[
\langle \Delta v_t^N \rangle = \int \int d\Omega \Delta v_t^N \sigma |v_t - v_f| f_f , \quad f_f = f_f(x, v_f, t)
\]

The term \( \langle \Delta v_t^N \rangle dt \) represents the mean value of the \( N \)-th order dyadic of velocity increment resulting from all encounters of the test particles with the field particles during the time interval \( dt \).

Fokker-Planck equation was originally derived to explain Brownian motion, i.e. the random movement of particles suspended in a fluid. Similar equation for plasmas was derived independently by Landau and therefore this equation is sometimes called Fokker-Planck-Landau [93]. On the right hand side of Fokker-Planck equation the first term is associated with dynamical friction and the second term with diffusion in the velocity space. When a fast test particle is injected into a bath of field particles which are in thermal equilibrium it is slowed down due to the friction and its velocity distribution spreads as a consequence of diffusion in the velocity space. As demonstrated in Figure 3.11 after some time the test particle is thermalized and its distribution function approaches equilibrium with the distribution of the bath. The rate of thermalization of the test particle in a bath of field particles is expressed using the collisional frequency \( \nu \) which will be introduced later.

Assuming pure Coulomb interaction between two point charges Rutherford cross section can be used for \( \sigma \) and the \( N \)-th order velocity increments can be integrated over the solid scattering angle \( \Omega \). However, when this integration is carried out over the entire sphere it diverges. Therefore, two cutoffs are usually introduced on the polar scattering angle which is

\textbf{Figure 3.11}: Demonstration of the temporal evolution of test particle velocity distribution in the bath of field particles with another distribution.
3.4. ELASTIC COLLISIONS

Figure 3.12: Illustration of cumulative collision with charged particles within the Debye sphere. The cumulative collision is a sum of many distant and a few close collisions.

the scattering angle in the scattering plane. The large angle cutoff is introduced to omit close encounters. In these encounters the trajectories of scattering particles cannot be assumed straight. If the trajectory is described correctly as hyperbolic the large angle cutoff is not needed. However, the influence of few close encounter is often assumed to be negligible in comparison with many distant ones in plasma. Therefore, integration is limited to encounters with maximum polar scattering angles corresponding to impact parameter of $max\{b_0, \lambda_B\}$ as discussed above.

On the other hand the integration diverges due to very distant encounters as well. Scattering angles due to these encounters are infinitesimally small but the number of such encounters grows more rapidly with the volume over which integration is performed in the case of long range potentials. Nevertheless, it is known [176] that these distant encounters are screened in plasma on a distance significantly longer than the Debye length ($\lambda_D$), (3.2). Hence the small scattering angle cutoff is usually set to correspond with the impact parameter of $max\{\lambda_D, r_i\}$. The term $r_i$ is the ion sphere radius and it is introduced to account for dense plasmas where the Debye length could be too short because the Debye-Hückel model is not applicable in this domain. The cutoffs usually applied to the impact parameter are illustrated in Figure 3.12. Recently, it has been demonstrated [179] that it is more correct to introduce the cutoff on the small velocity change ($\Delta v$) than on the small scattering angle. However, this new approach does not seem to bring significant difference in our case.

After the integration over the solid scattering angle is carried out the friction and the diffusion term can be expressed using the so called Rosenbluth potentials [180]. In the respective
order these terms are

\[ \langle \Delta v \rangle = \Gamma \frac{\partial H(v)}{\partial v} , \quad \langle \Delta v \Delta v \rangle = \Gamma \frac{\partial^2 G(v)}{\partial v \partial v} , \quad \Gamma = \frac{4 \pi q f \ln \Lambda}{\{4 \pi \varepsilon_0 \}^2 m_t^2} , \]  

and the potentials \( H \) and \( G \) are

\[ H(v) = \left( 1 + \frac{m_t}{m_f} \right) \int dv' \frac{f_f(v')}{|v - v'|} , \quad G(v) = \int dv' f_f(v') |v - v'| \]

The term \( \ln \Lambda \) is called the Coulomb logarithm and because it only weakly depends on its argument it is often regarded as constant. Using the small and large angle cutoffs for the possible impact parameters this logarithm is expressed as

\[ \ln \Lambda = \ln \left( \frac{b_{\text{max}}}{b_{\text{min}}} \right) . \]

From the analysis of plasma temperature equilibration in binary collisions [181] it results that the best, general, enough accurate and relatively simple model for evaluation of the Coulomb logarithm, which takes into account hyperbolic trajectory of colliding particles in close collisions and accounts for dense plasma as well as quantum effects, can be expressed as

\[ \ln \Lambda = \frac{1}{2} \ln \left( 1 + \frac{r_i^2 + \lambda_D^2}{b_0^2 + \lambda_B^2} \right) . \]

It is often feasible to assume at least as a first approximation that the distribution of field particles is isotropic and Maxwellian. Than the Rosenbluth potentials can be integrated and the friction and diffusion terms are further simplified [52, 182]. The friction term becomes

\[ \langle \Delta v \parallel \rangle = - \left[ \frac{m_t}{\mu} \psi(x) \right] v_0 v_t , \]

where \( \mu \) is the reduced mass and the components of the diffusion term along and perpendicular to the test particle velocity are

\[ \langle \Delta v^2 \parallel \rangle = 2 \left[ \psi(x) \left( 1 - \frac{1}{2x} \right) + \psi'(x) \right] v_0 v_t^2 , \quad \langle \Delta v^2 \perp \rangle = \left[ \frac{\psi(x)}{x} \right] v_0 v_t^2 . \]

In the above expressions \( x \) is called relative speed parameter \( (x = v_t^2/v_{fT}^2, v_{fT} \text{ is the thermal velocity of field particles}) \) and function \( \psi(x) \) is the so called Maxwell integral defined as \( (\psi'(x) \) is its derivative with respect to \( x) \)

\[ \psi(x) = \frac{2}{\pi} \int_0^x dt \sqrt{t} e^{-t} . \]

The friction and diffusion coefficients (3.54) and (3.55) express the rates of momentum
loss (slowing down) and parallel and perpendicular velocity diffusion respectively. In these expressions the frequency \( \nu_0 \) of test particle collisions with the field particles of the density \( n_f \) is introduced

\[
\nu_0 = \frac{4\pi n f q^2 q_i^2}{(4\pi\varepsilon_0)^2 m_i^2 v_i^2} \ln \Lambda . \tag{3.57}
\]

Care must be taken here to explicate the meaning of the collisional frequency. Even if in the theory of Coulomb collisions it is supposed that collisions are binary and therefore distinct event in real plasma the deflection of test particle is more likely continuous than stepwise process. Therefore, the collisional frequency does not represent the rate at which collisions occur but the rate at which many distant collisions produce significant deflection of the test particle.

If quasineutrality is assumed the electron-ion collision frequency is \( Z \) times higher than the frequency of electron-electron collisions, where \( Z \) is the average ion charge. Therefore, it is often sufficient to take into account only electron-ion collisions. Electron-ion collisions are indeed important in collisional absorption of laser radiation. Because the component of electron velocity associated with the oscillatory motion in the laser field is the same for all electrons locally, this component is zero in the center of mass frame of two electrons, where the deflection takes place. Therefore, electrons can exchange only the thermal component of velocity among themselves. On a short time scale which is of particular interest in this work it is possible to further assume that ions are immobile (i.e. they have infinite mass and zero velocity). In this case the reduced mass \( \mu \) becomes the electron mass \( (m_e) \), the Maxwell integral \( \psi \) is equal to one and its derivative \( \psi' \) and the terms divided by \( \chi \) vanish. The collisional model which assumes immobile ions is called Lorentz model. Lorentz collisional model is yet enough simple but it can still serve as reasonable approximation of Coulomb collisional processes in short pulse laser produced plasma.

Langevin equation

Fokker-Planck-Landau equation is probably the most widespread equation used to describe the evolution of collisional nonequilibrium plasma. Therefore most collisional models used in PIC simulations prove their reliability through some kind of correspondence with this equation. One of the characteristic equations of the Fokker-Planck-Landau collisional term is equivalent to the Langevin equation. Langevin equation is a stochastic differential equation and it was proposed to study Brownian motion as well [93]. For a particle with charge \( q \) this equation can be write as

\[
\frac{dp}{dt} = q(E + v \times B) + P(v) , \quad P_i(v) = F_i(v) + D_{ik}v_k \xi_k , \tag{3.58}
\]
3.4. ELASTIC COLLISIONS

where \( \mathbf{F} \) is a velocity dependent vector connected with the friction force and \( \mathbf{D} \) is a velocity dependent matrix connected with the velocity diffusion. The vector \( \xi \) is a Gaussian white noise with the properties

\[
\langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t) \xi_k(t + \tau) \rangle = \delta_{ik} \delta(\tau), \quad \int_{t}^{t + \tau} \xi_i(t') dt' = p_i \sqrt{\tau},
\]

where \( p_i \) is normally distributed random number. The functions \( \mathbf{F} \) and \( \mathbf{D} \) are related to the Fokker-Planck-Landau friction and diffusion terms denoted here as \( \mathbf{A} \) and \( \mathbf{B} \) respectively.

\[
\| D_{ik} \| = \| B_{ik} \|^{1/2}, \quad F_i = A_i - \chi D_{jk} \frac{\partial D_{ik}}{\partial v_j}.
\]

The matrices \( \mathbf{B} \) and \( \mathbf{D} \) are symmetric non-negative and definite and the parameter \( \chi \) ranges from 0 to 1 and depends on the definition of the stochastic integral (\( \chi = 0 \) Ito approach, \( \chi = 1/2 \) Stratonovich approach).

In the case of Lorentz collisional model (i.e. immobile ions) the approach utilizing Langevin equation to treat electron-ion collisions is indeed simple [183]. Using the Stratonovich symmetric definition of the stochastic integral (\( \chi = 1/2 \)) the governing equation of particle motion is obtained in the form

\[
\frac{d\mathbf{v}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) - \sqrt{\frac{a}{|v|^3}} \mathbf{v} \times (\mathbf{v} \times \xi), \quad a = \frac{\omega_p^2 Z \ln \Lambda}{4\pi n_e}.
\]

The general approach which accounts also for electron-electron collisions is however relatively complicated. Either the local velocity distribution of electrons must be decomposed into several Maxwell distributions each with separate temperature and drift velocity, or the Rosenbluth potentials must be evaluated numerically. When the distribution can be regarded as isotropic evaluation of these potentials is more simple. However, as the velocity distributions of particles in PIC simulation are not always represented enough accurately, evaluation of Rosenbluth potentials may introduce a significant error. Because of limited number of particles in the simulation and the stochastic manner of the force introduced in the Langevin equation energy and momentum conservation are not guaranteed and have to be somehow restored [184].

Nevertheless Coulomb collisional approach through Langevin equation is interesting for its close relation with Fokker-Planck-Landau equation in the sense that the test particle feels some stochastic scattering force and its average properties are well defined by the friction and the diffusion terms. The Langevin approach has been attracting attention of many authors in recent years [141, 183, 184, 185].
Binary collisions

The idea behind the binary collision approach to Coulomb collisions is to handle the deflection resulting from multiple distant encounters through a single collision with another particle. In this approach particles are locally grouped into pairs (or if their number is odd the last group contains three particles) and in these pairs they are deflected the one from the other. The deflection angle is essentially random but with a given statistical properties so that correspondence with the Fokker-Planck-Landau equation in the limit of short interval time and high number of particles is approached.

The cornerstone of the binary collision approach to Coulomb collisions is the multiple or plural scattering theory. It has been demonstrated for example in [186] that the cumulative deflection angle, resulting from multiple scattering where individual deflections are small, is characterized by the Gaussian distribution with zero mean and variance equal to two times the mean square scattering angle $2\langle \theta^2 \rangle$. In Coulomb collisions this mean square scattering angle is indeed related with the collision frequency $\nu$ (3.57) multiplied by the time step $\Delta t$. However, the approximation of small angle deflection hold only until $\nu \Delta t \ll 1$ and therefore applicability of this approach is limited to a very short time step.

The binary collision approach to treat Coulomb collisions in particle simulations was proposed by Takizuka & Abe [104]. Upon scattering the velocities of colliding particles are given as

$$v' = v \pm m\mu \left[ g(1 - \cos \theta) + h \sin \theta \right],$$

where $\mu$ and $g$ are the reduced mass and the relative velocity of colliding particles, $\theta$ is the polar scattering angle and the sign $\pm$ means that for one particle the second term is incremented while for the other one it is subtracted. The vector $h$ is designed to maintain energy conservation and its Cartesian components are

$$h_x = g_\perp \cos \psi,$$
$$h_y = -(g_x g_y \cos \psi + g_z g_y \sin \psi),$$
$$h_z = -(g_x g_z \cos \psi - g_y g_z \sin \psi),$$

where $g_\perp = (g_y^2 + g_z^2)^{1/2}$ and $\psi$ is the azimuthal angle of the collision plane. This angle can be arbitrary, wherefore it is a random variable uniformly distributed between 0 and $2\pi$. As stated above polar scattering angle $\theta$ is random Gaussian variable. In the approach of Takizuka & Abe $\tan(\theta/2)$ is obtained in the collisional center of mass reference frame through random sampling Gaussian distribution with zero mean and variance $\nu_0 \Delta t/2$, where $\nu_0$ is the collisional frequency given in (3.57) and $\Delta t$ is the time step. Because of the center of mass frame, mass and velocity are replaced by the reduced mass and the relative velocity of colliding particles.
in the expression for collisional frequency. The method is valid for $\nu_0 \Delta t \ll 1$ and the check of its reliability was provided through simulations of slowing-down and energy exchange rates of test particles in a thermal bath which were successfully compared with those in Fokker-Planck-Landau equation.

The binary collision model proposed by Takizuka & Abe became very widespread as it can be relatively easily implemented and the it guarantees exact energy and momentum conservation, as the correct collisional model should. The main disadvantages of the model come from the condition $\nu_0 \Delta t \ll 1$ which may imply a very short time step, and from its inaccuracy if the number of particles is low. The binary collision model is also sometimes criticized for the absence of physical arguments justifying grouping of particles into pairs.

Recently, the properties of cumulative scattering angle resulting from many small angle collisions in plasma have been studied by Nanbu [187]. The expectation of $\sin^2(\theta/2)$ after many small angle collisions, with $\theta$ being the cumulative polar scattering angle, has been proposed as

\[
\left\langle \sin^2 \frac{\theta}{2} \right\rangle = \frac{1}{2} \left( 1 - e^{-s} \right),
\]

(3.64)

where $s = \nu_0 \Delta t$ (in the expression for $\nu_0$ mass and velocity are again replace by reduced mass and relative velocity). The distribution of cumulative scattering angle is approximated by

\[
f(\theta) = \frac{A}{4\pi \sinh A} \exp(A \cos \theta) \approx \frac{A}{2\pi} \exp \left[ -A(1 - \cos \theta) \right] \text{ (for } A \gg 1),
\]

(3.65)

where $A$ is obtained as solution of the equation

\[
\coth A - \frac{1}{A} = e^{-s}.
\]

(3.66)

For $s < 1$ the solution of equation (3.66) can be approximated as $A = 1/s$ with reasonable accuracy. In the limit $s \ll 1$ and with the assumption of small scattering angle, i.e. $\cos \theta \approx 1 - \theta^2/2$, the distribution becomes

\[
f(\theta) \approx \frac{A}{2\pi} \exp \left( -A \frac{\theta^2}{2} \right).
\]

(3.67)

Hence the Gaussian distribution for $\theta$ is recovered. In the other extreme $s \gg 1$ the distribution tends to isotropic which is expected for cumulative scattering angle after many successive collisions. The model proposed by Nanbu is therefore extension of the Takizuka & Abe model to much longer time steps. Reliability of this model was proved through its first order (in $\Delta t$) correspondence to the Fokker-Planck-Landau collisional term [188].

Binary collisional approach to Coulomb collisions in plasma can be applied also for the case
of Lorentz model in which elastic scattering of electrons from stationary ions are treated. In this case the algorithm is significantly simplified as there is no need for grouping particles.

3.4.2 Close encounters - Elastic electron–atom scattering

In plasma where the interaction potential of particles is of long range (of order of \( \lambda_D \)) the deflection resulting from the cumulative effect of many distant encounters usually outweights the deflection resulting from less numerous close encounters. In neutral matter the potential is essentially short range (of order of the atom size) and the effect of close encounters is important as well. In short pulse laser target interactions the matter is quickly ionized and turned into plasma. However, until this happens elastic scattering of electrons from neutral atoms can play an important role in particular cases. In this work electron-atom scattering is taken into account in connection with high current fast electron beam propagation in a cold dielectric target where the process of turning the matter into plasma must be treated in details. Nevertheless, even in this case it is not necessary to describe electron-atom collisions very precisely and hence they are treated in an approximate manner. The angular shape of the effective cross section of electron–atom scattering assumed here depends on electron energy and takes the form

\[
\frac{\text{d} \sigma_{\text{en}}}{\text{d} \cos \theta} = \frac{\sigma_t}{4\pi \ln(1 + E)} \left[ 1 + E \sin^2(\theta/2) \right],
\]

where \( \theta \) is the polar deflection angle, \( E \) is the electron kinetic energy in eV, and \( \sigma_t \) is the corresponding integral cross section. This analytical expression was used to describe screened Coulomb collisions in [189] and it captures the main features of electron-neutral atom scattering, i.e. it is approximately isotropic at low energies and it becomes increasingly peaked in the electron propagation direction as the energy increases. In the paper [189] the formula (3.68) was given without explicit derivation. Recently, it has been pointed out in [190] that this expression is ad hoc and not exactly physically correct. The difference between the formula (3.68) and the corrected one propose in [190] cannot influence our results significantly. In future, when elastic electron-atom collisions would be taken into account, the correct formula will be employed.

The probability of electron-atom scattering is expressed in terms of frequency as well. The collisional frequency for electron-atom scattering is obtained as

\[
\nu_{\text{en}} = v n \sigma_t,
\]

where \( v \) is electron velocity and \( n \) is the density of atoms.
3.4. ELASTIC COLLISIONS

3.4.3 Implementation of elastic collisions

The size of the computational cell should be of the order of the Debye length in PIC simulations. Thus the electromagnetic field can be separated into two parts, the macroscopic part which stands in the Lorentz force equation, and the field on the scale length shorter than the Debye length which is accounted for in the collisional part. This choice of the cell size is also consistent with the small angle cutoff introduced in Coulomb logarithm.

The Coulomb logarithm is supposed to be constant in space and time and its value varies between 2 and 5 in our simulations. Particular choice of the value depends on the temperature and the maximum density of plasma considered in the simulation. Approximately, the argument in the Coulomb logarithm is $9 \times$ the number of ions in the Debye sphere and hence the lower value of 2 corresponds to only one ion per Debye sphere (this value is already on or even slightly beyond the borderline of validity of the above given models).

The collisional frequency is calculated according to equation (3.57). It is lower than plasma frequency, yet in a dense low temperature plasma it can be also very high. For example, for solid density aluminum with temperature 100 eV and mean ion charge 5 the Coulomb collision frequency is as high as $4 \times 10^{16} \text{ s}^{-1}$. However, it scales with the plasma density and the inverse third power of the velocity of colliding particles. Therefore, in the laser target interaction region collision frequency can be even three orders of magnitude lower (Ti:Sapphire laser is assumed). As all collisional algorithms in PIC simulations are very computationally expensive, collisions are taken into account only when necessary to handle important physical processes correctly and not for all species of particles (e.g. collisions of ions are always neglected).

Coulomb collisions were successfully implemented into our PIC simulation code using the Takizuka & Abe approach in the frame of diploma thesis [14]. Some other approaches were also discussed in this work. The binary collisional algorithm was later extended to the relativistic domain in the frame of diploma thesis [13].

In the frame of this work the Coulomb collision model has been revised. The collisional model proposed by Nanbu seems to be least restrictive than other approaches and the most part of this model is suitable for either Coulomb or elastic electron-atom collisions. Consequently, this model has been chosen as the most suitable one for the moment. Nevertheless, several recent works have demonstrated successful applicability of the Coulomb collision model which employs Langevin equation. Therefore, we do not utterly disqualify the Langevin model for future consideration.

Coulomb collisions take place every time step for every particle of the species for which collisions are not neglected. The polar scattering angle $\theta$ is randomly sampled from the distribution (3.65). With a uniformly distributed random number $RND$ ranging between 0 to 1,
cosine of the scattering angle is obtained as

$$\cos \theta = \frac{1}{A} \ln \left( e^{-A} + 2 \text{RND} \sinh A \right).$$

(3.70)

The azimuthal scattering angle is uniformly distributed between 0 and $2\pi$ (obtained as $\psi = 2\pi \text{RND}$). Post-collision velocities are calculated according to equation (3.62) and they are rescaled (with the propagation direction conserved) to guarantee energy conservation, which can be violated due to rounding errors.

For elastic scattering of electrons by neutral atoms, Monte Carlo algorithm similar to that used for collisional ionization is employed. The collisional frequency is calculated from the formula (3.69) where the total cross section for elastic collision is taken from the tables [191] which have been evaluated using the Dirac partial wave method with screened potentials obtained from Dirac–Hartree–Fock atomic electron densities. As there are no precise data in the energy range below 100 eV we suppose that the product $\sigma_t v$ in the collisional frequency is constant there. This assumption is not too restrictive. With decreasing electron energy the cross section $\sigma_t$ increases while the velocity $v$ obviously decreases. For example, the collisional frequency for 100 eV electron in solid density aluminum is 19 fs$^{-1}$. On the other hand it takes about 0.1 fs for 10 eV electron to pass the distance between two atoms and thus the corresponding maximum collisional frequency should be about 10 fs$^{-1}$.

The probability of elastic collisions is again expressed as $\nu_{en} \Delta t$ and randomly sampled. If the collision takes place the polar scattering angle is found from the distribution (3.68) using random number $\text{RND}$ as

$$\cos \theta = \frac{1}{E} \left[ E + 2 - 2(1 + E)^{\text{RND}} \right].$$

(3.71)

The rest of the electron-atom collisional algorithm is the same as for Coulomb collisions except that atoms are always assumed immobile (zero velocity and infinity mass). In comparison with Coulomb collisions the main differences are that elastic electron-atom collisions take place during the given time step only with certain probability and the distribution for polar scattering angles is not so much peaked at small angles like the one for Coulomb collisions.

3.5 Short review of existing PIC codes

PIC simulation codes used for calculations of short pulse laser target interaction or wakefield acceleration of electrons in which the ionization is implemented and the results with ionization have been published are reviewed in Table 3.2. As one can see, there are only few of them and most of the codes are two-dimensional. Nevertheless, almost all the results of simulations
Table 3.2: Short review of existing PIC simulation codes with variable plasma ionization implemented and utilized in the frame of high energy density physics science (laser plasma, dense charged particle beams).

with variable plasma ionization published until now have been calculated in one-dimensional geometry.

PIC simulations with variable ionization are also used in low temperature low density plasma to study discharges (for example PIC-MC method in [192, 193]). However electric fields in these simulations are much lower and the ionization process is mainly due to inelastic collisions. In PIC-MC codes several more processes are usually implemented including excitation, recombination and plasma-wall interactions and evolution of plasma is followed over longer time interval with much longer time step. These codes are not included in Table 3.2.

3.6 Monte Carlo electron transport calculations

Simulations based on the Monte Carlo (MC) approach are usually used to study detailed transport of fast particles in a cold solid matter. These simulations enable to follow ionization and local energy deposition (heating) in the material as well as characteristic and bremsstrahlung radiation produced during particle transport. In the frame of this work MC simulations are employed to study K-\(\alpha\) emission induced by hot electrons in short pulse laser irradiated targets in the next chapter. The MC code used here was developed in the frame of the author’s diploma thesis [197] in 2003. Since then only minor improvements have been done in the code.

In contrast with the PIC method the MC particle transport method completely neglects self-consistent electric and magnetic fields produced as consequence of charged particle motion. Trajectories of individual particles are therefore mutually independent. In the MC code used in this work individual elastic and some inelastic collisions of fast electrons with the background formed by stationary atoms are treated. The code is based on the single scattering approach. In between of two successive collisions electrons move on straight line trajectories with constant
speed.

The probability of electron elastic scattering is calculated from the screened Rutherford or Mott cross section and it is expressed as the mean free path. For inelastic collisions, the cross sections are based on quantum mechanical approach which utilizes generalized oscillator strength. These cross sections are doubly differential in the energy loss and the scattering angle. Bremsstrahlung radiation is neglected and therefore our code is applicable only to lower and mid Z elements. The energy losses due to bremsstrahlung generation are taken into account in the continuous slowing down approximation and a tabulated stopping power is utilized.

For ionization of K shells of target atoms semiempirical cross section proposed by Casnati [198] is used. Atom with a vacancy in the K shell relaxes immediately to a lower energetic state with the probability of emission of K-\(\alpha\) photon expressed as the fluorescence rate. Emission of K-\(\alpha\) radiation is isotropic and attenuation of K-\(\alpha\) radiation intensity during the transport inside the target is approximated using the Beer's law of exponential attenuation. Our code enables to simulate K-\(\alpha\) emission from the target with temporal as well as three-dimensional spatial resolution and also to regard target boundaries as reflecting or absorbing for fast electrons.
4 RESULTS AND DISCUSSIONS

As our PIC code includes variable plasma ionization, elastic collisions and it is able to treat multiple species of particles we concentrate particularly on problems where these processes and features are important. As illustrated in Figure 4.1 the following chapter is divided into three parts according to the location where the processes of particular interest take place:

- In the first part of this chapter we study the processes taking place on the laser side of a solid target when a short high intensity laser pulse strikes upon it. Primarily, we concentrate on the influence of variable plasma ionization on energy and angular distributions of accelerated electrons. This influence seems to be significant and might be important for applications where hot electron beam accelerated during laser target interaction is utilized.

- In the second part we study propagation of high current fast electron beam in dielectric target. The processes of electric field and collisional ionization as well as all other kinds of collisional processes are indeed important to describe the transition of initially cold nonconducting matter into dense relatively hot and conducting plasma in this context.

- In the last part we concentrate on the TNSA mechanism responsible for ion acceleration from the rear surface of laser irradiated foils. The interplay of different species of ions is very important in ion acceleration process and it may eventually result in formation of relatively narrow peak in the energy distribution of lighter ions. In the process of ion acceleration charge to mass ratio is the crucial parameter. The process of electric field ionization is therefore important to describe how individual charge states of ions are populated during acceleration in time and space.

4.1 Acceleration of electrons

Acceleration of electrons is the key issue in the short high intensity laser pulse interactions with solid targets. This is due to the fact that the significant part or even the bulk of laser energy absorbed in the target goes directly into hot electrons. For this reason, many other processes studied in connection with short pulse laser solid target interactions are in one or the another way connected with laser accelerated hot electrons, e.g. acceleration of ions, generation of X- and γ-rays, rapid isochoric heating of matter.

The results of our calculations presented in the following part are performed for a Ti:Sapphire
4.1. ACCELERATION OF ELECTRONS

Chapter 4 is divided into three parts concerned with acceleration of electrons in the laser target interaction region, transport of hot electron beam inside the target, and acceleration of ions from the target rear side.

Figure 4.1: Chapter 4 is divided into three parts concerned with acceleration of electrons in the laser target interaction region, transport of hot electron beam inside the target, and acceleration of ions from the target rear side.

Laser with wavelength $\lambda = 800$ nm and the $\sin^2$ temporal profile of the pulse. To make the total fluence of the $\sin^2$ pulse identical to the Gaussian pulse with the same peak intensity, duration of the $\sin^2$ pulse is set to $\tau_{\sin^2} = 2.13$ FWHM$_{\text{Gauss}}$ (where FWHM mean Full Width at Half Maximum).

The peak intensity of the laser pulse in our simulation ranges between $10^{16}$ and $10^{19}$ W/cm$^2$. For such high laser intensities it is reasonable to assume that there is a preplasma on the surface of the target already before the arrival of the main laser pulse. As discussed in Section 2.3 the preplasma is created either by Amplified Spontaneous Emission (ASE) or by the uncompressed pedestal of the main pulse. Its characteristic properties, density profile, temperature, and ionization depend in particular on the properties of the laser system, target material, and experimental arrangement.

According to the isothermal model of plasma expansion described in Section 2.3 the density profile is assumed to have exponential shape. However, the model of isothermal plasma expansion is sometimes oversimplified. When a more precise approximation to the density profile of plasma is needed, we resort to hydrodynamic simulations. The characteristic length of the exponential density profile is defined as follows

$$ L = \left. \left| \frac{d(\ln n_e)}{dx} \right|^{-1} \right|_{n_e}, \tag{4.1} $$

where $n_e$ is the electron density and the derivative is evaluated at critical surface where $n_e = n_c$. For the Ti:Sapphire laser critical density is approximately $1.75 \times 10^{21}$ cm$^{-3}$. At this point it should be noted that in plasma with variable ionization it is more reasonable to define the density scale length via ion density as this density is almost constant throughout the interaction.
Electron plasma density on the other hand quickly rises in consequence of rapid ionization. Its growth is not necessarily uniform especially in front of the critical surface where the laser and the strongest plasma fields are localized. The density scale length can thus vary significantly during the interaction. In literature density scale length is always defined by means of electron plasma density because the density profile of electrons is tightly connected with the absorption mechanism of laser radiation. We will comply with this convention here and use the term density scale length for the scale length of initial exponential electron density profile before the ionization set up.

The density profile of plasma on the target surface is rather steep and its scale length is usually comparable to the laser wavelength in short pulse laser target interactions. As the laser pulse absorption and electron acceleration take place only in front and in the vicinity of the critical surface, our simulations cover only a narrow region of the target behind this surface. Therefore, the maximum plasma density is mostly less than $10^{22} \text{ cm}^{-3}$, i.e. much below the solid state density. At these densities the Coulomb collision frequency for thermal electron is of the order of 0.1 per femtosecond or even less when the electron temperature of order of hundred eV is assumed. Such temperature is often achieved during the short pulse high intensity laser solid target interactions. Collisionless absorption processes which take place on the temporal scale of the laser period (2.67 fs for the Ti:Sapphire laser) are therefore predominant while the collisional effects are of secondary importance and they are neglected.

Similar argument applies to ionizing collisions as well. For example, according to the Lotz cross section (3.38) the maximum frequency of ionizing collisions in the vicinity of critical surface is 0.07 per femtosecond for an ion with the ionization potential 40 eV and 6 equivalent electrons in the outermost shell (e.g. Al$^{3+}$ ion). Lower ionization potential are not taken into account in these simulations as we suppose that preplasma is already partially ionized due to absorption of laser prepulses. In our calculations electric field ionization predominates over the collisional ionization process everywhere except where the laser pulse does not penetrate and plasma field is low. For this reason, collisional ionization can be neglected here. To check this claim we have performed some simulations with collisional ionization included and found out that the average ion charge does not change significantly in the interaction region due to ionizing collisions.

According to our results the influence of variable plasma ionization on acceleration of electrons can be organized into three categories:

- **No significant influence of variable ionization on electron acceleration evidenced.**
  In particular the case when the density profile of plasma on the target surface is very steep ($L < \lambda$) falls into this category. In this case laser penetrates only into a very thin plasma region. As a consequence of electric field ionization electron density increases
over all this region. However, the electron density profile does not change significantly (except of the almost uniform increase) and the influence of ionization on either energy or angular distribution of accelerated electrons is not important.

- **Variable plasma ionization affects mainly the energy distribution of accelerated electrons.**
  This category refers in particular to the situation when the density profile is longer \((L > \lambda)\) and when acceleration of electrons is due to resonance absorption near the critical surface. Obviously, obliquely incident \(p\)-polarized laser wave is necessary for the resonance absorption. In particular, the efficiency of transformation of laser energy into hot electrons is influenced by ionization in this case. Namely, this efficiency may drop down several times. This situation is presented and discussed in details in Section 4.1.1.

- **Variable plasma ionization affects mainly angular distribution of accelerated electrons.**
  Variable plasma ionization has a significant impact on the angular distribution of accelerated electrons when the preplasma density profile is long \((L > \lambda)\) and the peak laser pulse intensity is so relativistic that there is a strong relativistic ponderomotive force. This case is presented and discussed in section Section 4.1.2.

### 4.1.1 Energy distribution of hot electrons

The simulations presented in this section are performed in accordance with experiments carried out in the Max-Born Institute in Berlin by the group of Dr. Zhavoronkov [199]. First of all let us summarize the experimental setup and the main results obtained by Dr. Zhavoronkov.

The Ti:Sapphire laser system employed in the experiment produces relatively low energy pulses, less than 5 mJ per pulse, but with a very high repetition rate of 1 kHz. Laser pulses produced by the system are \(p\)-polarized and 45 fs long (FWHM). These pulses are focused at an angle of 20° onto the surface of thin metal foils. This angle of incidence is chosen so that K-\(\alpha\) radiation is emitted from the laser irradiated target with the highest efficiency in the experiment. Most results were obtained with copper foils thus this is the material assumed in our simulations.

In the experiment the focal spot size on target was about 6.7 \(\mu\)m (FWHM) and the peak laser intensity on target reached almost \(10^{17}\) W/cm\(^2\). In addition to the main laser pulse the system produced also an intrinsic laser prepulse located approximately 5.5 ps ahead the main pulse. The intensity contrast ratio of the prepulse was about \(10^{-5}\) in comparison with the main laser pulse. The ASE preceding the main laser pulse lasted typically several nanoseconds and its intensity contrast ratio was measured to be about \(10^{-7}\).
The main objective of these experiments was to characterize laser-irradiated metal foils as sources of characteristic K-α radiation, which can be subsequently applied in other measurements. K-α radiation coming from the rear side of foil targets is more suitable for subsequent application because of experimental layout and better contrast in comparison with thermal radiation coming from plasma on the laser side. The thickness of target foils was varied between 10 and 40 \( \mu m \) not to attenuate the intensity of K-α radiation along its passage through the target too much.

K-α emission was measured from either side of the target, from the laser side at angle 45° with respect to the laser incidence direction, from the rear side in the laser transmission geometry. About \( 5 \times 10^6 \) K-α photons per steradian and per shot were detected in both forward and backward directions and the emission spot size on the rear side was measured to be approximately round with the radius of about 10 \( \mu m \). In the experiments spectra of bremsstrahlung radiation were also measured and from these measurements temperature of hot electrons was estimated to be at least 19 keV. By the word temperature we mean the parameter in the exponential energy distribution of hot electrons which characterizes its scale. More details about the experiments and their results can be found in [199].

We have employed the adapted PIC code as well as 1.5-dimensional atomic/hydrodynamic code Ehybrid [31] and the MC code [197] described in the Section 3.6 to simulate this experiment. The code Ehybrid has been utilized to calculate absorption of laser prepulses and to describe the preplasma formed on the target surface before the impact of the main laser pulse. The results calculated by the code Ehybrid, namely the density profile of preplasma, have been taken as a starting point in some PIC simulations. The PIC code has been applied to calculate absorption of the main laser pulse and acceleration of hot electrons. In these simulations hot electrons escape from the rear side of the simulation box and they are substituted by thermal ones. These hot electrons are recorded and subsequently postprocessed by the MC electron transport code. Similar simulation procedure is often applied to calculate K-α emission from short pulse laser-irradiated targets, see e.g. [65,200].

We have used just exponential plasma density profile on the target surface in PIC simulations at the beginning. Moreover, we supposed that the density scale length of this profile should range between 0.1\( \lambda \) and \( \lambda \) (\( \lambda \) being the laser wavelength). According to the model of isothermal expansion the scale length of \( \lambda \) corresponds for example to electron temperature of 5 eV, average ion charge 2 and the expansion time of 200 ps. This seems to be quite reasonable for the ASE fluency in the experiment.

However, we were not able to reproduce the experimentally measured K-α emission even roughly using the exponential density profile with scale length in the above given range. The number of K-α photons emitted from either side of the target per steradian was always almost order of magnitude higher in our model. The MC code used to calculate K-α emission was
4.1. ACCELERATION OF ELECTRONS

previously calibrated against other experimental measurements [201] (see [197]) and we expect that its maximum error is always less than a few tens of percents for copper. Likewise, we do not expect that the overestimate of K-α emission could come from the neglectation of self-consistently induced electric and magnetic fields that are not incorporated in MC simulations. Copper is a well conducting material and the flux of hot electrons is not huge enough to produce fields that could significantly influence hot electron transport on a distance of a few tens of microns. The overestimate must therefore come from the laser absorption and hot electron acceleration process in PIC simulation. We have to note at this place that our PIC code calculates hot electron energy distributions in a good agreement with other PIC codes and theoretical estimates of laser absorption [13] in the range of parameters given above. The results are neither influenced by ionization in the range of density scale lengths given above as will be show later. For these reasons the overestimate should come from initial conditions and most probably from the density profile, as this profile has the most profound influence on the electron acceleration process.

Plasma density profile on the target surface - hydrodynamic simulations

Laser prepulses and particularly ASE may very significantly influence the number of K-α photons emitted from solid targets irradiated by short laser pulses according to experiments [27]. This observation has been tentatively explained by the absorption of the relatively long lasting ASE prepulse which heats, melts, and evaporates some material from the target surface even before the target surface is turned into plasma. Once the cloud of vapor in front of the target is ionized by intrinsic prepulse or the rising edge of the high-intensity pulse it may significantly influence the main laser pulse interaction with target.

We have employed the hydrodynamic code Ehybrid to gain a better insight into this evaporation and plasma formation process and to find more proper shape of the preplasma density profile as well as its temperature and ionization. The code Ehybrid was originally designed for simulations of coherent X-ray radiation emission (X-ray lasing) from laser irradiated targets. Since copper was not interesting for such application there are no input data for this element available. Instead of copper we have therefore used silver and germanium, silver being an element in the same group in the periodic table and having similar electrical and thermal conductivity while germanium being close to copper and thus having similar atomic number and weight. As the results of Ehybrid calculations for both elements are quite similar it is reasonable to expect that the behavior of copper would not be significantly different. In the Ehybrid simulation we assume 1 ns long laser pulse with constant intensity of $10^{10} \text{ W/cm}^2$. The preplasma density profile as calculated by the Ehybrid code is plotted in Figure 4.2.

In panel a) of Figure 4.2 temporal evolution of the electron density profile is plotted. The target surface is located at 0 μm at the beginning. Electron density is in the logarithmic scale
4.1. ACCELERATION OF ELECTRONS

Figure 4.2: Plasma density profile calculated by the Ehybrid code for irradiation of germanium target with 1 ns long Ti:Sapphire laser pulse with intensity \(10^{10}\) W/cm². Temporal evolution is plotted in panel a) and the resulting profile at the end of simulation in panel b). In panel a) the dashed line denotes the critical surface while the solid line denotes position where ion density is equal to \(1.7 \times 10^{20}\) cm\(^{-3}\). Approximation of the density profile calculated by the Ehybrid code which is further used in PIC simulations is included in panel b).

in the units of cm\(^{-3}\). Behind the critical surface which is denoted by dashed black line heating and ionization are insignificant and free electron density quickly drops to zero (dark blue color). The solid black line denotes position where ion density is \(1.7 \times 10^{20}\) cm\(^{-3}\) (i.e. about \(10 \times\) less than critical density). During the main laser pulse interaction with the target the region behind this line may already become overcritical. As will be shown later ionization due to the electric field of the main laser pulse is so strong that the average ion charge reaches 11 in the interaction region near the laser pulse maximum. From the results of Ehybrid simulations it is possible to conclude that even the low intensity laser prepulse may cause significant evaporation of the material from the target surface even if the vapor is still transparent to laser radiation as it is only lowly ionized.

Both electron and ion density profiles, as resulting at the end of Ehybrid simulation, are plotted in panel b) of Figure 4.2. The preplasma density profile as calculated in the hydrodynamic simulation is practically exponential in the vicinity of critical surface \(1.75 \times 10^{21}\) cm\(^{-3}\) and hence in agreement with the isothermal model of plasma expansion. Density scale length near the critical surface is about \(0.6\lambda\), which is in the range \(0.1\lambda - \lambda\) as expected.

However, in the undercritical part of the profile the density decrease is not so steep and it is more likely linear than exponential. Similar plasma density profiles were also evidenced in
some experiments yet the conditions of these experiments \cite{202,203} are not fully comparable with the situation studied here. Likewise in the experiment \cite{204} a strong correlation between proton acceleration from the rear side of titanium foil with ASE duration was reported. Proton measurements were found to correlate with the pedestal of the XUV signal at 13.5 nm coming from the target indicating preplasma formation due to ASE prepulse of similar intensity as the one in experiments of Dr. Zhavoronkov. However, no direct comparison of the density profile calculated by the Ehybrid code with experimental measurements is possible as up to know and to our knowledge no density profile measurements covering the region around the critical surface have been reported for short pulse laser solid target interactions.

The ion density profile around the critical surface can be with a nice accuracy approximated by a sum of linear and exponential functions. This approximation is also included in panel b) of Figure 4.2. In the hydrodynamic simulation the average ion charge is approximately 3. It rapidly drops down to zero behind the critical surface while in the undercritical region it slightly increases with the distance from the target surface. We further assume a constant ion charge 3 overall the preplasma profile. This assumption is reasonable as the ion charge adjusts self-consistently when the main laser pulse strikes the target and starts to ionize, no matter how low the initial ion charge is. Electron density profile corresponding to the ion density profile and constant charge of 3 is plotted in Figure 4.2 panel b) for comparison.

The above described approximation of the preplasma density profile was used as the initial profile of plasma in PIC simulations. For the sake of simplicity we will refer to this approximation as ”Ehybrid” further in the text. The ion charge 3 is relatively low and it is reasonable to expect that it will further increase during the main laser pulse interaction. PIC simulations are accordingly performed with variable ionization while comparison with the results calculated with constant ionization is also provided.

**Electron acceleration - PIC simulations**

The main laser pulse interaction with the plasma, absorption of laser energy, and acceleration of electrons has been calculated using the PIC code. The parameters used in our simulation are practically identical to those of the experiment. P-polarized 45 fs long laser pulse with peak intensity $10^{17}$ W/cm$^2$ and wavelength 800 nm strike the copper target under the angle of 25°. Preplasma on the surface of the target has either exponential density profile with scale length 0.7$\lambda$ or 0.07$\lambda$, or the approximation to the profile calculated by the code Ehybrid is used. PIC simulations with the exponential density profiles are calculated with either constant ion charge ranging between 3 and 10 or with variable plasma ionization with initial ion charge 3 assumed. However, in this case no significant influence of the ion charge or the ionization process on hot electron energy distribution is observed.
Density plateau is assumed in our simulations at the back of the exponential part of the profile. This plateau is introduced to guarantee enough free electrons in the simulation box to form the return current neutralizing the hot electron flux. At the end of the plateau hot electrons are absorbed and substituted by thermal electrons. The plateau is also plotted in the approximation of the ion density in Figure 4.2 panel b). Ion density in this plateau is set to critical density, i.e. about 50 times lower than solid density of copper, however the plasma is obviously overdense for laser radiation because ions are multiply ionized. It is necessary that the distribution function of electrons is sufficiently represented in the vicinity of critical surface to calculate electron acceleration properly, i.e. multiple electrons per one simulation cell are required in this region. If the distribution is not represented precisely enough a single electron produces a significant step in the electron density profile which may cause increasing perturbations and instability, especially when the electric field ionization is in play. This is the reason for the density profile cutoff at the density much lower than solid density. With increasing density the number of particles per simulation cell increases and treating the density profile up to solid density imposes too huge requirements on computer performance and simulation time.

Figure 4.3: Energy distribution of hot electrons accelerated in PIC simulations with and without variable plasma ionization and with several different density profiles. Copper target is irradiated by 45 fs p-polarized obliquely incident (25°) laser pulse with wavelength 800 nm and intensity $10^{17}$ W/cm². In PIC simulations either exponential plasma density profile or the profile plotted in Figure 4.2 is used in panel a). Hot electron energy distribution deduced from bremsstrahlung measurement is included. In panel b) the results are calculated with ionization and with the same parameters like in panel a) but the Ehybrid density profile is slightly modified (see below).
Distributions of hot electrons as calculated in the PIC simulations are plotted in Figure 4.3. In panel a) we compare the distributions calculated with the exponential density profile with respective scale length with distributions calculated with Ehybrid profile with both variable and constant ionization. Intensity of the laser pulse is not relativistic and the main absorption and electron acceleration mechanisms is expected to be due to resonance excitation of electron plasma wave at the critical surface. For the short plasma density profile \((L = 0.07\lambda)\) laser absorption is most likely due to vacuum heating while for longer profiles resonance absorption is more efficient and the maximum energy of accelerated electrons is higher. This can be seen comparing the distributions calculated with exponential density profiles. According to the formula (2.10) the density scale length of \(0.7\lambda\) is optimum for the \(25^\circ\) angle of incidence for the resonance absorption to take place.

Energy distribution of hot electrons calculated with the Ehybrid profile and with constant ionization is very similar to the one calculated with exponential density profile with \(L = 0.7\lambda\). This results from the fact that both profiles are similar around the critical surface. It is also possible to conclude that the underdense part of the Ehybrid profile does not have significant influence on the hot electron energy distribution except for some increase in its high energy tail which may be due to parametric decay instabilities. However, a very strong reduction of number of accelerated electrons overall the energy distribution is found when variable ionization is taken into account in simulations with the Ehybrid profile. Nevertheless, the hot electron temperature seems not to change indicating the same acceleration process with reduced efficiency.

For comparison we include the exponential distribution resulting as the best fit to the distribution of bremsstrahlung radiation measured in the experiment. When comparing either of the distributions calculated by our PIC code with the fit to the bremsstrahlung spectra reasonable agreement is found only with the distribution calculated with Ehybrid profile and variable ionization. This indicates that we are on a good way. In the experiment measurements of bremsstrahlung radiation are limited by the effective range of the detector to photon energy below 150 keV and therefore the bremsstrahlung spectra cannot involve the high energy tail observed in our calculations.

Comparing the results calculated with and without ionization it is obvious that ionization has profound effect on electron acceleration in the case of Ehybrid profile. At this place let us demonstrate that the effect of ionization does not apply only to the specific Ehybrid profile used in our calculations but more likely to a class of density profiles with similar shape.

We present comparison of hot electron energy distributions calculated with ionization for the Ehybrid profile and three other similar profiles in Figure 4.3 panel b). The distribution calculated with Ehybrid profile is plotted in blue. The distribution calculated with the same ion density but with two times higher initial ion charge (i.e. \(Z=6\)) is plotted in green. In red we depict the results calculated with Ehybrid profile where the ion density in the linear
4.1. ACCELERATION OF ELECTRONS

(a) Electron density and electric field

(b) Mean ion charge

**Figure 4.4:** In panel a) electron density profile and longitudinal electric field induced in plasma, in panel b) mean ion charge in the PIC simulation with Ehybrid profile and variable plasma ionization. Simulation parameters are the same as in Figure 4.3. Electron density is normalized to critical density and time is measured in laser periods \( \tau \approx 2.7 \text{fs} \). Laser pulse arrives from the left.

The processes of ionization and electron acceleration in the simulation with Ehybrid profile are demonstrated in Figure 4.4. The electron density profiles and the longitudinal electric fields in the simulation are presented in panel a) in several time instants. The longitudinal electric field is the field induced in plasma and directed along the incident laser pulse. In particular this field is responsible for acceleration of electrons.

Before the main laser pulse strikes the target \((t = 6\tau, \tau\text{-laser period})\) electron density in the linear part of the profile is undercritical and laser wave may penetrate almost up to the critical surface. Notice that obliquely incident laser wave is reflected already in front of the critical surface at the point where electron density equals \(n_c \cos^2 \theta\) (in our case 0.82\(n_c\)), see
Section 2.4.1. The critical surface is located at 7 µm initially. Further in time \((t = 18\tau)\) but still before the laser pulse maximum strikes the target we observe that electron density in most of the linear part of the density profile is already higher than critical density. After the laser pulse maximum electric field ionization process stops and the ion charge and electron density remain almost constant until the end of the interaction. This can be seen comparing the electron density profiles at 18\(\tau\) and 30\(\tau\).

In these two time instants we include also the longitudinal electric fields in panel a) of Figure 4.4. In the time 18\(\tau\) a small amplitude resonant field is observed near the former critical surface at 7 µm. In the linear part of the density profile the electric field is due the longitudinal component of the electric field of the laser wave, due to the electron plasma wave propagating from the critical surface, and also due to the space charge separation induced by the ponderomotive force. However, overall the interaction region amplitude of the longitudinal electric field is relatively low and the field does not give rise to significant acceleration of bulk number of electrons as will be demonstrated later. After the laser pulse maximum at 30\(\tau\) the resonant field has much higher amplitude. In this time it is located at about 4 µm that is much farther from the target surface.

Explanation of the effect observed in our simulations rely on electric field ionization in the linear part of the density. Rapid ionization in the first half of the laser pulse causes that both the laser reflection point and the critical surface shift toward vacuum. The resonant field is attenuated during the ionization phase and only a minority of electrons are accelerated. After the laser pulse maximum the processes of ionization and shifting of critical surface turn off and a stable resonant field rises at the new critical surface. Similar situation is observed for exponential density profiles as well. However, in this case ion density in the undercritical part of the density profile drops down more quickly and the effect of ionization is of minor importance unless the density profile is long enough \((L \gg \lambda)\).

Temporal evolution of average ion charge in the Ehybrid density profile is demonstrated in panel b) of Figure 4.4. Average ion charge and free electron density increase very rapidly in the interaction region in the first half of the main laser pulse. Near the laser pulse maximum average ion charge reaches 11 while it was only 3 at the beginning. In consequence, free electron density is almost 4 times higher. At \(Z = 11\) the ionization process practically stops. This is not surprising as in this state copper ions have closed outermost shell, namely the 3p shell. The ionization potential grows significantly from 266 eV at \(Z = 10\) to 367 eV at \(Z = 11\) and therefore the probability of further ionization becomes very small. A pronounced peak in the average ion charge is found at the initial position of the critical surface. This is due to the fact that not only the optical laser field but also the plasma field can ionize and the field induced in plasma usually peaks around the critical surface.

In Figure 4.5 the difference in the electron acceleration process when ionization is constant
4.1. ACCELERATION OF ELECTRONS

(panels a) and variable (panel b) is illustrated on the electron phase space plots. In both cases Ehybrid profile is used in PIC simulations. The electron phase space in panel a) is plotted at \( t = 24 \tau \) which is about the time when the laser pulse maximum is at the critical surface at \( 7 \mu m \). In the vicinity of critical surface motion of electrons in the resonantly driven plasma wave can be seen. The wavebreaking process resulting in acceleration of electrons toward vacuum is also clearly distinguishable (electrons with the highest negative velocity).

In panel b) the field is plotted at \( t = 18 \tau \), i.e. more early. A regular oscillatory motion of electrons like in panel a) is observed only in a short front part of the density profile. The closer the distance to the target surface the more chaotic behavior of free electrons is observed. This chaotic behavior is introduced by electric field ionization. It comes from the fact that electrons released by electric field ionization are not necessarily in phase with other free electrons which will be demonstrated later in Section 4.1.2. Thereby the higher number of newborn electrons the higher is the degree of stochasticity in the electron oscillatory motion and finally the oscillatory motion is effectively smoothed out close to the former critical surface. In fact some wavebreaking is observed in this case as well (follow the electrons with the highest negative velocity in the figure) but the number of accelerated electrons as well as their velocities are lower. One more fact is readily observed from the phase space plots. The longitudinal electron temperature is evidently much higher in the case when ionization is taken into account.

When electron released by electric field ionization is not in phase with the electron plasma wave it always gains some energy from this wave. Notice that newly released electrons have

![Figure 4.5: The electron phase space in PIC simulation with Ehybrid profile with constant and variable ionization. In panel a) the phase space is plotted at \( t = 24\tau \), in panel b) at \( t = 18\tau \). Simulation parameters are the same as in Figure 4.3, velocity is normalized to the speed of light, spatial coordinate to the laser wavelength.](image)
zero or almost zero energy initially so that their energy can only increase. The electron plasma wave is thus partially depleted through interactions with these newborn electrons. In some way this process is a bit similar to collisional absorption. In collisional absorption of electrostatic or electromagnetic wave electron is put out of phase with the oscillating field by elastic collision. In this case the newly released electron could be out of phase already initially. Hence it is in some way equivalent to a free electron after elastic collision.

Accordingly, the transverse temperature which is due to electrons out of phase with the laser wave is higher in panel b) of Figure 4.5 than in panel a). The above mentioned effect of an increase in electron plasma temperature as a consequence of field ionization is known at nearly similar conditions in the context of short wavelength recombination lasers [205]. There the additional thermal energy of electrons is called residual energy.

We are recording not only the velocity components of hot electrons in our calculations but also the time when they cross the rear boundary of the simulation box. Then we are able to plot the velocities of hot electrons against the time. However, there is no direct correspondence between this time and the time of electron acceleration. One can only see whether electron acceleration is a continuous process. The longitudinal velocity of hot electrons against the time when they cross the rear boundary of the simulation box is plotted in Figure 4.6 panel a).

Again the results come from PIC simulations with the Ehybrid profile with either ionization on or off. Hot electrons arrive to the rear boundary in two groups when ionization is taken into account. The first group of them comes at about $t = 40\tau$ but they are less in number and their velocity is not very high. This group is accelerated by the resonant field at the former critical surface in the first half of the laser pulse. The other group which contains the most energetic electrons comes about $20\tau$ later. These electrons are accelerated by the resonant absorption at the new critical surface at $4 \mu$m (see Figure 4.4 panel a). This indicates the correctness of our interpretation that the resonance absorption is temporally suppressed due to ionization, because such effect is not observed in simulation with constant ionization.

To conclude the part about the influence of ionization on electron acceleration we present in Figure 4.6 in panel b) energy distributions of hot electrons calculated by PIC code with Ehybrid profile and variable ionization for different peak laser intensities. The temperature of hot electrons does not scale faster than with the square root of laser intensity in the theory as well as simulations of resonance absorption [206]. Therefore, the difference in hot electron temperature should not be higher than 1.3 between the peak laser intensities $6 \times 10^{16} \text{ W/cm}^2$ and $10^{17} \text{ W/cm}^2$. However, we observe that the temperature of hot electrons differs more than 2 times in our simulations. We conclude that electron acceleration process strongly depends on the peak laser intensity like the electric field ionization process does when variable plasma ionization is taken into account and the plasma density profile is similar to the Ehybrid one.
4.1. ACCELERATION OF ELECTRONS

(a) Velocity of hot electrons versus the time when they cross the rear boundary of simulation box

Figure 4.6: In panel a) velocity of accelerated electrons is plotted against the time when they cross the rear boundary of the simulation box. The results come from PIC simulations with Ehybrid profile and both constant and variable ionization. Time is normalized to laser period and velocity to the speed of light. Energy distributions of hot electrons calculated by PIC code with variable ionization and Ehybrid profile are plotted in panel b) for several laser intensities. The best fit to experimentally measured bremsstrahlung radiation is included again. Other simulation parameters are the same as in Figure 4.3.

K-α emission - MC simulations

The distributions of hot electrons calculated by PIC code have been postprocessed by our MC code. As the result the temporally dependent fluency of K-α radiation emitted from the target has been obtained. This emission was also measured in the experiment [199] and thus the results of our calculations could have been directly compared with the experimental ones.

As we have shown in Figure 4.6 panel b) the distribution of hot electrons strongly depends on the peak laser intensity. It is therefore indeed important to estimate the average laser intensity on target in the experiment. The laser pulse is 45 fs long (FWHM of a Gaussian temporal profile) and its spatial profile can be approximated by a Gaussian function with FWHM of 6.7 µm in the focal spot. The peak laser intensity in the central part of the spot is $10^{17}$ W/cm$^2$ and it drops down with the distance relatively quickly. At about the distance of 4 µm from the center the intensity is reduced to $3.5 \times 10^{16}$ W/cm$^2$ and the spot with radius of 4 µm contains about 63% of the laser pulse energy. It is also possible to conclude from Figure 4.6 panel b) that the number of hot electrons with energy above the K-shell binding energy of copper is negligible below the intensity of $3.5 \times 10^{16}$ W/cm$^2$ and so is their...
contribution to K-α emission. Assuming the radius of the effective interaction area of 4 µm, the average intensity in this focal spot is approximately $6 \times 10^{16}$ W/cm$^2$. We have used the hot electron distribution resulting in the PIC simulation with this intensity for K-α emission calculation.

Our MC results of K-α emission are in relatively good agreement with experiments. Comparison between calculated and measured K-α emission is provided in Figure 4.7 for various copper foil thicknesses. The K-α emission calculated in our simulations is still about 2 times higher than the experimental one, nevertheless it is much better agreement than the emission calculated for exponential density profiles or without ionization. In these cases K-α emission is about $8 \times$ higher. The very steep ($L = 0.07\lambda$) exponential density profile is an exception. However, this case can be excluded due to the fact that for such short density profile resonance absorption and consequently also K-α emission are maximum for the angle of incidence $> 60^\circ$. We remind that maximum K-α emission is observed for the $20^\circ$ angle of incidence in the experiment. Qualitatively our results of K-α emission are very similar to the experimental ones for different foil thicknesses. This indicates that the energy distribution used in our calculations has the correct shape (temperature). From Figure 4.7 it is possible to conclude that most of K-α photons originate from the region near the surface of the target. With increasing foil thickness the signal at the rear side is significantly attenuated while the signal coming from the front side remains almost unchanged.

The quantitative disagreement of our simulations and experiments indicates that we are still slightly overestimating electron acceleration in PIC simulations or that the peak laser intensity or the effective interaction area are smaller. Decreasing the effective area to only 3 µm in radius the agreement is already within a few tens of percents. Some uncertainty is due to the Ehybrid profile as well. The hydrodynamic code Ehybrid was not designed specially for simulations with such low intensity as the one used here and the particular shape, duration, and intensity of the ASE in the experiment are not precisely known. On the other hand our results do not
4.1. ACCELERATION OF ELECTRONS

Figure 4.8: Temporal and spatial profiles of K-α pulses emitted from copper foils as calculated by our MC code. Both profiles are calculated for hot electrons calculated in PIC simulations, see Figure 4.3 panel a) for energy distributions. K-α pulse with similar temporal profile is emitted from either side of the foil - rear side emission is plotted here. K-α emission spot is shifted in the laser propagation direction.

depend strongly on the specific density profile when it is similar to the Ehybrid one. There is one more evidence which supports our calculations and interpretations of the experiment. The angle 20° was used in the experiment for the reason that K-α emission measured for this angle of incidence was the strongest. The maximum laser absorption is obtained for approximately the same angle of incidence in our PIC simulations with the Ehybrid profile and variable ionization.

Electron acceleration takes place on a very short temporal scale which is comparable with the laser pulse duration in short pulse laser target interactions. The pulses of K-α photons are therefore very short because hot electrons thermalize due to inelastic collisions during their transport in the solid target relatively quickly. This is one of the reasons why K-α emission from short pulse laser irradiated targets is very interesting. In other experiments [64] K-α pulses shorter than 350 fs were reported whereas simulations predict that K-α pulses can be even shorter, of order of a few hundreds of fs [63].

We present the temporal profiles of K-α emission from the rear side of the copper foil target calculated for exponential ($L = 0.7\lambda$) and Ehybrid (with variable ionization) hot electron energy distributions in Figure 4.8 panel a). For the exponential density profile the K-α pulse is about 150 fs long (FWHM) while in the case of the Ehybrid profile the pulse is about 250 fs long (FWHM). Explanation is obvious from the Figure 4.6 panel a) - the two temporally separated groups of hot electrons.
Our MC code supplies spatially resolved K-α emission data and thus we have calculated the K-α emission spot for comparison with the experiment. In this calculation we assume a point source of hot electrons and make a convolution of the resulting K-α emission with the Gaussian profile of laser intensity on target. The resulting spatial K-α emission profile is plotted in Figure 4.8 panel b). The diameter of the emission spot is approximately 10 µm, almost independent of the foil thickness or the target side (front/rear). This result is consistent with the experiment. We would like to point out that in simulations K-α emission spot on the target front side (rear side as well in the case of a thin foil) is determined in particular by the laser intensity profile, see e.g. [67]. The central peak of the emission spot is slightly shifted from zero in our simulations. Hot electrons do not propagate exactly perpendicularly to the target surface if they are accelerated by an obliquely incident laser field. Their propagation direction is shifted toward that of the incident laser pulse.

To summarize this section we have studied acceleration and propagation of hot electrons as well as emission of K-α radiation induced during the interaction of short laser pulse with copper foil target. Our simulations have been performed for conditions of experiments [199] carried out in Max Born Institute in Berlin by the group of Dr. Zhavoronkov. Simulations using a 1.5 dimensional hydrodynamic code Ehybrid predict that due to absorption of ASE preceding the main laser pulse the preplasma density profile has a long undercritical part where ion density decreases almost linearly. In PIC simulations where this density profile is employed we have observed that the electric field ionization process in the undercritical part of the profile has a profound effect on electron acceleration, namely it inhibits resonance absorption significantly. K-α emission calculated with the hot electron distribution resulting from PIC simulations with Ehybrid density profile and variable plasma ionization are in the best agreement with the experiment. More precisely, this is the only reasonable situation where a relatively good agreement with experimental measurements is obtained from all the situations we have considered. This brings us to belief that our interpretations are correct. Our simulations predict that transformation of laser energy into K-α emission would be more efficient if ASE can be suppressed. However, this is relatively complicated and impossible to realize at this moment.

### 4.1.2 Angular distribution of hot electrons

The influence of ionization on electron acceleration studied in detail in the preceding subsection relied on particular experiment. On the other hand our simulations in the following section are not based upon conditions of any particular experiment. Nevertheless, we pay attention to choose such interaction parameters which are often encountered in experiments nowadays. This section is devoted to the influence of variable plasma ionization on angular distribution of hot electrons in short pulse laser solid target interactions. In fact this study is inspired by
what we have observed in PIC simulations with the Ehybrid profile.

Here we assume a short ($\approx 50$ fs) laser pulse produced by Ti:Sapphire laser. The intensity on target is assumed to be relativistic ($\approx 10^{19}$ W/cm$^2$) and therefore electron acceleration is not only due to resonance absorption or vacuum heating but also due to relativistic ponderomotive force and probably also by other processes, e.g. Raman scattering, stochastic acceleration. Ionization in the laser target interaction region can on one hand suppress some mechanisms producing hot electrons, e.g. resonance absorption, while on the other hand it may enhance some other ones, e.g. stochastic acceleration. The influence of ionization on hot electron energy distribution is therefore weaker. To be more specific we did not find any situation where the influence of ionization on hot electron energy distribution is very significant.

Nevertheless, we demonstrate that ionization may have a significant effect on the hot electron angular distribution. In our simulations this effect applies only to a smaller number of hot electrons however the question whether it can influence the bulk in some particular situation is still open. The effect of ionization on hot electron angular distribution is interesting for different reason. A part of hot electrons released by electric field ionization around the laser pulse maximum propagate in directions which are forbidden if ionization is not taken into account in the simulation.

**Ejection angle of hot electrons**

First of all let us briefly summarize some important theoretical results which will be important in the reminder of this subsection. If the radiative reaction effects are neglected the motion of a free electron in a plane electromagnetic wave in vacuum can be solved analytically. The solution is given for example in [58]. Of particular interest is that some quantities are invariant along electron trajectory.

As a consequence of symmetry of the laser field the transverse component (with respect to laser wavevector) of the canonical momentum of free a electron oscillating in the laser wave is conserved. This canonical momentum is expressed as

$$p_t(t) + \frac{q}{c} A(\eta(x,t)) = \text{const.} = p_t(0),$$  \hspace{1cm} (4.2)

where $p_t(0)$ is the initial transverse momentum before the laser is turned on, $A$ is the vector potential, and $\eta(x,t)$ is the instantaneous phase of the field at the electrons position $x$. The vector field potential defines the electric and magnetic components of the laser field as $E = -\partial_t A/c$ and $B = \nabla \times A$. The second constant of electron motion is

$$\gamma - p_l = \text{const.},$$  \hspace{1cm} (4.3)
where $\gamma$ is the electron relativistic factor, and $p_l$ is the normalized momentum along the laser pulse propagation direction (further denoted as longitudinal). This invariant is a consequence of the $\omega t - kx$ dependence of the phase of the harmonic laser wave.

Using the invariant (4.3) and the definition of $\gamma$ one can find the relation between the longitudinal and the transverse momentum components of electron being ejected from the laser pulse. The ejection angle for electron which was initially at rest is

$$\tan \theta = \sqrt{\frac{2}{\gamma - 1}}.$$ 

(4.4)

This relation has also a quantum mechanical interpretation based on the nonlinear Compton scattering. Free electron in vacuum cannot gain energy simply by absorbing a photon but only by scattering and due to momentum conservation electron gains some additional transverse momentum as well. Very high energy electrons are ejected almost along the laser pulse as the net multiphoton momentum transfer tends to zero while low energy electrons are ejected almost perpendicularly to the laser propagation direction. Expressions similar to (4.4) are often applied to study laser acceleration of electron in vacuum and they essentially tell in which direction one can expect electrons with given energy, e.g. $[207, 208]$.

In the laser target interaction the momentum components (longitudinal and transverse) are usually defined with respect to the target surface. Further there is not only the forward propagating but also the specularly reflected wave and than the vector field potential accounts for both. If the plasma field is neglected the situation is similar to two intersecting laser beams in vacuum. The ejection angle of electron can be written as $[209]$

$$\tan \theta = \pm \left[ \frac{\gamma^2 - 1}{(\gamma \sin \alpha + C)^2 - 1} \right]^{-1/2}, \quad (4.5)$$

where $\alpha$ is the laser incidence angle with respect to the target normal. The constant $C$ is a constant of electron motion. For $\alpha > 0$ it is given by (4.3) while for normal incidence it is the constant (4.2). Defining the momentum parallel to the target surface $p_{||}$, $C$ is written in the compact form as $C = p_{||}(t) - \gamma(t) \sin \alpha = p_{||}(0) - \gamma(0) \sin \alpha$, where $\gamma$ is the electron rel-

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{laser_target_interaction.png}
\caption{Laser target interaction geometry, $\alpha$ is the angle of laser pulse incidence and $\theta$ is the ejection angle of accelerated electron both with respect to the target normal. The components of electron momentum are defined with respect to the target surface as parallel $\parallel$ and perpendicular $\perp$.}
\end{figure}
4.1. ACCELERATION OF ELECTRONS

ativistic factor. Expression (4.4) is recovered setting \( \alpha = \pi/2 \), \( \gamma(0) = 1 \), and transforming \( \theta \rightarrow \pi/2 - \theta \). The interaction geometry is demonstrated in Figure 4.9 for illustration. In order to avoid misunderstanding the momentum components of electron defined with respect to the target surface are called perpendicular and parallel and denoted by \( p_\perp \), \( p_\parallel \) respectively. We recall that the momentum defined with respect to laser propagation direction are called longitudinal and transverse. The scattering angle \( \theta \) in equation (4.5) is also defined with respect to the target and if the case of single laser pulse in vacuum should be recovered (\( \alpha = \pi/2 \)) the scattering angle \( \theta \) must be transformed correspondingly.

According to (4.5) the high energy electrons propagate again mainly along the incident or reflected laser pulse (\( \tan \theta \rightarrow \tan \alpha \) for \( \gamma \rightarrow \infty \)) while the low energy electrons propagate mainly perpendicularly to the target surface (\( \tan \theta \rightarrow 0 \) for \( \gamma \rightarrow 1 \)) irrespective of laser incidence angle. Note that all angles greater than \( \alpha \) are forbidden.

Expression (4.5) has been derived for plane laser wave neglecting the effect of plasma fields. However, even if the plasma field is present the expression for electron ejection angle (4.5) is still reasonable approximation. The ejection angles of hot electrons against their energy are plotted in Figure 4.10 and the expression (4.5) is included for comparison. Hot electron distributions are taken from simulations presented in the previous section, see Figure 4.3 panel a). At very high energies the agreement between theory and our PIC simulation results is excellent. The effect of plasma field is more significant at lower energies as one can see in [210]. Moreover, there is also some thermal random component which may contribute to the spread of the angular distribution of hot electrons.

Normal incidence

For the sake of simplicity let us first discuss the case of normal laser incidence and assume that the laser wave is linearly polarized. Note that \( p_t = p_\parallel \) in (4.2) and \( p_t = p_\perp \) in (4.3) in this case. Moreover only one component of the vectors in (4.2) is important. In the case of normal
4.1. ACCELERATION OF ELECTRONS

incidence the formula for electron ejection angle \((4.5)\) reduces to

\[
\tan \theta = \pm \left[ \frac{\gamma^2 - 1}{p_\parallel^2(0) - 1} \right]^{-1/2}.
\]  \tag{4.6}

If the component of electron momentum parallel with the target surface is initially zero then electron leaves the interaction region only in the direction normal to the target surface no matter what energy it gains. Actually, this is what we observe in our PIC simulations when electric field ionization is omitted.

Now suppose that a new electron is injected into the simulation box upon being released from its parent ion by the strong electric field. As already mentioned newly released electrons have very small energy initially so we can assume that their momentum is \(p(t) = 0\) in the instant \(t\) when they are born. Further, let us assume that the newly released electron is not in phase with other free electrons in the same simulation cell, meaning that its parallel momentum is significantly different from the average parallel momentum of other free electrons. Let us postpone the question of how can it happen for later discussion.

Hereafter, we suppose that the momentum difference between the newborn electron and the other free electrons is equivalent to the situation in which the newborn electron is free already before the laser pulse arrives to the target, but it has some nonzero initial momentum, whereas the other free electrons are at rest. Recalling equation \((4.2)\) we can approximately find this nonzero initial momentum. While for the free electrons which have been at rest before the interaction (indicated with prime in the equation) we have

\[
p'_\parallel(t) + \frac{q}{c}A(\eta(x,t)) = p'_\parallel(0) = 0,
\]  \tag{4.7}

for the newborn electron we can write down

\[
0 + \frac{q}{c}A(\eta(x,t)) = p_\parallel(0),
\]  \tag{4.8}

in the instant \(t\) when the new electron is released. This implies that \(p_\parallel(0) = -p'_\parallel(t)\). Thus using this initial value for the parallel momentum of the newborn electron it is possible to find its ejection angle from \((4.6)\). This ejection angle is plotted as a function of the momentum \(p_\parallel(0)\) and the final relativistic factor \(\gamma\) in Figure 4.11.

The black region near the horizontal axis in Figure 4.11 cannot be described by equation \((4.6)\) as the final \(\gamma\) is less than the initial one \(\gamma(0) = (1 + p_\parallel^2(0))^{1/2}\). From Figure 4.11 one can conclude that the momentum \(p_\parallel(0)\) of the newborn electron must be relatively high to result in a large ejection angle. This is in a good agreement with what we have observed in our calculation results as the ejection angles of newborn electrons are not significantly different in simulations with subrelativistic laser intensities like in the case described in previous section.
4.1. ACCELERATION OF ELECTRONS

\[ \approx 10^{17} \text{ W/cm}^2 \].

Let us proceed to numerical results. In the following we assume that preplasma on the target surface has an exponential density profile with scale length of \(4\lambda\) and the initial ion charge is always 3. The length of the density profile may seem relatively high. However, such value is necessary for the impact of the electric field ionization to show up significantly. Aluminum and titanium are selected as two representative and widely used target materials. In simulations for aluminum target the laser pulse is 45 fs long and its peak intensity is \(10^{19} \text{ W/cm}^2\). For titanium target we use 65 fs long laser pulse with peak intensity \(7 \times 10^{18} \text{ W/cm}^2\). In either case normally incident linearly laser wave is assumed and the results with both constant and variable plasma ionization are provided for comparison. Any types of collisions are omitted in all the simulations presented in this section.

Due to the strong dependence of the electric field ionization rate on the amplitude of the instantaneous electric field it is clear that new electrons are released almost entirely around the electric field maxima of each laser cycle. In the harmonic electric field of the incident laser wave with slowly varying envelope free electrons have zero or nearly zero transverse momentum (parallel to the target surface) in the instants of maximum electric field. Note that the vector potential \( A \) in the invariant (4.2) is

\[ A(\eta(x,t)) = -c \int_{-\infty}^{t} E(\eta(x,t'))dt' \],

(4.9)

so the transverse kinetic momentum in (4.2) should be zero in the electric field maxima of a slowly varying harmonic field. The transverse momentum of electrons in the PIC simulation with titanium target is plotted together with the laser field in Figure 4.12 in several time instants. The red lines denote positions of several laser field maxima. It can be seen that the transverse momentum is really zero around the electric field maxima in panels a) and b). For this reason the newly released electrons born around the field maxima are in phase with other
4.1. ACCELERATION OF ELECTRONS

Figure 4.12: The transverse (with respect to the laser wave) momentum of free electrons in the simulation with titanium target in four time instants. The electric field of the laser wave (both incident and reflected) is included. Red lines denote several positions of the electric field maxima. These fields and electron phase spaces come from the PIC simulation with titanium target (normal incidence, linear polarization, $\lambda = 800$ nm, $I = 7 \times 10^{18}$ W/cm$^2$, $\tau = 65$ fs).

electrons and ionization does make anything unexpected only the average ion charge and the number of free electrons both increase.

However, laser field reflected from the target comes into play later in time and the conditions change. We would like to point out that the phase of the reflected field can be shifted from the phase of the incident wave for example due to temporally varying refractive index or position of the critical surface [211, 212, 213]. Moreover, in general the reflected field is not
monochromatic. It usually contains many harmonic fields with frequencies of multiples of
the incident field frequency. As a consequence, the electric field in front of the target is not
harmonic and free electrons have often nonzero transverse momentum in the field maxima.
This is demonstrated in Figure 4.12 in panels c) and d).

In Figure 4.13 we present two examples of the newborn electrons that demonstrate the
correctness of the theory given above. This figure is taken from simulation with titanium
target. It depicts the electron momentum phase space in two simulation cell in the underdense
plasma. The simulation time is about $30\tau$ and in this time instant a new electron is just released
due to electric field ionization in both these cells. In panel a) the transverse momentum of
the newborn electron (blue spot) is significantly displaced from the momentum of other free
electrons (black squares). Because free electrons are initially almost at rest their transverse
momentum is given by the local instantaneous vector potential of the laser electric field is
accordance with (4.2). They all have approximately the same transverse momentum with the
average $p_{\parallel}'(t) = 0.7$. Consequently, we can assume that the newborn electron behaves like
if it has been present already at the beginning of the interaction but with initial transverse
momentum $p_{\parallel}(0) = -0.7$ (4.8).

Particles are numbered in our PIC simulation and accordingly one can distinguish them.
A part of electrons that are in the particular time instant in the simulation cell plotted in
Figure 4.13 panel a), are accelerated and their momentum is recorded when they reach the
rear boundary of the simulation box. We include the final momentum of these accelerated
electrons in the figure (denoted as after ejection). As free electrons are at rest before the
interaction they should end up with zero transverse momentum and consequently their ejection
angle should be zero. As can be seen in the figure this is confirmed in our simulation. On the
other hand the newborn electron keeps its transverse momentum difference and it is ejected
at angle $45.4^\circ$. This is in excellent agreement with the angle given by equation (4.6) which is
$44.8^\circ$ for $p_{\parallel}'(0) = -0.7$ and the final relativistic factor of the newborn electron $\gamma = 1.41$.

We demonstrate the situation in another cell in the same time instant in panel b) of
Figure 4.13 for comparison. Now the newborn electron is almost in phase with other free
electrons and consequently it ends up with almost zero transverse momentum and its ejection
angle is small. Our understanding to the question, where does the different ejection angle of
some electrons in our simulations come from, is therefore correct.

So far we did not discuss the field induced in plasma. Due to strongly nonlinear plasma
dynamics this field is not necessarily in phase with the field of the incident laser wave. Moreover,
the electric field induced in plasma can be of the same magnitude as the field of laser wave
itself and consequently it is also able to ionize. Then the instant when the newborn electron
is released is generally unpredictable as the local vector field potential also is in that time
instant. The ejection angle of newborn electrons is therefore arbitrary in principle. However,
4.1. ACCELERATION OF ELECTRONS

(a) Newborn electron out of phase with free electrons

(b) Newborn electron in phase with free electrons

Figure 4.13: Electron momentum phase space in two simulation cells in the under-critical plasma. The time is $30\tau$ and in both cells new electron is just released by optical field ionization. The data are taken from PIC simulation with variable ionization for titanium target, same parameters as in Figure 4.12. In panel a) the newborn electron is out of phase from other free electrons, in panel b) the newborn electron is in phase. Final momentum of the accelerated electrons is included for illustration.

we remind that the difference in the transverse momentum and the ejection angle is significant only when the electric field is strong (see Figure 4.11). Therefore, almost entirely only those electrons released around the peak of the laser pulse have arbitrary ejection angles and other electrons released earlier behave ordinary just like the initially free electrons.

Electrons from the inner shells (e.g. 3s, 2p shell of titanium) are mostly ionized around the laser pulse maximum as the outer shells are largely depleted in this time. The electric field ionization process is fastest at the rising edge of the main laser pulse and electrons released around the peak of the pulse are in minority in general. Therefore, the newborn electrons usually do not change the overall angular distribution of hot electrons substantially.

The velocity and momentum distributions of hot electrons accelerated into the target in PIC simulation with titanium are plotted in Figure 4.14. Electrons are accelerated only in the direction normal to the target surface in simulation with constant ionization. On the other hand there are also many electrons with different ejection angles in the case of variable ionization as can be seen in panel a). The ejection angles of some electrons almost reach $\pm \pi/2$ and these electrons propagate essentially along the target surface. The pattern of accelerated electrons is symmetrical around $v_y = 0$ ($v_y$ being the component of velocity along the target surface). It is important to take into account that the ‘yellow’ electrons are covered by the red ones so there are many ‘yellow’ electrons propagating normally to the target surface as well. The
ejection angles all lie in the laser polarization plane as the laser pulse is linearly polarized. In the velocity distribution the high energy tail of hot electrons cannot be seen in enough details. Therefore, momentum distribution of hot electrons is included in panel b). Considering this momentum distribution it seems that the newborn electrons with high ejection angles are not the highest energy electrons. This is partially true. The transverse momentum of electrons is limited by the potential of the laser wave whereas the momentum along the target normal is determined by the acceleration process and it can be significantly higher. The ejection angle of high energy electrons is therefore limited and it decreases with electron energy. Nevertheless, some individual 'yellow' electrons, which are possibly not enough clearly seen, are distributed all over the phase space plotted in this figure.

The same phase spaces are plotted for aluminum target in Figure 4.15. One finds a significant difference in the angular distribution of hot electrons comparing between the results obtained for aluminum and for titanium targets with similar laser pulses. This difference is explained by the unlike behavior of both elements during the process of ionization by the laser field. The ionization potentials of all electrons bound in aluminum atom, except for the two innermost ones, lie below 450 eV. Therefore, aluminum is almost completely ionized up to the ion state $\text{Al}^{+11}$ well before the laser pulse maximum. On the other hand, further ionization is improbable even around the peak of the laser pulse as the ionization potential for 1s electron is more than 2 keV for which the field is not strong enough. Contrariwise the 4s, 3d, 3p and possibly 3s shells of titanium with ionization potentials below 300 eV are depleted during the rising edge of the similar laser pulse while the 2p shell (with ionization potential in the range

**Figure 4.14:** Velocity and momentum phase space of electrons accelerated in PIC simulation for titanium target. Simulation parameters are the same as in Figure 4.12. 'Yellow' electrons lie also below the 'red' ones.
4.1. ACCELERATION OF ELECTRONS

(a) Velocity phase space

(b) Momentum phase space

Figure 4.15: Velocity and momentum phase space of electrons accelerated in PIC simulation for aluminum target. Simulation parameters are: normal incidence, linear polarization, $\lambda = 800$ nm, $I = 10^{19}$ W/cm$^2$, $\tau = 45$ fs. 'Yellow' electrons lie also below the 'red' ones.

787 - 1221 eV) is left almost intact until the peak of the pulse arrives. This explains why the velocity and the momentum distributions of hot electrons in Figure 4.15, which are accelerated in aluminum target, are not influenced by ionization so significantly like hot electrons accelerated by similar laser pulse in titanium.

It follows that the angular distribution of hot electrons may significantly depend on the target material. In a simplified manner it is possible to relate the number of hot electrons with nonzero ejection angle with the number of electrons that are released around the peak of the laser pulse. The ionization impact on the angular distribution can thus be more profound if the laser pulse is significantly shorter than the pulses considered here. However, the influence of laser pulse duration has not been studied yet and presently we are not able to discuss this question.

The case of linearly polarized laser wave has been considered first because there the presented phenomenon can be described most easily. Next we briefly discuss how the situation changes in the case of circularly polarized laser wave. Amplitude of the electric field of the circularly polarized wave changes only smoothly. Therefore, the electric field ionization process is more continuous-like than step-like process. Moreover, free electrons never have zero transverse momentum (with respect to laser wave) in this case and therefore the newborn electrons are always out of phase with other free electrons. Consequently the influence of ionization on angular distribution of hot electrons should be more profound which is exactly what we observe. As an example we present the results of PIC simulation with circularly polarized laser
wave in Figure 4.16 for aluminum target, for which the effect of ionization is only weak in the case of linearly polarized wave. Except of laser wave polarization all other parameters are the same as in previous simulations.

The momentum distribution of hot electrons plotted in panel b) is particularly interesting. Here one can see that the maximum transverse momentum \( p_y \) is limited to about \( \pm m_c \) (i.e. \( \text{max } p_y \approx a_0 \)). This indicates that the electric field ionization process terminates when the laser intensity reaches about \( 2 \times 10^{18} \, \text{W/cm}^2 \). This is in a good agreement with the appearance intensity for \( \text{Al}^{11+} \) ion calculated using (3.29) \( (U_i = 442 \, \text{eV}, Z = 11) \) which is about \( 1.3 \times 10^{18} \, \text{W/cm}^2 \). Accordingly, we have confirmed that the ionization process in aluminum stops well before the peak of the laser pulse.

At this place we should make a short comment on what can be seen in the momentum phase space in panel b) of Figure 4.16. The fringes in the high energy tail of hot electron momentum distribution are not physical. They come from the roundoff when hot electrons are recorded. The velocity of hot electrons is recorded with precision of three decimal places in the output files which is evidently not sufficient for this simulation. This will be corrected in future.

Finally, the angular distributions of hot electrons are compared in Figure 4.17 panel a) for all the above presented cases. The influence of electric field ionization on angular distribution of hot electrons is clearly seen here as well as its dependence on target material and

(a) Velocity phase space
(b) Momentum phase space

Figure 4.16: Velocity and momentum phase space of electrons accelerated in PIC simulation for aluminum target and circularly polarized laser wave. Other simulation parameters are the same like in Figure 4.15. 'Yellow' electrons lie also below the 'red' ones.
4.1. ACCELERATION OF ELECTRONS

(a) Angular distribution  
(b) Energy distribution

Figure 4.17: Angular and energy distributions of electrons accelerated in the above presented PIC simulations. For parameters see captions of Figure 4.12 and Figure 4.15. Angular distributions are presented for both targets and polarizations, energy distributions are presented only for the case of linearly polarized laser wave.

We conclude that the angular distribution of hot electrons may become significantly wider due to electric field ionization. Namely, for linearly laser wave and titanium target about 14% of hot electrons with energy higher than 100 keV propagate outside the cone with an opening angle of 30° around the target normal whereas in theory it is often assumed that hot electrons are confined in this cone. For circular polarization and aluminum target the number of electrons outside the cone is more than 20%.

In the beginning of this section we have pointed out that the energy distribution of hot electrons is not notably influenced by electric field ionization in the case of relativistic laser intensity. To verify it we plot the energy distributions of hot electrons in Figure 4.17 panel b) for the case of linear polarization and both target materials. Although, there is some difference in hot electron energy distributions it seems not to be too important and the hot electron temperatures are essentially the same irrespective of the ionization process. The hot electron temperature is higher for aluminum as the laser pulse is more intense. It is about 0.94 MeV whereas the hot electron temperature estimated from the formula (2.14) is about 0.7 MeV. For the titanium target the hot electron temperature is 0.63 MeV and the ponderomotive temperature (2.14) is about 0.54 MeV. In addition to the ponderomotive acceleration some other electron acceleration process is possibly taking place in our simulations (e.g. Raman scattering or stochastic heating). However, detailed analysis of the electron acceleration process is not of prime importance in the scope of the presented results and it is postponed for the future.
4.1. ACCELERATION OF ELECTRONS

Oblique incidence

Analysis of the above presented phenomenon is more complicated in the case of oblique laser incidence. The mechanism producing electrons with different ejection angles is the same in principle. The equation (4.5) determining the ejection angle now depends on the initial momentum $p_{∥}(0)$ as well as the initial relativistic factor $\gamma(0)$ through the constant $C$. Nevertheless, $C$ is still a constant of electrons motion and it is equal to $- \sin \alpha$ for an electron initially at rest. Therefore, we can again regard the newborn electron as if it has been free already initially but with possibly different constant of motion $C$. The constant of motion of the newborn electron can be determined from other free electrons in the instant of the new electron release similarly to the parallel momentum in the case of normal incidence. In the instant $t$ when the newborn electron is released the other free electrons (indicated with prime), which have been initially at rest, have

$$C = p_{∥}(t) + \frac{q}{c} A(\eta(x,t)) \cos \alpha - \gamma'(t) \sin \alpha = p_{∥}'(0) - \gamma'(0) \sin \alpha = - \sin \alpha ,$$  (4.10)

where $p$ is the kinetic momentum. The newborn electron can be regarded as being at rest in the instant when it is released and thus we can write

$$C_{\text{new}} = p_{∥}(t) + \frac{q}{c} A(\eta(x,t)) \cos \alpha - \gamma(t) \sin \alpha = \frac{q}{c} A(\eta(x,t)) \cos \alpha - \sin \alpha ,$$  (4.11)

and thereout

$$C_{\text{new}} = \sin \alpha (\gamma'(t) - 2) - p_{∥}'(t) .$$  (4.12)

Figure 4.18 reflects the situation in the instant when a new electron is born in one particular cell in the underdense plasma. Again the simulation time is close to the peak of the laser pulse about 30τ. The presented electron momentum phase space plot is taken from the simulation for titanium target with the same parameters as in the previous part with exception of the laser incidence angle which is now 45°. As all free electrons were at rest before the laser pulse arrived, they all lie on the parabola given by $p_y - \gamma \sin \alpha = - \sin \alpha + qA/c \cos \alpha$, where $p_{∥}$ is now denote $p_y$ to correspond with the figure. To demonstrate the difference in the ejection angle both the accelerated free electrons and the newborn electron are plotted also with their final momenta after they are ejected into the target. Free electrons stay on a similar parabola upon acceleration as well however the newborn electron is ejected into significantly different direction. Its ejection angle is 61.7°. The ejection angle determined using equation (4.5) with $\gamma = 2.72$ and $C_{\text{new}} = 0.31$ (which is calculated from (4.12) using the momenta of other free electrons) is 62°. Hence the agreement between simulation and theory is very good if $C_{\text{new}}$ is known.
4.1. ACCELERATION OF ELECTRONS

The reasons for the release of new electron out of phase with other free electrons, i.e. with different constant $C$, are essentially the same as in the case of normal incidence (e.g. anharmonic electromagnetic field, plasma field). According to the equation (4.11) one would expect that in a symmetric field of electromagnetic wave the constant $C_{new}$ of the newborn electrons should be equally distributed below and above $-\sin \alpha$ which is the value corresponding to free electron initially at rest. Yet this is true only in the absence of plasma field. The invariant $C$ accounts only for the plane electromagnetic wave in vacuum and if there is a nonzero plasma field it is not always an invariant. Let us assume that the potential $A$ in both equations (4.10) and (4.11) is a function which accounts for both the laser and the plasma field potential. Than the final equation for $C_{new}$ (4.12) remains unchanged. However, the plasma field potential may show itself in the ejection angle through $\gamma'$ which includes $p_{x}'$. To demonstrate the dependence of the value of $C_{new}$ on $p_{y}'$ and $p_{x}'$ (denoted as $p_y$ and $p_x$ respectively) as given by equation (4.12) we plot it in panel a) of Figure 4.19.

The black border line in this figure represents the position of free electrons in the momentum phase space where the newborn electron is in phase with other free electrons, i.e $C_{new} = -\sin \alpha$. Let us denote this value $C_0$ in the following. The gray part of momentum phase space above this line is the region where $C_{new} < C_0$ while in the color part $C_{new} > C_0$. One can expect that if there is a strong plasma field potential $|p_x|$ is high and then the constant $C_{new}$ will be more probably higher than $C_0$. This is also the case for situation presented in Figure 4.18. Consequently, it seems that the plasma field may introduce asymmetry in the ejection direction of newborn electrons with respect to the ejection direction of other free electrons.

In panel b) of Figure 4.19 we include the ejection angle dependence as given by (4.5) on the constant $C$ and the final relativistic factor $\gamma$ of electron leaving the laser target interaction region. The black line denotes the position where $C = C_0$ (approximately $-0.707$ for $\alpha = 45^\circ$). From this figure one can readily conclude that the value of $C$ higher than $C_0$ results in ejection...
4.1. ACCELERATION OF ELECTRONS

(a) Constant of electron motion $C_{\text{new}}$

(b) Ejection angle

Figure 4.19: In panel a) the constant of electron motion $C_{\text{new}}$ (4.12) is plotted against the initial electron momenta. The constant of motion $C_0$ of free electrons initially at rest is denoted by black line. In the gray region $C_{\text{new}} < C_0$ while in the color region $C_{\text{new}} > C_0$. In panel b) the ejection angle calculated using (4.5) is plotted against the constant $C$ and the final relativistic factor of ejected electron $\gamma$. The black vertical line denotes position where $C = C_0$.

of accelerated electrons more along the target surface.

In Figure 4.20 the velocity and the momentum distributions of electrons accelerated in PIC simulation for titanium target are presented. All parameters except of the laser incidence angle $45^\circ$ are the same as in the case of normal incidence. In the simulation with constant ionization low energy electrons propagate almost normally with respect to the target surface as one can see in the velocity distribution in panel a) while the direction of propagation of high energy electrons tends to the laser incidence direction. In the case of variable ionization the propagation angle of accelerated electrons can exceed the laser incidence angle and reach almost $90^\circ$. As discussed above the ejection angle of newborn electrons is not symmetric around the direction of ejection of other free electrons but the newborn electrons are ejected preferentially with high angles. One must again take into account that ‘yellow electrons’ are covered by red ones when their propagation directions are the same. The most of lower energy electrons in the case of variable plasma ionization are thus hidden below the electrons resulting in simulation with constant ionization. This is reasonable as again the mayor part of electrons are either free initially or released early during the interaction and thus in phase with free electrons.

In panel b) of Figure 4.20 the momentum distributions of electrons accelerated in PIC simulation with constant and variable ionization are compared with the theoretical formula (4.5). In the case of constant ionization the agreement of simulation results with theory is very
4.1. ACCELERATION OF ELECTRONS

(a) Velocity phase space
(b) Momentum phase space

Figure 4.20: Velocity and momentum phase space of electrons accelerated in PIC simulation for titanium target. Simulation parameters are the same as in Figure 4.12 except of the 45° angle of incidence. ‘Yellow’ electrons lie also below the ‘red’ ones. In panel b) theoretical curve calculated from equation (4.5) is added for comparison.

good. In the case of variable ionization one can see many electrons ejected into significantly different directions. In comparison with the case of normal incidence the momentum parallel with the target surface is significantly higher here (compare with Figure 4.14 panel b) and it is not limited by the laser field potential. Nevertheless, the highest energy electrons tend slowly to the laser incidence direction, again indicating that at very high electron energies the initial conditions are washed out. This is in agreement with equation (4.5).

Angular distributions of accelerated electrons with energy higher than 1 MeV are compared in Figure 4.21 panel a). We include the results of simulation with titanium target with both constant and variable ionization. The results calculated with carbon target and similar laser parameters are added for comparison. The ejection angles of all hot electrons lie in between 20° and 44° and the beam is well collimated in the case of titanium target without ionization. However, if ionization is taken into account the peak in the angular distribution spreads into two peaks which are separated by the laser incidence angle (indicated with black line). We recall that ejection angles higher than the laser incidence angle are forbidden if ionization is not considered. Therefore, the second peak in the angular distribution is only due to electrons released by electric field ionization out of phase with other free electrons. This second peak is relatively wide and it contains number of hot electrons comparable to the first peak.

The angular distribution of hot electrons depends on the target material significantly as demonstrated in the case of normal incidence. Similar effect is observed in the case of oblique incidence. In the case of carbon target plasma is ionized at the very beginning of the main
laser pulse and only a minority of 1s electrons (with ionization potentials 392 eV and 490 eV) remain bound until the laser field is high enough and anharmonic. Consequently, there is only a very small influence of ionization on the angular distribution of hot electrons, yet some other peak due to the ionization process is also visible in the angular distribution. We believe that the results presented in this subsection can be utilized to select target materials for experiments where better collimation of laser accelerated hot electron beam is desired (e.g. Fast ignition, TNSA).

The energy distribution of electrons accelerated into the titanium target in the simulations with and without ionization are presented in panel b) of Figure 4.21. We conclude that the ionization process does not inhibit acceleration of electrons in the high intensity laser solid target interaction.

Our basic conclusions claim that electrons produced by electric field ionization of inner atomic shells may contribute to angular spread of hot electrons accelerated in high intensity laser solid target interactions. The resulting angular distribution depends strongly on laser polarization, angle of incidence and target material. The influence of ionization on hot electron angular spread is more profound in higher Z materials.

The boost frame technique is used to describe the obliquely incident laser wave in our

![Figure 4.21: Angular and energy distributions of electrons accelerated in PIC simulations for titanium target and 45° angle of incidence. For parameters see captions of Figure 4.12. Angular distributions include only electrons with energy higher than 1 MeV. The distribution calculated for carbon target with the same laser pulse is added for comparison. Black vertical line denotes the laser propagation direction. Energy distributions are presented only for titanium target.](image)
4.2 Propagation of hot electrons inside the target

In high intensity laser solid target interactions a significant part of energy of the laser pulse is converted into beam of hot relativistic electrons. Compared with other conventional particle accelerators energies of hot electrons are usually lower however their flux is very intense. Laser
accelerated hot electron beams are thus characterized by very high charge and current density. The propagation of such electron beam is accompanied by significant space-charge separation which gives rise to a strong quasistatic electric field. The missing charge must be neutralized otherwise this electrostatic field will decelerate the beam and stop it and finally it will revert its propagation direction.

The space-charge neutralization is carried out by shifting free electrons. If there is sufficient number of these electrons in the target the space-charge is neutralized relatively easily. This is the case of plasmas or well conducting materials like metals. Electrostatic field produced in consequence of charge separation accelerates free electrons into the region where hot electrons are missing. However, free neutralizing electrons are losing some momentum of their directed motion in collisions. Thus their drift motion is being gradually turned into the chaotic motion, heat. Therefore, some nonzero residual electrostatic field must remain in the target to supply free electrons with the lost directed momentum of their drift motion. The neutralizing current of free electrons is called the return current, $j_r$, and the electrostatic field necessary to sustain this current can be expressed from the Ohm’s law as (e.g. [216])

$$ E = \frac{j_r}{\sigma}, $$(4.13)

where $\sigma$ is the electrical conductivity of the target material. As electron-electron collisions conserve momentum and do not impede the flow of current, electron-ion or electron-atom collisions produce all the electrical resistance. The conductivity of plasma can be expressed using the electron-ion collisional frequency $\nu_{ei}$ as

$$ \sigma = \frac{e^2 n_e}{m_e \nu_{ei}}. $$(4.14)

Even if the space-charge is neutralized and the residual electric field is low there is another factor inhibiting electron beam from free streaming propagation. In one-dimensional model the return current must flow through the same volume as the current of the electron beam. This means that charge neutralization implies perfect current neutralization as well. However in more dimensions the neutralizing electrons do not necessarily take the same path as the beam electrons. The return current may flow around the hot electron beam especially if conductivity is higher there for some reason (e.g. cold metals are better conductors than low temperature plasmas). In such case the beam current is not completely neutralized and thus it gives rise to the azimuthal magnetic field according to Faraday’s induction law. The magnetic field induced around the hot electron beam is proportional to the nonneutralized current it encloses. It has been found by Alfvén [217] that there is a limiting maximum noncompensated current and higher current is not possible on a longer time scale. The reason for this limiting current is that the magnetic field near the edges of the hot electron beam would otherwise be so strong that it deflects hot electrons near the beam edges inhibiting their further propagation with the
beam. Alfven current depends only on the energy of beam electrons not on the current density or the beam cross section and it reads

$$I_A = \frac{4\pi\varepsilon_0 m_e c^3 \gamma \beta}{e} \approx 17\gamma \beta \text{ kA}, \quad (4.15)$$

where $\gamma$ is the relativistic factor and $\beta$ is the velocity of beam electrons normalized by the velocity of light. The magnetic field may on one hand deflect some electrons near the beam edges but on the other hand it may confine collimated propagation of the rest of the beam.

The system consisting of an electron beam and a return current formed by free electrons is in general unstable. In reality every possible unstable mode allowed by Maxwell equations will grow exponentially while only the most unstable one will shape the beam. Among the most unstable modes filamentation, Weibel and two-stream instabilities are widely considered [218, 219, 220, 221, 222]. These instabilities pertain to different orientations of wave vector and various kinds of waves (filamentation – $k \perp x$ and $E \parallel x$, Weibel – $k \parallel x$ and $E \perp x$, two-stream – $k \parallel x$ and $E \parallel x$, where $x$ is the beam propagation direction). If the instability growth rate is high and it has enough time to develop it may result in a significant energy loss of the beam or it can break the beam into filaments.

Last but not least collisions of the beam electrons are also important especially if beam electrons are not very energetic and their propagation on a longer distance in the dense material is studied.

### 4.2.1 Hot electron beam propagation models

General numerical solution of the problem of electron beam propagation in matter including all the above mentioned processes is practically impossible especially on longer temporal and larger spatial scales. According to the current $I_b$, and current density $j_b$ of the beam and the conductivity $\sigma$ of the surrounding material, it is possible to classify the problem of electron beam propagation into one of the following categories and apply corresponding simplifications ($|j_r| = |j_b|$ is assumed):

- $I_b \ll I_A$ and $j_b/\sigma$ is small so that energy losses due to Ohmic heating are much lower than collisional ones
  
  In this case the influence of self-consistent electric and magnetic fields can be neglected and electron transport is dominated by collisions. The trajectories of individual beam electrons are mutually independent and it is possible to apply the MC electron transport approach described in Section 3.6.

- $I_b \simeq I_A$ and (or) $j_b/\sigma$ is higher but the material is still a relatively good conductor (e.g. plasma)
In this case energy loss of the beam due to Ohmic heating is comparable with energy loss due to collisions. The same may apply to the deflection of beam electrons due to self-induced magnetic field and due to collisions. As the influence of collisions and self-induced electric and magnetic fields is comparable one must resort to a hybrid model. An example of such model is presented in [223]. The body of the model consists of collisional MC electron transport algorithm. In this model however electrons do not propagate on straight line trajectories with constant velocities between two successive collisional events. The self-induced electric and magnetic fields are solved on a spatial grid with some reasonably long time step and they are taken into account in the equations of electrons motion. In this model the conductivity is also temperature dependent and when it is evaluated energy deposition by the beam is taken into account. However, the spatio-temporal resolution of such models is limited and they are not able to handle the effect of fields on the spatial scale of the Debye length and temporal scale of the plasma frequency.

- $I_b \gg I_A$ and (or) $j_b/\sigma$ very high ($\rightarrow \infty$)

In this case the propagation of electron beam is dominated by the self-induced electric and magnetic fields. Electron trajectories are not mutually independent but they are interconnected with each other. Thus the self-induced fields must be described properly but on the other hand collisions of beam electrons can be disregarded. Kinetic treatment of the hot electron beam and the return current is necessary and either PIC or Fokker-Planck simulation must be applied.

In this work our PIC code is applied to study high-current relativistic electron beam propagation in cold dielectric target. This subject is of prime importance in connection with recent experiments related to Fast Ignition of Inertial Confinement Fusion targets. In these experiments [224, 225] stronger filamentation of the hot electron beam was observed in dielectric targets in comparison with metals. Recently proposed explanation of this effect relies on ionization instability of hot electron beam propagating in dielectric target [226]. This instability is supposed to develop due to corrugation of the ionization front. The corrugation may be enhanced if there is a dependence of hot electron beam propagation velocity on the beam density in dielectric target. One of the major objective of our work is to demonstrate such dependence. In particular we identify the effect of the field ionization in the head of the beam as a dominant process which defines the effective velocity of the beam propagation and its energy losses. The work has been done in collaboration with prof. Tikhonchuk from the CELIA laboratory at the University of Bordeaux and his PhD student Debayle. In accordance with our PIC simulations our colleagues from CELIA have developed a theoretical model describing hot electron beam propagation in dielectric target analytically. Their analytical model will not be presented here. Nevertheless, to demonstrate the correspondence of both model comparison will be provided. For more details about the analytical model we refer to our joint publication [2].
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

4.2.2 Hot electron beam studied in this work

First of all let us specify the hot electron beam whose propagation is studied in our work and compare it with electron beams obtained in recent short-pulse high-intensity laser solid-target interaction experiments. Energy distribution of hot electrons obtained in experiments can be usually approximated by Boltzmann, Maxwell or relativistic Maxwell distribution with hot electron temperature given by formula (2.14). The density of hot electrons in the beam can be estimated as \( n_b = I\eta/(cT_h) \), where \( I \) is laser intensity and \( \eta \) is the laser energy absorption into hot electrons. In the relativistic regime laser absorption into hot electrons \( \eta \) of about 20% is evidenced in experiments. The electron acceleration process takes place in the vicinity of critical surface so the maximum beam density should not be higher than critical density. In experiments the density of hot electron beam is more likely below \( 10^{20} \text{ cm}^{-3} \). Hot electrons are relativistic and their velocity approaches the velocity of light. Thus the beam current density can be estimated as \( j_b = en_b c \) and it can be as high as several hundreds of GA/cm\(^2\). The length \( l \) of hot electron beam is proportional to the duration of the acceleration process and it is approximately \( l = c\tau_l \) where \( \tau_l \) is the laser pulse duration. Finally, as already mentioned in previous subsection the beam divergence is supposed to be less than 30°. For more details about laser accelerated hot electron beams see e.g. [227, 228, 229].

<table>
<thead>
<tr>
<th></th>
<th>Experiments</th>
<th>Our model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy / velocity</td>
<td>Boltzmann,</td>
<td>homogeneous in velocity</td>
</tr>
<tr>
<td>distribution</td>
<td>Maxwell,</td>
<td>ranging between 0.7 and 0.9 c</td>
</tr>
<tr>
<td></td>
<td>relativistic Maxwell</td>
<td>about 0.5 MeV</td>
</tr>
<tr>
<td>Average electron</td>
<td>up to several MeV</td>
<td></td>
</tr>
<tr>
<td>energy</td>
<td>( T_h = m_e c^2(\sqrt{1 + a_0^2} - 1) )</td>
<td></td>
</tr>
<tr>
<td>Beam density</td>
<td>up to ( 10^{20} \text{ cm}^{-3} )</td>
<td>( 10^{18} - 10^{20} \text{ cm}^{-3} )</td>
</tr>
<tr>
<td></td>
<td>( n_b = I\eta/(cT_h) )</td>
<td>homogeneous along the beam</td>
</tr>
<tr>
<td>Beam intensity</td>
<td>up to order of ( 10^{18} \text{ W/cm}^2 )</td>
<td>( 2 \times 10^{15} - 2 \times 10^{17} \text{ W/cm}^2 )</td>
</tr>
<tr>
<td></td>
<td>( I_b = I\eta = n_b T_h c )</td>
<td></td>
</tr>
<tr>
<td>Beam current density</td>
<td>up to 400 GA/cm(^2)</td>
<td>4 - 400 GA/cm(^2)</td>
</tr>
<tr>
<td></td>
<td>( j_b = e n_b c )</td>
<td></td>
</tr>
<tr>
<td>Beam length</td>
<td>several tens of ( \mu \text{m} )</td>
<td>8 ( \mu \text{m} )</td>
</tr>
<tr>
<td></td>
<td>( l = c\tau_l )</td>
<td></td>
</tr>
<tr>
<td>Beam divergence</td>
<td>( \leq 30^\circ )</td>
<td>zero, 1D model</td>
</tr>
</tbody>
</table>

Table 4.1: Comparison of hot electron beam parameters obtained in recent experiments with the parameters used in our model. For parameters characterizing hot electron beams in experiments see e.g. [227, 228, 229, 230].
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

The beam assumed here has a homogeneous velocity distribution ranging between 0.7 and 0.9 velocity of light. The average hot electron energy is thus about 0.5 MeV. The beam density ranges between $10^{18}$ and $10^{20}$ cm$^{-3}$ and it is uniform along the beam propagation direction. Correspondingly, the beam current density ranges between 4 and 400 GA/cm$^2$. A lower beam intensity is assumed here in comparison with experiments. The beam density is comparable with the one obtained in experiments and the difference in the beam intensity is due to the lower kinetic energy of the beam electrons. Hot electrons are only moderately relativistic in our work. The computational performance limits the propagation distance on which we are able to follow the beam in our simulations. Lower beam electron energy is thus advantageous because the beam dynamics changes more rapidly and on a shorter distance. The hot electron beam is just 8 $\mu$m long in all the cases considered here. This length approximately corresponds to 30 fs laser pulse. The limit on the beam length comes again from computational constraints. Finally, the divergence of hot electron beam is zero in our one-dimensional model. For clarity the characteristics of hot electron beam assumed in our work are compared in Table 4.1 with characteristics of electron beams usually obtained in experiments.

We chose polyethylene with a relatively simple chemical composition CH$_2$ as a representative dielectric material. The density of polyethylene is about 0.9 g/cm$^3$ which corresponds to about $0.3 \times 10^{23}$ CH$_2$ molecules per cm$^3$. For definiteness we note that the electrical conductivity of polyethylene at normal conditions (room temperature, atmospheric pressure) is approximately of the order $10^{-11}$ ($\Omega$m)$^{-1}$ [230].

4.2.3 Computational model of electron beam propagation

Complete kinetic simulations of the hot electron beam propagation are not accessible yet because of large disparity between the densities and electron energies of the beam and the solid material. To keep the computational cost of our PIC simulations on a reasonable level some simplifying assumptions have to be made. These assumptions and their validity are discussed here.

In our simulations the beam and the plasma electrons are treated as separate species. Collisions of hot electrons are neglected and therefore we keep only one velocity component of the beam particles. Consequently, we take into account only the electric field component directed along the beam propagation axis. Magnetic field effect on the hot electron beam propagation cannot be described by our one-dimensional model. In one dimension, charge neutralization always implies current neutralization and therefore there is no net magnetic field once the space-charge is neutralized. The neutral atoms and ions are treated as immobile stationary background. This crucial simplification is justified by two arguments supported by the simulation result: first, the amplitude of the self-consistent electric field remains always well below the atomic field; second, its existence in any particular place is temporally limited.
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

The simulation box consists of two spatial regions of different solid density materials. The first one is the injection region - a thin aluminum foil, where the hot electron beam is initiated. It is followed by the propagation region composed of polyethylene. The length of the injection layer is equal to the length of the beam (8 \( \mu m \)). The injection layer contains both cold and beam electrons. The number density of cold electrons is \( 1.8 \times 10^{23} \, \text{cm}^{-3} \), corresponding to the solid density aluminum with three free electrons per ion. Initial electron temperature of cold aluminum electrons is set to 50 eV. Beam electrons are distributed among the cold ones and they are assigned random velocity, uniformly distributed between 0.7 and 0.9 speed of light, in the beam propagation direction. The density of electrons in the beam is also initially uniform along the propagation direction except for the first and the last micron where it linearly increases or decreases, respectively. As the density of the beam in this study, \( 10^{18} - 10^{20} \, \text{cm}^{-3} \), is much lower than that of solid aluminum and as the number of beam electrons is desired to be high to have a good statistics of their distribution function and a smooth profile of the electric field, we initiate beam electrons with a lower numerical weight and keep the number of macroparticles comparable for cold and hot electrons.

The size of the computational cell as well as the time step used in PIC simulation should be proportional to the electron Debye length (3.2) which depends on electron density and temperature. The Debye length in a real low temperature solid density aluminum plasma is of order 0.1 nm. This is beyond our available computational resources and also near the limit of validity of the Debye-Hückel model. However, what happens in the aluminum layer is not important in our study except for a short time at the beginning until the beam leaves it. Moreover, the plasma which develops during the beam propagation in polyethylene is of lower density. For these reasons, we consider a higher initial electron temperature in aluminum, about 50 eV, and we are using the cell size of 1 nm. The cell size is constant but the Debye length in the dielectric part of the target continually changes as the number of free electron increase. Therefore, one must verify if numerical heating is not too significant in the simulation. The

\[ v = 0.7c \text{ to } 0.9c \]

**Figure 4.22:** Illustration of our hot electron beam propagation model. The beam is initiated in a thin aluminum layer and it propagates in the polyethylene target.
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

Calculations presented here provide a sufficient accuracy as the total energy in the simulation box does not deviate from the initial value more than 1% during the whole simulation. The polyethylene layer is usually 50 µm long and it contains only neutral atoms initially. The simulation setup is demonstrated in Figure 4.22 for convenience. The two most important processes which take place in this part of the simulation box during electron beam propagation, the ionization, and the collisions of newly produced cold electrons, are described next.

Ionization model

When the hot electron beam enters the cold dielectric material electrostatic field is induced in consequence of charge separation. Its magnitude can be roughly estimated from the beam intensity as

\[ E = \sqrt{\frac{2I_b}{\varepsilon_0 e}} \approx \sqrt{\frac{n_b I_b}{\varepsilon_0}}. \]  \hspace{1cm} (4.16)

For the beam densities assumed in our simulation magnitude of the electric field should approximately range between 0.1 and 1 TV/m. If the space-charge is not neutralized this field will stop the beam on a distance of several µm. However, as there are no free charge carrier in cold dielectric material initially ionization must take place first and foremost.

In our case there are three important processes which may produce free electrons in the dielectric target. Namely, these are the electric field ionization, the collisional ionization by the beam electrons and the collisional avalanche ionization by the return current. The number of free electrons in the target obeys equation

\[ \frac{\partial n_e}{\partial t} = (w_f + w_b + w_r)(n_a - n_e), \]  \hspace{1cm} (4.17)

where \( n_a \) is the density of atoms and \( w_f, w_b \) and \( w_r \) are the rates of change of free electron density due to electric field ionization, collisional ionization by the beam and collisional ionization by the return current respectively. Single ionization of atoms is assumed here. The ionization of the outermost electron is the most probable and the density of free electrons produced by this ionization is usually sufficient for the return current.

To estimate the importance of the above mentioned ionization processes let us assume for the moment that the target consists only of hydrogen atoms and their density is \( 10^{23} \text{ cm}^{-3} \), approximately corresponding to the density of atoms in polyethylene. We demonstrate the dependence of the ionization rates employed in equation (4.17) on the free electron density for the beam density \( 10^{19} \text{ cm}^{-3} \) in Figure 4.23. The rate of collisional ionization by beam electrons
is independent of free electron density. It is calculated as

\[ w_b = n_b v_b \sigma , \quad (4.18) \]

where the ionization cross section \( \sigma \) is evaluated using the Lotz cross section (3.38). Energy of 0.5 MeV is assumed for the beam electrons. The rate of collisional ionization due to the return current scales linearly with free electron density \( n_e \) and it is evaluated in a similar way

\[ w_r = n_e v_e \sigma . \quad (4.19) \]

The return current electrons are assumed to have energy of 15 eV. In the simulation results it will be seen that this assumption is quite reasonable. The rate of ionization by the electrostatic field depends on the field strength only and it is calculated using the Landau-Lifshitz formula (3.13). The electrostatic field is estimated as

\[ E = \min \left\{ \frac{n_b T_b}{\varepsilon_0}, \frac{n_b c m_e v_{ei}}{e n_e} \right\} . \quad (4.20) \]

The first term on the right hand side is the estimate of the maximum electrostatic field (4.16) when the space-charge is not neutralized while the second term corresponds to the field which is necessary to drive the return current equal to the current of the beam \( (j_r = j_b) \) given by the Ohm’s law (4.13). In (4.20) electron-ion collisional frequency is assumed constant with a reasonable value of \( 10^{15} \text{ s}^{-1} \).

It is clear that as long as the density of free electrons is low the dominant ionization process is due the electrostatic field (see Figure 4.23). The electric field continuously increases while the head of hot electron beam enters the dielectric material. As soon as the electric field reaches some threshold value, ionization by this field becomes very fast. The electric field at the head of the beam will not reach the maximum value given by equation (4.16) because by that time free electron density will already be high and the space charge will be easily neutralized. Electric field ionization creates a seed population of free electrons which gain their energy from the same field. Kinetic energy of the newborn
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

electrons rapidly overcomes the threshold for collisional ionization and the population of free electron further increases due to ionization by the return current.

Both the electric field ionization and the collisional ionization by the return current must be taken into account. If only electric field ionization is taken into account and collisional ionization by the return current is omitted, the conductivity of plasma produced in the dielectric target is too low and energy of the beam is dissipated by Ohmic heating rapidly. On the other hand, collisional ionization by the beam electrons is not important for the beam density $10^{19} \text{ cm}^{-3}$ and it can be neglected. Similar situation applies to the whole beam density range $10^{18} - 10^{20} \text{ cm}^{-3}$ assumed here. As we are dealing with simulation times of order of tens of femtoseconds and the dielectric target is usually not completely ionized during this time the complementary process of three body recombination is omitted.

The field ionization process included in our PIC code is described in Section 3.3.2. To calculate the ionization rate we use the instantaneous ADK tunneling ionization rate (3.25). In our model we assume that only the outermost shell of carbon atoms can be ionized ($Z = 1$) and for the ionization potential we use an average value between carbon and hydrogen, $U_i = 12.8 \text{ eV}$. These approximations seem to be quite reasonable because the dependence of the ionization probability on the ionization potential is highly nonlinear and secondary ionization does not set up. The simulation results do not depend on the ionization potential if we vary it in the domain between the values for carbon and hydrogen. The field in our simulations is always lower than the critical field (3.27), (3.28) at which the barrier suppression ionization sets up. Therefore, application of the ADK tunnelling ionization rate is justified.

The difference in the numerical weight of beam and cold electrons must not be too big, otherwise a single cold electron would affect the electric field too much. On the other hand, the number of new free electrons per simulation cell is limited by the computational performance. As we will show later, the final ionization state of the initially neutral polyethylene target depends on the beam density. Roughly, the density of plasma created by the beam is 1000 times higher than that of the beam. Consequently, we are using 4000, 1000 and 400 cold electrons per simulation cell to represent a singly ionized solid density polyethylene for the beam densities $10^{18}, 10^{19}$ and $10^{20} \text{ cm}^{-3}$ respectively. Then the number of cold electrons per simulation cell in plasma behind the beam is usually in the reasonable range of values between 70 and 400.

We recall here that atoms and ions are treated as immobile in our simulations and they serve only to provide an appropriate resolution for sampling the ionization probability. Using the same number of atoms per cell as the number of cold electrons would impose unnecessary constrains on the computational performance. For this reason, we use just 200 equally spaced atoms per cell in every simulation and let each of these atoms be ionized several times, strictly speaking 20, 5 and 2 times, with the same ionization potential. The atoms ‘remember’ how
many times they were already ionized and when ionization probability for the electric field ionization is calculated, it is always multiplied by the number of electrons that can still be released from the corresponding atom. The newborn electrons are initiated with velocity randomly sampled from the Maxwellian distribution with temperature 7 eV. This nonzero initial velocity does not significantly affect the overall energy balance and it is essential for the collisional algorithms.

The energy spent for ionization is subtracted from the field using an artificial ionization current. In these simulations, the part of electric field energy spent for ionization is indeed important. In the runs where the ionization current is neglected, the field amplitude and correspondingly the number of new free electrons at the head of the beam is significantly higher.

Implementation of the process of ionization due to inelastic electron collisions is described in Section 3.3.4. The cross section for ionizing collision is calculated using an analytical fit to the Bethe binary encounter cross section (3.35) for ionization of polyethylene. Currently, we assume that only the outermost shell of carbon atoms can be ionized. This assumption is valid for the beam densities below $10^{20}$ cm$^{-3}$. For higher densities it is not exactly correct, as the single ionization is almost completed at the rear part of the beam, while the temperature of cold electrons is sufficiently high for the secondary ionization of carbon atoms. This assumption could be easily corrected in future, however we are not considering such very high beam densities here.

Newborn electrons released in ionizing collisions are assigned kinetic energy which is randomly sampled from Maxwellian distribution with temperature 2 eV. The ionization energy and the kinetic energy of the newborn electron are both subtracted from the kinetic energy of the electron that ionized the atom. The collisional ionization leads to plasma cooling as a counterpart of the Joule heating by the return current.

**Collisional model**

As the collisional algorithm in the PIC code is computationally very expensive, we do not use collisions for every species of particles. All ions and atoms are immobile and therefore collisionless. Moreover, we assume their temperature to be low during the beam propagation and therefore they are having zero velocities. Propagation of the beam is predominantly influenced by the self-induced electric field and therefore beam electrons are also considered as collisionless. Cold electrons in aluminum are highly collisional but the aluminum layer is included just to provide initial conditions for hot electrons and to avoid the disruption of the beam at boundary between the two materials. Therefore, there is no need to know their distribution function exactly. They have initially Maxwellian distribution and the Joule heating in alu-
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

Aluminum is insufficient to heat them up or to change their distribution significantly. However, their collisions must be taken into account to damp the oscillations at plasma frequency that are otherwise present. We treat their collisions with ions with constant collisional frequency of 2 fs$^{-1}$. This value is realistic and it is sufficient to damp the oscillations, but does not inhibit the return current in aluminum. Therefore, cold electrons in polyethylene are the only species for which collisions are essential and must be treated in detail.

The collisional algorithm used here is described in Section 3.4.3. The frequencies of electron-atom or electron-ion collisions in solid density material are very high, of order of 1 fs$^{-1}$. Correctness of our Monte Carlo approach for such high collisional frequencies is guaranteed by a very short simulation time step of the order of $10^{-3}$ fs. Collisions with neutral atoms play the most important role in the front part of the beam, where electron and ion densities and also the Coulomb collision frequency are low. If collisions with neutral atoms are not included, cold electrons would gain too high velocity from the field just after ionization and the electric field behind the ionization front starts to oscillate at plasma frequency. Because of higher velocities, electrons are less collisional during the whole simulation in this case and plasma oscillations are damped only slowly. The frequency of collisions with neutral atoms is calculated using the total cross section for elastic electron scattering in polyethylene as $\nu_{en} = n_e n_m (\sigma_C + 2\sigma_H)$, where $n_m$ is the number density of CH$_2$ molecules, which is initially $0.3 \times 10^{23}$ cm$^{-3}$, and $\sigma_C$ and $\sigma_H$ are the total cross sections for elastic scattering for carbon and hydrogen, respectively. The Coulomb electron-ion and electron-electron collisions set up behind the ionization front where the density of free electrons and ions is high enough. Electron-electron collisions drive the distribution of cold electrons toward Maxwellian but as they conserve momentum, they do not impede the return current. However, we are also interested in the distribution of cold electrons and therefore these collisions cannot be omitted. In our binary collision algorithm electrons collide in pairs while in electron-ion collisions we use again the assumption of static scattering centers. Therefore, there is no need to group ions in pairs with electrons. In the collisional model applied here, the frequency of Coulomb collisions $\nu_e$ depends on the local cold electron density and electron velocity. In practical units it is $\nu_e = 1.6 \times 10^6 n_e v_e^{-3} \text{ s}^{-1}$, where the velocity of electron is in m/s and the electron density is in m$^{-3}$. In our simulations the collisional frequency is kept in the range $1 - 1000$ ps$^{-1}$.

4.2.4 Results of hot electron beam propagation and their discussions

The results of our simulations of the relativistic electron beam propagation in dielectric target and their interpretations are presented next. Our objective is to study the dependence of the ionization front velocity, of the beam energy dissipation, and of the plasma parameters behind the beam, on the beam density. The density of the beam in our simulations is $10^{18}$ cm$^{-3}$, $10^{19}$ cm$^{-3}$ or $10^{20}$ cm$^{-3}$. 
Characteristics of the beam and dependence on the beam density

A. Ionization process

The ionization process, which takes place in the polyethylene target during the propagation of relativistic electron beam, is demonstrated in Figure 4.24 in the simulation time 74 fs. The whole beam is already inside the dielectric part of the target which begins at 8 µm. The electric field, blue curve in panel a), grows rapidly at the head of the beam. Once the field reaches the value of about 20 kV/µm, the field ionization, blue curve in panel b), starts and the field growth slows down, until it stops. Depending on the beam density, the maximum field in the ionization front is between 23 kV/µm and 38 kV/µm. This is less than 10% of the atomic field. More than 100 new electrons per one beam electron are produced by the field ionization. These new electrons are accelerated by the electric field and neutralize the space-charge and the beam current. Then the electric field drops down and the field ionization stops. Collisions of newborn cold electrons play a very important role behind the beam front. It was checked in a special run that if plasma is considered collisionless, the electric field drops down to zero or even changes its sign and starts to oscillate. This is the process of the plasma wake formation behind the electron beam. It operates in a low density plasma but it is suppressed in solid targets because of their high collisionality.

While neutralizing the beam current, cold electrons rapidly gain kinetic energy higher than the ionization potential and start to ionize neutral atoms behind the front. The collisional ionization frequency for an electron with the kinetic energy of tens of eV is very high, of the order of several fs$^{-1}$. Therefore, the collisional ionization by plasma electrons, green curve in Figure 4.24 b), sets up almost immediately after the field ionization. The collisional ionization process is so important that at the end of the ionization front the total cold electron density, red curve in Figure 4.24 panel b), is already doubled, compared with the cold electron density produced just by the field ionization.

After the initial stage of rapid ionization, the resistivity of plasma drops down and correspondingly the electric field needed for the current neutralization inside the beam is low, about 6 kV/µm. The average energy of cold electrons decreases to 7 eV, below the ionization potential, red curve in Figure 4.24 panel a), and the collisional ionization rate decreases. Nevertheless, collisional ionization behind the ionization front persists, the density of cold electrons increases and the resistivity decreases a few times. Finally, behind the beam, the electric field drops down to zero, as the current density of the beam has been neutralized, and both the heating of plasma and the further increase of number of cold electrons stop there.

The density of new free electrons produced by the electric field ionization is approximately 10% of the total density of new electrons at the tail of the beam for all three beam densities considered here. The electric field ionization process dominates the collisional one in the head
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

(a) Electric field and cold electron energy  
(b) Cold electron density produced by ionization

Figure 4.24: Demonstration of the ionization process. The relativistic electron beam with the density $10^{19}$ cm$^{-3}$ propagates from the left and the snapshot is taken in the time 74 fs. All curves are normalized to the maximum values given in legends. The number of electrons produced by the field and the collisional ionization processes are normalized to the total cold electron density in panel b).

of the beam. It defines the velocity of ionization front. However, the collisional ionization by the return current takes place in the whole region behind the ionization front and consequently produces from 80% to 90% of free electrons.

B. Dependence on the beam density

Comparing the electric field induced by the beam in plastic target, it is observed in Figure 4.25 panel a) that with the decrease of the beam density, the maximum electric field in the ionization front also decreases, while the thickness of the ionization front increases. A lower amplitude of the electric field implies a lower field ionization rate and therefore the thickness of the ionization front must be bigger to provide the field with more space for ionization and production of enough new free electrons. For all three beam densities, distinct change in the slope of the cold electron density is observed just behind the ionization front in panel b). It corresponds to the switch from electric field to collisional ionization.

The position of the ionization front in Figure 4.25 panel a) depends on the beam density. This is due to the dependence of the ionization front velocity on the beam density. The velocity of the ionization front is smaller than the velocity of fastest beam electrons. It can be defined as the mean velocity of the beam electrons inside the strongest field region. The number of hot electrons at the head of the beam creating the strong field, which ionizes the matter, depends
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

(a) Electric field
(b) Cold electron density

Figure 4.25: Comparison of the electric fields (panel a), and the cold electron densities \(n_e\) produced by the field and avalanche ionization (panel b), for the relativistic electron beam densities \(n_b = 10^{18}, 10^{19}\) and \(10^{20}\) at the time 74 fs.

weakly on the beam density. Therefore, the velocity distribution of beam electrons inside the ionization front contains more slower electrons and the propagation of the ionization front is correspondingly slower when the density is lower.

For the beam densities \(10^{18}, 10^{19}\) and \(10^{20}\) cm\(^{-3}\), the density of cold electrons behind the beam is about 1700 times, 1400 times and 1000 times the density of the beam respectively, see Figure 4.25 b). We must point out that the cold electron density for the beam density \(10^{20}\) cm\(^{-3}\) could be even higher if the secondary ionization will be allowed in our model. However, we do not expect any dramatic change in the results. Even if all carbon atom would be doubly ionized, cold electron density would increase only by 30%.

C. Two-stream instability

The electric fields presented in Figure 4.25 panel a) is smoothed over an interval of about 0.1 \(\mu m\). For the beam densities \(10^{18}\) and \(10^{19}\) cm\(^{-3}\), the non-averaged fields are similar but more noisy. For the beam density \(10^{20}\) cm\(^{-3}\), the average field is accompanied by a regular oscillations demonstrated in Figure 4.26. Their wavelength is about 70 nm and their amplitude is comparable with the electric field in the ionization front. This oscillating field is due to the two-stream instability which is the only instability that might be excited in one spatial dimension. This instability is related to excitation of the plasma waves in the body of electron beam. The time of the beam propagation is rather short and only very fast growing instability can be excited. In this situation, the beam energy spreading and the electron thermal motion...
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

in plasma can be neglected and the dispersion relation for the two-stream instability follows from the continuity equations for both electron species, their equations of motion and from the Poisson equation as

\[ 1 - \frac{\omega_b^2}{\gamma_b^4(\omega - kv_b)^2} - \frac{\omega_p^2}{\omega(\omega + iv_{ei})} = 0, \]  

(4.21)

where \( \omega_{b,p}^2 = e^2 n_{b,e}/\epsilon_0 m_e \) are the plasma frequencies of the beam and the cold electrons. An unstable solution can be found near the plasma resonance with the beam mode, \( \omega \simeq \omega_p \simeq kv_b \), where the phase velocity of electron plasma waves is approximately the velocity of the beam. The frequency of the oscillating field calculated from the simulation data is about 18.5 fs\(^{-1} \). It is in a reasonable agreement with the electron plasma frequency that is about 18 fs\(^{-1} \). In the absence of electron collisions the maximum growth rate for the two-stream instability is well known (e.g. [216])

\[ \text{Im} \omega_{max} = \frac{3}{\gamma_b} \left( \frac{\omega_b^2 \omega_p}{16} \right)^{1/3}. \]  

(4.22)

The maximum growth rate of two-stream instability increases with plasma density and in the case of the beam density \( 10^{20} \text{ cm}^{-3} \), it can be as high as \( \text{Im} \omega_{max} \sim 1 \text{ fs}^{-1} \). It is comparable to the collisional frequency of cold electrons which is also of the order of fs\(^{-1} \). The electron collisions have to be accounted for if \( v_{ei} > \text{Im} \omega_{max} \). They decrease the growth rate but do not suppress the instability. For the lower beam densities \( 10^{19} \text{ and } 10^{18} \text{ cm}^{-3} \), the two-stream instability is not observed. The growth rates are 3.3 and 10 times smaller, respectively, in these two cases and the instability has not enough time to develop due to the short beam length.

The formula for the instability growth rate is valid if the beam velocity spread is sufficiently small, \( \text{Im} \omega_{max}/\omega_p \lesssim \Delta v/v_b \). In the opposite case the instability develops in the kinetic regime and the growth rate is much smaller. The two-stream instability growth rate decreases in our simulation in later times because of beam energy losses and larger velocity spread of the beam. Nevertheless, this instability might produce a significant energy dissipation of the beam if its
length is large and the instability has enough time to grow.

D. Heating of thermal electrons

The average drift velocity of cold plasma electrons streaming against the beam and their average kinetic energy are presented in Figure 4.27. In the region behind the electron beam, where the average velocity is zero, the average energy corresponds to the temperature of plasma. The drift velocity attains its maximum in or slightly behind the ionization front and then it gradually decreases to zero. There is only a small difference in the return current drift velocity for the different beam densities. The higher current needed to neutralize the beam with higher density is therefore associated with higher cold electron density.

The average cold electron energy also attains its maximum in the ionization front but we recall that the number of cold electrons is strongly increasing behind this point due to collisional ionization. Then the kinetic energy of electrons decreases below the ionization potential and it remains at this level throughout the beam. The case of the beam density $10^{20} \text{ cm}^{-3}$ is an exception. Here additional heating at the end and behind the beam is due to the two-stream instability.

The energy distributions of cold electrons are demonstrated in Figure 4.28 in more details for the lowest and the highest density beam in the simulation time 74 fs. The case of the beam

![Figure 4.27: Average cold electron drift velocity in the direction opposite to the beam propagation (panel a) and the average cold electron energy (panel b) at the time 74 fs. The beam is propagating from left, the plastic part of the target begins at 8 $\mu$m, and the end of the beam is at about 16 $\mu$m.](image-url)
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

Figure 4.28: Energy distributions of cold electrons generated by the field and the collisional ionization in a plastic target at the simulation time 74 fs for the beam densities $10^{18}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$. The plots are normalized to the maximum values.

Density $10^{19}$ cm$^{-3}$ is very similar to the case of the beam density $10^{18}$ cm$^{-3}$. The tail of the beam is at the spatial position of about 16 µm and the distribution of cold electrons behind the beam is almost Maxwellian for the beam densities $10^{18}$ and $10^{19}$ cm$^{-3}$. It is established due to elastic and ionizing collisions. For the beam density $10^{20}$ cm$^{-3}$, the distribution function demonstrates a high energy tail related to acceleration of plasma electrons in the electric field generated by the two-stream instability.

Temporal evolution of the beam and plasma parameters

The simulation results presented above at the time of 74 fs demonstrate general characteristics of the beam propagation. The temporal evolution of the average beam and plasma parameters is shown in Figure 4.29. The simulation results, solid lines with markers, are compared with the results of the analytical model, dashed lines. The analytical model is stationary and therefore parameters of the beam are constant. Although the qualitative behavior is similar, there are some evident quantitative differences between the two models.

The analytical approach assumes a stationary situation where the beam has already evolved so that only the fastest electrons can penetrate the peak field. Moreover, hot electrons that lose their kinetic energy in the ionization front are always replaced by new fresh ones. In the simulation, there are electrons from the whole range of velocities at the head of the beam initially. The fastest ones propagate in front of the field and do not lose almost any energy. The spatial profile of the beam density is smoothed, linearly increasing from zero to the maximum
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

density on the distance of 1 µm, at the beginning of the simulation. Also, in the simulation, the source of fastest electrons in the beam is not infinite and the energy losses play an important role on the longer time scales as will be seen later.

A. Temporal evolution of the average characteristics

The maximum electric field in the ionization front, Figure 4.29 panel a), increases with the beam density and in the simulation, it remains almost constant during the whole time. It agrees rather well with the predictions of the analytical model. The thickness of the ionization front presented in panel b) is measured from the absolute head of the beam to the point where electric field attains its maximum. The initial front thickness in simulations with the beam densities $10^{19}$ and $10^{20}$ cm$^{-3}$ agree well with the analytical approach. For the beam density $10^{18}$ cm$^{-3}$, the analytical model overestimates the thickness two times because it neglects collisional ionization which contributes already in the ionization front. It is observed that the thickness of the ionization front increases with time. This is due to precursor electrons that propagate at the beam head in front of the electric field. These electrons approximately keep their initial velocity during the whole simulation. Their initial velocity is close to 0.9 of the speed of light and they are faster than the ionization front. The maximum electric field, i.e. the ionization front, propagates on the other hand with lower velocity and therefore the thickness of the ionization front increases with time.

In the simulation, the velocity of ionization front, Figure 4.29 panel c), is calculated from the positions of the maxima of the electric field in two different times. For the two higher beam densities, the field peaks are very narrow and therefore front velocity is calculated with enough precision using this approach. For the lowest beam density however the region around the electric field maximum is significantly wider and therefore the velocity is calculated with less precision and there is an error of approximately $2 \times 10^6$ m/s. Another possible approach is to calculate the average front velocity from the widening of the ionization front. As stated previously, the ionization front widens due to the difference in the velocity of the precursor electrons (0.9 velocity of light) and the peak field (front velocity). Using this approach, the average front velocity in the time interval between 20 fs and 160 fs is $2.2 \times 10^8$ m/s, $2.36 \times 10^8$ m/s and $2.43 \times 10^8$ m/s for the beam densities $10^{18}$ cm$^{-3}$, $10^{19}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$, respectively.

The initial values of the ionization front velocity in simulations are in reasonable agreement with the ones calculated analytically. With time however front velocity in our simulations decreases and the beam propagation becomes slower. The decrease in the ionization front velocity is associated with the decreasing number of the fastest electrons in the beam and hence with the dissipation of the beam energy. Temporal evolution of the velocity distribution of beam electrons is demonstrated in Figure 4.30.
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

(a) Maximum electric field

(b) Ionization front thickness

(c) Ionization front velocity

Figure 4.29: Temporal evolution of the peak electric field induced by the beams propagating inside the plastic target (panel a), the thickness (panel b), and the velocity (panel c) of the ionization front. The ionization front thickness is measured from the position of the beginning of the beam to the position of the field maximum. The front velocity is calculated from the positions of the field maxima in two adjacent times. Solid lines with markers represent numerical results, dashed lines with the corresponding markers represent the values given by the analytical model.

B. Beam velocity distribution

The strongest temporal evolution of the beam velocity distribution is observed for the beam density $10^{18}$ cm$^{-3}$, Figure 4.30 panel a). As in the beginning of the simulation, electrons from the whole range of velocities, i.e. from 0.7 to 0.9 velocity of light, are at the head of the beam in the ionization front, these electrons are losing energy almost equally. Later in time,
propagation of hot electrons inside the target

(a) Beam density $10^{18}$ cm$^{-3}$

(b) Beam density $10^{20}$ cm$^{-3}$

Figure 4.30: Temporal evolution of the beam velocity distribution for the beam densities $10^{18}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$. The distribution is initially uniform and all electrons are equally decelerated. Further in time, only faster electrons are at the head of the beam where the electric field is higher and they are decelerated more strongly.

however, preferentially the fastest electrons are slowed down, as they are mostly the ones, which propagate faster than the ionization front and therefore they can get into the regions where the field is the highest. In the simulation time 160 fs, the precursor electrons are also clearly seen. They are not stopped in the ionization front and they propagate freely in front of it.

Temporal evolution of the beam velocity distribution for the higher beam density $10^{20}$ cm$^{-3}$, panel b), exhibits similar features, however, changes in the distribution are much weaker. There are two reasons for this slower evolution. First, when integrating the electric field in the ionization front for different beam densities, it is found that the lower the beam density, the higher the electric field potential. The second reason is that the higher the front velocity, the shorter the time needed for electron to cross the front. Both these factors together result in the energy losses that are more significant when the density of the beam is lower. Therefore, comparing the distributions in Figure 4.30 in panels a) and b), not only the numbers of decelerated electrons but also the velocities of the slowest electrons are different.

C. Beam current evolution and the current neutralization

Temporal evolution of the beam current density is demonstrated in Figure 4.31. In simulation time 80 fs, the return current is also shown. Current neutralization is quite good except of the
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

smallest beam density and the front region. Temporal evolution of the beam current density is due to two effects, the ballistic evolution and the electric fields. At the head of the beam in the ionization front, hot electrons are decelerated below the average velocity of the beam and they are caught up by the rest of the beam, increasing the beam density behind the ionization front. As the deceleration of the beam electrons is the strongest for the lowest beam density $10^{18}$ cm$^{-3}$, the beam current density behind the ionization front is increased in this case by almost 40%. In later time, however, the ballistic spreading predominates and current density decreases inside the whole volume of the beam.

In Figure 4.31 panel a), the precursor electrons in the simulation time 160 fs are clearly distinguishable. The electric field induced by these electrons is independent of the beam density and its value in this time is about 9 kV/µm. The average separation of precursor electrons from the region, where quasi-neutrality is restored, is approximately half the difference between the initial thickness of the ionization front and the thickness in the time 160 fs. This is about 3.6 µm for the beam density $10^{18}$ cm$^{-3}$. Substituting this distance and the electric field stated above into the Poisson equation one can estimate the average density of the precursor electrons. For the beam density $10^{18}$ cm$^{-3}$, it is about 14% of the initial beam density, while for the beam densities $10^{19}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$, it is only 2.1% and 0.2%, respectively. Therefore, the current of precursor electrons is limited by the value of $\sim 1$ GA/cm$^2$. 

Figure 4.31: Temporal evolution of the beam current density for the beam densities $10^{18}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$. The return current is also shown at the time 80 fs to demonstrate the current neutralization. The beam electrons that are slowed down in the peak field in the ionization front appear inside the beam and increase its current density. Precursor electrons are seen for the beam density $10^{18}$ cm$^{-3}$.
D. Energy dissipation

The distribution of beam electrons in the phase space is demonstrated in Figure 4.32 in the simulation time 160 fs for all three beam densities. The figure in each panel covers the same area and the color represents the same number of simulation electrons in all four panels. The horizontal line in panels b), c), and d) represents the actual front velocity, while the vertical line denotes the position of the peak electric field in the ionization front. In panel a) the initial beam distribution is plotted for comparison. The whole beam is in aluminum layer and its

![Figure 4.32: Distribution of the beam electrons in the phase space in the initial time (panel a) and in the time 148 fs for the beam densities $10^{18}$ cm$^{-3}$, $10^{19}$ cm$^{-3}$ and $10^{20}$ cm$^{-3}$. Colors represent the normalized number of beam electrons and the figure in each panel covers equal area.](image-url)
distribution is uniform with only slightly smoothed borders in this panel. In the time 160 fs, the rhomboid-like shape of the distribution is due to the ballistic evolution. Hot electrons with velocity higher than the front velocity penetrate into the ionization front and are slowed down by the electric field. They leave the front and are caught up by the beam again. They accumulate behind the ionization front and form the peak which is seen in the current density plots in Figure 4.31. In all three panels, the precursor electrons are clearly seen.

The lowest beam density, $10^{18} \text{ cm}^{-3}$, corresponds to the highest energy dissipation. In the time 160 fs, there are no more electrons with the velocity 0.9 velocity of light in this distribution and therefore the velocity of the ionization front is already relatively low. On the other hand as the velocity of the ionization front is the lowest in this case during the whole simulation, the fastest electron get into the ionization front from the beam earlier, they propagate with the front for a longer time, and their energy losses are the highest. For the highest beam density, $10^{20} \text{ cm}^{-3}$, the tail of the beam distribution is also significantly disturbed. This is the result of the two-stream instability.

In Figure 4.33, energy losses of the beams with different densities are demonstrated against the propagation distance measured at the position of the ionization front. The beam with the density $10^{18} \text{ cm}^{-3}$ loses about 50% of its total energy on the distance of about 40 $\mu$m. This explains why the velocity of the ionization front of this beam decreases significantly. The energy lost by the beam is transferred into the kinetic energy of cold electrons and as long as there are enough neutral atoms in the target, this energy is used for additional ionization.

As the electric field behind the ionization front is approximately the same for all three beam densities, see Figure 4.25 panel a), (except for the highest beam density where the two-stream instability is excited), the field inside the ionization front is responsible for different energy losses. From the energy losses of the beam in Figure 4.33, we can calculate the average stopping power acting on a beam electron. It is about 4.9, 3.6 and 2.4 keV/$\mu$m for the beam densities going up from $10^{18}$ to $10^{20} \text{ cm}^{-3}$.
4.2. PROPAGATION OF HOT ELECTRONS INSIDE THE TARGET

$10^{20} \text{ cm}^{-3}$. This is more than ten times higher than the classical stopping power of a single electron due to binary collisions, which is less than 0.3 keV/µm for 0.5 MeV electron in polyethylene. It is a clear manifestation of the collective effects in high-current density electron beam propagation in dielectric target.

**Scaling of beam propagation characteristics**

The velocity distribution of beam electrons chosen here allows one to see the various physical processes clearly. However, it is not as relativistic as the ones obtained in recent high intensity laser target interaction experiments. The energy flux corresponding to the highest density beam is only about $10^{17}$ W/cm$^2$ here. The calculations with more energetic uniform beam velocity distributions (with velocities between 0.9 and 0.99 velocity of light) confirm that the physical processes are similar as the ones described above. Only the velocity of the ionization front is higher and energy losses of the beam do not significantly influence its propagation on the temporal scales which we are able to simulate.

Finally, we want to point out that our simulations are currently limited to the range of the beam current densities $4 - 400$ GA/cm$^2$ used here. The lower or higher beam densities can be only accessed by the analytical model at this moment. In particular, for higher densities one or two more electrons per atom will be liberated due the collisional ionization by the return current. Because of increase in the ionization potential, the cold electron temperature will increase, which will lower their collisionality. On the other hand, as additional ionization will be more difficult, electric field behind the ionization front may be higher and this may increase energy losses of the beam. Finally the two-stream instability (as well as other multi-dimensional instabilities) will be excited more strongly increasing the stopping power even more. For the lower electron beam current densities, electric field ionization will not provide sufficient number of cold electrons for the return current and the stopping of the beam by the electric field will be very strong.

4.2.5 Summary and conclusions about hot electron beam propagation

Our numerical model of hot electron beam propagation in dielectric target takes into account the processes of electric field ionization in the head of electron beam and the subsequent collisional ionization of the insulator by secondary electrons. The processes of current and charge neutralization take place in the ionization front and the thickness of the front is adjusted self-consistently. Heating of the plasma electrons by the return current is identified as a major source of the secondary ionization and the beam energy losses. Simulations show that the self-consistent electric field in the head of the beam plays an important role in hot electron transport, defining the average beam propagation velocity and providing the initial population
of plasma electrons. Its amplitude is saturated at the level of about 10% of the atomic electric field and it never provides complete ionization. The density of plasma electrons created in the ionization front is typically 100 times the density of the beam. Collisional ionization takes place mainly in the beam body where the electric field is strongly reduced.

The average velocity of hot electron beam is an increasing function of the beam current density for the currents larger than a few tens of $\text{GA/cm}^2$. Such dependence may cause filamentation instability in the ionization front predicted in [226] and already observed in the experiment [225]. This two-dimensional effect is not described within our one-dimensional model. Nevertheless, our model demonstrated an important effect of excitation of a large-amplitude plasma wave due to the two-stream beam-plasma instability. It is excited in the case of current densities $\sim 400 \text{ GA/cm}^2$ and it enhances the beam dissipation rate and leads to acceleration of plasma electrons to keV energies.

The simulations demonstrate a complicated electron beam dynamics related to the ionization process in the beam head. The fastest electrons, which are moving with the velocities higher than the ionization front, are entering the front and loosing a significant part of their energy to support the strong electrostatic field and the ionization process. Therefore, efficient beam propagation is maintained as long as the electron beam can supply enough energetic electrons. For an electron beam of a finite length the propagation would be strongly inhibited at the moment when all energetic electrons will cross the front. This effect can be used to control the propagation length and the deposition rate of high current electron beams.

Finally, a significant electron heating takes place in the beam tail behind the ionization front. The level of electron plasma temperature is controlled by the collisional ionization and it is kept below the ionization potential as long as the ionization is not completed. This process could play an important role also in metallic target providing an increased ionization level for higher beam currents.

### 4.3 Acceleration of ions from the rear surface of thin foil target

As we have demonstrated in the preceding section, propagation of laser accelerated high current hot electron beam is not significantly inhibited by either self induced fields or collisions on a distance shorter than a few tens of $\mu\text{m}$ in a solid target even if it is dielectric. Thus the hot electron beam may penetrate almost freely through a thin foil and the vast majority of hot electrons arrive to the rear surface of the foil wherefrom they are emitted into vacuum. As a consequence, strong electric field builds up between the negatively charged hot electron cloud in the vacuum and the positively charged target. We will show that this field is of much higher amplitude than the field formed during hot electron beam propagation in a dielectric. Duration of the field is also considerably longer and therefore this field accelerates ions very efficiently.
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

4.3.1 Target Normal Sheath Acceleration - theory and simple estimates

The process of ion acceleration from the rear surface of a laser irradiated thin foil target is called Target Normal Sheath Acceleration (TNSA) [77, 78, 79]. Actually, the situation is similar in some sense to the one described in the previous section. Hot electron beam is assumed collisionless and the dominant influence on its propagation is associated with self-induced fields again. The basic difference is that in this case there are neither free electrons nor any atoms that can be ionized in the vacuum behind the target. Therefore, both the space-charge and the current of the beam cannot be neutralized. Actually, the neutralization takes place but it is provided only by shifting target ions toward vacuum or by stopping hot electrons and accelerating them back to the target. Thus, the neutralization takes place on a much longer temporal scale.

At the head of the hot electron beam emitted from the target into vacuum electric field grows similarly like in the dielectric material studied in previous section. However, in vacuum the electric field growth is not terminated by the ionization process and therefore the amplitude of this field reaches the maximum value estimated in equation (4.16). For the highest beam density considered in the case of electron beam propagation (10^{20} cm^{-3}) and the hot electron energy used there, the electrostatic field behind the target can be as high as TV/m. The field can be even several times higher if the beam of hot electrons is more energetic or more dense.

Such a strong field stops even the multi-MeV electrons on a distance of several µm. Therefore, the bulk of hot electrons are trapped in the Coulomb potential in a thin layer behind the target where they are reflected back. Behind the target the beam of hot electrons constitutes an exponential sheath with the density described by the Boltzmann distribution

$$ n_b(x) = n_{b0} \exp \left( \frac{e\phi(x)}{T_h} \right) , $$

(4.23)

where $\phi$ is the electrostatic Coulomb potential and $T_h$ is the hot electron temperature. The Boltzmann distribution together with the Poisson equation constitute the bases of Debye-Hückel model which describes screening of macroscopic fields in plasmas. The spatial extent of the sheath of hot electrons is thus approximately given by the Debye length (3.2) of the hot electron cloud. This length is of order of micron for the beams whose propagation has been studied in the previous section.

Only hot electrons or accelerated ions may compensate the space-charge produced by the hot electron beam. The inertia of ions is much higher than that of hot electrons. Therefore, hot electrons respond to the field faster and tend to restore quasineutrality of the target first. In this simplified estimate let us assume for the moment that ions are stationary. Then the quasistatic electric field behind the target survives until hot electrons are returned back to the target. The excursion of majority of hot electrons in the sheath behind the target is very
short, of order of femtoseconds, and most of hot electrons propagate through the target with approximately the same velocity close to the velocity of light. Therefore, duration of the electric field behind the target should be approximately given by the duration of electron acceleration process which is approximately equal to the laser pulse duration. As long as acceleration of electrons persists in the laser target interaction region and new hot electrons are coming to the rear surface, quasineutrality is not restored. In a thin foil, hot electrons may circulate through the target being reflected from the field at the back of the target as well as from a similar field in the front of the target. This effect may even extend duration of the quasistatic electric field. On a longer time scale ion motion cannot be neglected and ions themselves contribute to the space-charge neutralization process. Nevertheless, it is still reasonable to expect that duration of the strong electric field behind the target is at least of the order of laser pulse duration.

In summary, the quasistatic electric field behind the target has amplitude of up to several TV/m, it extends from the target surface into vacuum to the distance of up to several microns and persists at least a few tens of femtoseconds. This field is strong enough to ionize atoms up to high charge states and accelerate the resulting ions to very high multi-MeV energies. For example, the field of 1 TV/m is the critical field \( (3.27) \) at which barrier suppression ionization produces \( \text{C}^{4+}, \text{O}^{6+}, \text{Al}^{6+}, \text{Ti}^{10+}, \text{Cu}^{10+}, \text{Ag}^{11+} \text{ or } \text{Au}^{13+} \) ions. However, these are only lower estimates as the electric field amplitude can be higher and tunneling ionization is efficient already well below the critical field.

For an ion of charge \( Z \) and mass \( m_i \) initially at rest, the time needed to cross the field (nonrelativistic velocity is assumed) is

\[
t = \sqrt{\frac{2\lambda_D m_i}{|e| Z E}},
\]

(4.24)

and the energy gained by an ion that crossed the field is

\[
E_{\text{ion}} = |e| Z E \lambda_D ,
\]

(4.25)

where \( \lambda_D \) is the Debye length of hot electrons. While this energy depends only on the ion charge the time needed to cross the field depends on the charge to mass ratio. If the charge to mass ratio of ion is high so that the time given by equation (4.24) is longer than the duration of the electric field the resulting ion energy will be lower which is mostly the case for higher \( Z \) atoms.

The highest charge to mass ratio of all ions have obviously protons and therefore they are most easily accelerated. Even if the target material does not contain hydrogen atoms, a thin layer of contaminants which is usually rich on hydrogen settles down on the target surface in the evacuated target chamber \([81,82]\). For example, the contamination layer on a thin gold foil in the vacuum of \( 2.6 \times 10^{-5} \) mbar was about 1.2 nm thick and consisted of 27% of gold,
61% of hydrocarbons and 12% of water in [231]. Consequently, mostly protons are measured in experiments with laser irradiated thin foil targets if the contamination layer is not removed prior to the interaction using some special technique, e.g. [83].

4.3.2 Energy distribution of accelerated ions

In the most of experimental and theoretical works devoted to ion acceleration from the rear surface of laser irradiated foils much attention is paid to find the conditions for acceleration of ions to highest possible energy e.g. [232, 233]. However, energy distribution of accelerated ions is of at least the same importance from the application point of view [83]. For targets composed of a single species of atoms the standard theory of isothermal rarefaction followed by a free expansion [30, 81] predicts that ions should end up with broad energy distribution corresponding to exponential distribution in velocity. However, the target contains fraction of hydrogen atoms and possibly some other species as well in most experiments. Hydrogen atoms are either present in a thin contamination layer on the target surface (further called as 'heterogeneous' target) or they are uniformly distributed in the whole volume of the target, e.g. water droplet, mylar foil (further called as 'homogeneous' target). Therefore, the process of ion acceleration mostly involves multiple ion species where the 'heavy' ions serve to maintain the field in which the 'light' ions are accelerated. This offers some possibility to control the energy distribution of 'light' ions and particularly to produce quasi-monoenergetic 'light' ion beams.

In recent experiments, light ions with quasi-monoenergetic distributions have been emitted from various kinds of heterogeneous as well as homogeneous targets, e.g. palladium foil with ultrathin layer of graphitic carbon on the rear side [83], titanium foil with PMMA microdots [234] or normal and heavy water droplets [235]. Our work is particularly focused on explanation of the quasi-monoenergetic behavior of the distribution of protons and deuterons in experiments with water droplets [235] but the same explanation can be applied to heterogeneous targets with thin surface layer of 'light' ions. Most of the theory and simulations explaining the quasi-monoenergetic feature of the distribution of 'light' ions have been done by Dr. Brantov and Prof. Tikhonchuk from the University of Bordeaux. Our PIC code is very expensive on computational time in the case of these simulations. Nevertheless, we were able to perform several calculations which confirmed that the less expensive simulation model used by Dr. Brantov accounts for the charge distribution of ions produced by field ionization on the rear surface of the target correctly. Moreover, we have performed an additional run for a heterogeneous target which demonstrates that the theory explaining formation of quasi-monoenergetic distribution of 'light' ions is applicable for heterogeneous targets as well. In this section we briefly summarize the theory and discuss the results calculated with our PIC code. For the full details and the results of simulations of Dr. Brantov we point to our joint
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

4.3.3 Laser irradiated water droplet experiments

The simulations are particularly intended to study the situation of experiment with laser irradiated water droplets performed in Max-Born Institute in Berlin [235]. Therefore, experimental conditions and results are briefly described first. Ti:Sapphire laser delivering energy of about 750 mJ in a 40 fs long laser pulse was focused onto water or heavy water droplets with 20 µm in diameter. Intensity of the main laser pulse on target was estimated to about $10^{19}$ W/cm$^2$ and the level of ASE was suppressed to be about $10^{-8}$ of the main laser pulse intensity. Ions were recorded with Thomson parabola coupled with microchannel plates in the direction of laser propagation (0°) and at an angle 135°. In many shots, the distribution of protons or deuterons accelerated in the laser propagation direction exhibited a quasi-monoenergetic structure and the central energy of the peak in the distribution was higher for deuterons than for protons. Shot to shot fluctuations in the distribution were associated with the laser pulse fluctuations and the inaccuracy of laser pointing to the target.

4.3.4 PIC model of TNSA

PIC simulations of TNSA are very complex, difficult, and time consuming. First of all, the simulation box must be very large so that ions and hot electrons have enough space for free propagation. The simulation box should be so large that only a small number of hot electrons can reach its boundary during the simulation time because neither reflecting nor absorbing boundary conditions describe the physical situation correctly. Therefore, the target is usually placed into a large volume of vacuum extending several tens of µm on both sides of the target in PIC simulation of TNSA.

Secondly, the simulation time should be several times longer than the laser pulse. The laser pulse must first propagate through the vacuum to the target which itself takes many time steps. Fortunately motion of particles can be neglected during this phase of simulation and therefore this part of simulation is not time consuming in one-dimensional case. Acceleration of electrons usually persists during the whole laser pulse and eventually some time after. Many electrons are accelerated into vacuum from the target front surface. Subsequently, they are reflected by the quasistatic field which forms in front of the target. However, their propagation in vacuum and reflection takes some time as well. Then hot electrons must fly through the target and create the field accelerating ions on the rear side. This does not take too much time for relativistic electrons. Nevertheless, there are many moderately relativistic electrons which arrive to the target rear side later. They determine the acceleration process in its later stage. Finally, it takes quite a long time to set ions in motion including some shorter time necessary
to ionize them. The distribution of accelerated ions strongly evolves and the simulation should not be stopped until some kind of quasisteady state in the distribution of ions separated from the target is reached. For these reasons, the simulation time in our PIC simulations of TNSA is about ten times longer than the laser pulse duration.

Thirdly, the whole target is present in the simulation box, not just the laser target interaction region like in the simulations of electron acceleration. The foil stroked by the laser pulse is of solid density which means that the density of ions is more than order of magnitude higher than the critical density for Ti:Sapphire laser pulse. The density of free electrons in the target can be more than two orders of magnitude higher than the critical density. It is necessary to have almost 2000 cells per \( \mu \text{m} \) even if electron temperature is set to a relatively high value of order keV, as the size of computational cell should be of order of the electron Debye length given by (3.2). The timestep is inversely proportional to the cell size \( \Delta t \approx \lambda_D/c \) and hence it is of order of attoseconds.

Finally, it is necessary to have sufficient resolution of the electron distribution function in the vicinity of critical surface to describe laser absorption process correctly. This implies that at least a couple of electrons per cell are needed around the critical surface. Than in the solid part of the target there are hundreds of electrons per simulation cell if all electrons are assigned the same numerical weight, which is the case of our simulations here. Last but not least, new electrons are injected into the simulation box when ionization is taken into account and the number of particles per cell strongly increases during the simulation.

This imposes huge demands on the computational performance and the simulation time. Our PIC simulations of TNSA last even several weeks on a single yet powerful CPU. For this reason, we have to simplify our computational model as much as possible. All kind of collisional processes are neglected in our TNSA calculations assuming that they are not of prime importance in the current context. The foil target is always very thin. It is only about 2 \( \mu \text{m} \) thick excluding the exponential plasma density ramp on the front surface. The laser pulse is very short in all our simulations (not more than 40 fs). Initial electron temperature of 2 keV is used to lower the number of simulation cells.

At this place, let us point out to the weak point which is often left out when one-dimensional PIC simulations of TNSA are discussed. As noted in the preceding section, transport of hot electrons produces very strong magnetic field if the current of the beam is not neutralized. In one dimension the current is always neutralized once the space-charge is neutralized. Now, let us assume that the electrostatic field in the sheath behind the target is essentially one-dimensional. This is supported by relatively good divergence of beam of accelerated ions observed in experiments, see e.g. [236]. Then every hot electron reflected in the sheath behind the target, which has nonzero component of the velocity along the target surface, will not return to the same place on the target surface, from which it was emitted. This may imply
that the current will not be exactly neutralized leading to strong magnetic field in later time. Such field may eventually deflect hot electrons in the later stage of TNSA. In future we will try to carry out some two-dimensional simulations to make sure whether this is a real problem. Nevertheless, one-dimensional simulations are still able to give new interesting information about the TNSA process as one can see below.

### 4.3.5 Results and discussions of PIC simulations of TNSA

**Influence of electric field ionization**

Firstly, the question of the importance of electric field ionization in TNSA will be addressed here. The simulations are performed with an ad hoc designed foil target which consists of aluminum and hydrogen. Both elements are homogeneously distributed in the whole volume of the target. The foil is 2 µm thick excluding the exponential ramp on the front surface. The density scale length of the exponential part of the density profile is equal to laser wavelength. The density of aluminum atoms is set to \(6 \times 10^{22} \text{ cm}^{-3}\) approximately corresponding to the density of solid state. The density of hydrogen is 6 times lower. In the front and at the back of the foil there are 15 and 25 µm of vacuum respectively. The initial ion charge of aluminum is set to 3 while hydrogen atoms are completely ionized already at the beginning. Initial electron temperature is 2 keV and the temperature of ions is 10 times lower.

The laser pulse used in this simulation is just 16 fs long with a box-like temporal profile (rising to the maximum respectively decreasing to zero in just 1/10 of the period). The maximum intensity is \(10^{20} \text{ W/cm}^2\) and the laser wave with the wavelength 800 nm is linearly polarized and normally incident on the target surface. For convenience we plot in Figure 4.34

![Figure 4.34: PIC simulation box shortly before the laser target interaction. The laser pulse with peak intensity \(10^{20} \text{ W/cm}^2\) has a box-like temporal profile and it is 16 fs long. Linearly polarized laser wave with wavelength 800 nm is normally incident on the target. The target consists of solid density aluminum with 16% of uniformly distributed protons and it is surrounded by a large volume of vacuum from both sides (behind the target vacuum is not shown).](image-url)
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

(a) Constant Al ion charge 3

(b) Variable ionization

Figure 4.35: Quasistatic electric field and electron and ion densities in PIC simulations of ion acceleration from the rear side of thin foil target. The simulation time is 260 fs after the laser target interaction. For simulation parameters and setup see Figure 4.34. The results calculated with constant ionization (Al charge 3) are plotted in panel a). Al ion charge may vary due to electric field ionization in the simulation presented in panel b).

the snapshot of a part of the simulation box taken shortly before the laser target interaction.

Absorption of the laser pulse, acceleration of electrons, and their transport through the target are of course very important in the scope of ion acceleration from the rear surface of a thin foil target. However, in this part we only care about the processes taking place on the target rear side. Therefore, we do not study where do the hot electrons come from, how did they gain their energy, or how did they get to the target rear side. It is sufficient to know that amplitude of the electrostatic field created behind the target is almost the same throughout the simulations with either constant or variable ionization. This indicates that the process of ionization does not significantly influence acceleration of electrons which is in agreement with the results presented in Section 4.1.2. We remind that the foil is very thin so that the energy of the beam of hot electrons is not significantly dissipated during its transport through the target.

In Figure 4.35 we demonstrate the situation on the target rear side some time after the beam of laser accelerated hot electrons has arrived there. The simulation time is about 260 fs after the laser interaction with the target. In panel a) of Figure 4.35 the snapshot is taken from PIC simulation with constant ion charge of aluminum ions (Al$^{3+}$). The snapshot in panel b) is taken from simulation where aluminum ion charge may vary due to electric field ionization.

In the simulation with constant ionization, acceleration of protons from the target rear side
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

is continuous and relatively more efficient. Aluminum ions have charge 3 and consequently their charge to mass ration is about 9 times lower than that of protons. That is why aluminum ions are accelerated much more slowly. The fastest protons are at the head of the proton bunch which gradually tends to separate from the exponential plasma density profile formed on the target surface. Most hot electrons are already stopped and reflected back by the strong electric field in the sheath behind the target in this time. Only the most energetic electrons are able to penetrate the sheath and get to the head of the proton bunch. The charge and current of hot electrons is partially neutralized by the proton bunch. Consequently, the field inside the proton beam is of lower amplitude and locally it even drops down to zero or changes its sign. However, this cannot be seen in the figure because of the logarithmic scale.

The situation in the case of variable ionization is significantly different. The density of free electrons and the average ion charge increase in the whole volume of the target very significantly in consequence of electric field ionization. Al$^{11+}$ is the dominant charge state in the exponential plasma density profile on the target rear side. This corresponds to aluminum ions with bound electrons only in the innermost 1s shell. The critical field for barrier suppression ionization of aluminum ions to charge state 11+ is about 3 TV/m according to (3.27) and therefore the presence of Al$^{11+}$ ions is not surprising.

More surprising is the presence of this charge state inside the solid part of the target although the dominant charge state in the most part is Al$^{10+}$. In both panels of Figure 4.35 a relatively noisy electric field with amplitude of the order of 0.1 TV/m is observed in the solid part of the target. Although we did not analyze this field in the scope of the present simulations, its tentative explanation presents itself readily from the preceding section of this work. Oscillating high amplitude electric field resulting from two-stream instability is observed there for the hot electron beam with high density. In the present simulation, the density of plasma is much higher as is probably also the density of the hot electron beam. Then the two-stream instability growth rate as well as the electric field

![Figure 4.36: Energy distributions of protons accelerated from the target rear surface into vacuum in the time 260 fs after the laser target interaction. The distributions are taken from PIC simulations with constant and variable ionization with the same parameters as in Figure 4.34. Only protons located behind the initial rear target surface (17.2 µm) are included.](image)
amplitude can be both very high. One must also take into account that the simulation time in Figure 4.35 is 260 fs after the laser target interaction so that the two-stream instability had enough time to grow and ionize the target.

The charge to mass ratio of Al$^{11+}$ ions is only 2.5 times lower than that of protons. Therefore, these ions are much more mobile in the strong electric field than Al$^{3+}$ ions in the case of constant ionization. Thus Al$^{11+}$ ions stay in a close touch with the bunch of accelerated protons for considerably longer time. It is observed that the bunch of fastest protons is confined in a relatively small volume in panel b) of Figure 4.35. Most of these protons were accelerated in the early stage before the ionization of aluminum ions reached its maximum value and Al$^{11+}$ ions were set in motion. It is also readily seen that the number of accelerated protons is lower than in the case of constant ionization while the number of accelerated aluminum ions is significantly higher. The density of aluminum is 6 times higher than the density of protons and as the charge to mass ratio is not very different for the case of Al$^{11+}$ ions, their acceleration consumes a serious part of energy of the electrostatic field.

Energy distribution of protons accelerated from the target rear side in simulations with constant and variable ionization are compared in Figure 4.36 in the same simulation time 260 fs after the laser target interaction. As one can see in Figure 4.35, amplitude of the electric field is about 1 TV/m in this time which is much lower than in the early stage of ion acceleration. Even though ion acceleration still persists, the energy distribution of ions does not change significantly from this time on. We include only the protons located behind the spatial coordinate 17.2 $\mu$m (see Figure 4.35), i.e. only those behind the former target surface, in the energy distribution presented here.

The distribution of protons is exponential in the low energy part in both cases and a significant quasi-monoenergetic peak is observed. The appearance of the peak in the energy distribution of protons will be explained later. At this place we only want to demonstrate

\[ \text{Energy distribution of protons accelerated} \]
\[ \text{from the target rear side in simulations with} \]
\[ \text{constant and variable ionization are compared} \]
\[ \text{in Figure 4.36 in the same simulation time 260} \]
\[ \text{fs after the laser target interaction. As one can see in Figure 4.35, amplitude of the} \]
\[ \text{electric field is about 1 TV/m in this time which is much lower than in the early stage of ion} \]
\[ \text{acceleration. Even though ion acceleration still persists, the energy distribution of ions does not} \]
\[ \text{change significantly from this time on. We include only the protons located behind the spatial} \]
\[ \text{coordinate 17.2 $\mu$m (see Figure 4.35), i.e. only those behind the former target surface, in the} \]
\[ \text{energy distribution presented here.} \]

\[ \text{The distribution of protons is exponential in the low energy part in both cases and a} \]
\[ \text{significant quasi-monoenergetic peak is observed. The appearance of the peak in the energy} \]
\[ \text{distribution of protons will be explained later. At this place we only want to demonstrate} \]
that electric field ionization has a profound effect on the target normal sheath acceleration of protons from homogeneous targets. Let us also point out that the quasi-monoenergetic peak at about 5 MeV in the case of simulation with constant ionization is due to protons which are located in the low field region between the spatial coordinates 21 and 24 µm in Figure 4.35. The quasi-monoenergetic peak in the case of variable ionization is obviously due to the proton bunch which is already separated from the target at the spatial position of about 26 µm.

As the process of proton acceleration is tightly connected with the presence of Al$^{+11}$ we have performed an additional shorter simulation run with constant ionization but with the initial ion charge of aluminum set to 11. The snapshot from this simulation is compared with the snapshot from the simulation with variable ionization in Figure 4.37. It is observed that the difference in proton acceleration is only small, much smaller than in the case of constant ionization and lower charge state of aluminum ions. It is possible to conclude that the process of proton acceleration from the target rear side can be approximately described using simulation with constant ionization if the ‘heavy’ ions near the target surface are assigned the proper value of charge.

**Quasi-monoenergetic spectrum of ‘light’ ions - water droplet targets**

The simulations of proton and deuteron acceleration from laser irradiated water and heavy water droplets have been performed according to the experiment [235] mentioned earlier. Water droplets are in situ prepared targets and therefore they are free of any surface contamination layer. However, they are homogeneous targets with higher density of light ions. Though, small water droplets are not one-dimensional targets by nature, let us approximate them by water foils in our simulations keeping in mind that this is a serious limitation of our approach. Nevertheless, the mechanism of quasi-monoenergetic peak formation in the distribution of light ions (protons or deuterons) demonstrated here is quite general.

We use the following parameters in these PIC simulations. The laser wave of wavelength 800 nm is again linearly polarized and normally incident. The peak intensity is $10^{19}$ W/cm$^2$ and the pulse is 40 fs long. The temporal shape of the laser pulse envelope is $\sin^2$. The target is 2 µm thick foil with exponential density ramp on the front side. The scale length of this ramp is equal to laser wavelength. The target consists of oxygen ions and protons or deuterons with the density of both elements approximately corresponding to density of corresponding atoms in water, i.e. $3 \times 10^{22}$ cm$^{-3}$ for oxygen ions and twice higher for protons or deuterons. Hydrogen atoms are again completely ionized from the beginning of the simulation while the initial charge state of oxygen is set to 2. The water foil is surrounded by a large volume of vacuum on both sides, about 10 µm on the front side and about 40 µm on the rear side. Initial electron temperature is set to 2 keV and the temperature of ions is 200 eV. PIC simulations are performed with variable ionization.
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

Figure 4.38: Snapshots of the rear surface of water targets taken from PIC simulation with variable ionization. The laser pulse is linearly polarized, 40 fs long and normally incident on the target. It has the wavelength of 800 nm and the peak intensity of $10^{19}$ W/cm$^2$. The target initially consists of O$^{2+}$ ions of the density of $3 \times 10^{22}$ cm$^{-3}$ and protons of the twice higher density. Time is measured with respect to the end of the laser target interaction.

We present four snapshots of the target rear side taken at different times in PIC simulation with water droplet (foil) in Figure 4.38. In panel a), the snapshot is taken immediately after the laser target interaction, i.e. relatively soon after the beam of hot electrons arrived to the target rear surface. The amplitude of the electric field behind the target is about 2 TV/m in this time. The strong field penetrates only into a very thin skin layer of the target while it is screened by plasma electrons deeper. Oxygen atoms are significantly ionized up to the charge
state $O^{6+}$ in this skin layer. We remind that $O^{6+}$ ions have only about 2.5 times lower charge to mass ratio than protons. It is thus possible to expect that this charge state will play an important role in the proton acceleration process and it will shape the energy distribution of accelerated protons.

Let us postpone further discussion of snapshots presented in panels b), c) and d) to a later time and draw your attention to the phase space plots of accelerated ions. Our colleagues from Bordeaux have found that these plots contain a very interesting information. The phase space plots are presented in Figure 4.39 in the time instants corresponding to the snapshots in Figure 4.38. In panels a) and b), i.e. in the early stage of proton acceleration, the situation is not too interesting. One can only see how quickly the velocity of accelerated ions increases with the distance from the target surface which is located at about 13.3 $\mu$m.

The phase space in later times presented in panels c) and d) is interesting indeed. It is readily seen that protons in some part of the phase space have nearly the same velocity. These are the protons in the quasi-monoenergetic peak in the energy distribution. The other important thing is that the plateau of protons in the phase space is always only a small step in front of $O^{6+}$ ions.

At this moment, let us return to the snapshots presented in Figure 4.38, particularly to the one in panel c). In this snapshot, it is observed that the density of accelerated protons exhibits a significant peak just in front of the first oxygen ions. As the proton beam is relatively dense in the place where all protons have nearly the same velocity, the quasi-monoenergetic peak in the energy distribution should be indeed significant and it should contain a relatively high number of particles.

The same snapshot shows where these protons come from. The electrostatic field exhibits a shock-like structure near the head of the beam of oxygen ions. The field is relatively high inside the bunch of oxygen ions while it decreases by almost an order of magnitude at the head of the bunch. The protons traveling with the bunch of oxygen ions are thus pushed by this field ahead of the oxygen bunch. Similar situation can be seen also in the snapshots in panels b) and d) of Figure 4.38, yet it is not so apparent there.

In fact, the light ion acceleration process consists of several stages. This is demonstrated on the temporal evolution of the energy distribution of protons in Figure 4.40. Light ions are much more mobile than the heavy ones initially, and since all of them are crossing the steep plasma edge, they acquire approximately the same energy and form the first quasi-monoenergetic peak. This peak can be seen in panel a) of Figure 4.40 in the time 80 fs. The mechanism of formation of the first monoenergetic peak works better if the charge density of light ions is much lower than the charge density of heavy ions, i.e. for example in the case of aluminum target with some admixture of protons mentioned earlier.
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

Figure 4.39: Temporal evolution of the phase space of accelerated protons and oxygen ions. The phase space plots are taken from PIC simulation of laser interaction with water target with the same parameters as in Figure 4.38 and in the corresponding times. Velocity of ions is normalized to the velocity of light.

The first quasi-monoenergetic peak is however not stable in our simulations. There is no plateau of light ions in the phase space plot in this time. Therefore, the monoenergetic peak is relatively dense. Since the Debye length of hot electrons is relatively long in comparison with the dimensions of the monoenergetic bunch of light ions, these ions experience a strong Coulomb repulsion due to non-neutralized positive charge. Together with the persisting ion acceleration process the repulsion destroys the monoenergetic spectrum on a relatively short time scale (see Figure 4.40 panel a) in the time 160 fs).

Light ion acceleration process continues after the first layer is torn off the target. Different
motion of light and heavy ions results in a spatial separation of both species and in the formation of the electrostatic shock. This results in the plateau formation in the phase space of light ions and a new quasi-monoenergetic peak appears in the energy distribution of light ions as one can see in panel a) of Figure 4.40 in the time 240 fs.

However, this is not the final stage of the acceleration process. Electrons are still relatively hot and they do not screen the charge of the monoenergetic bunch of light ions completely. Nevertheless, light ions with the same energy are now distributed over a larger volume and the bunch is less dense. Their charge is consequently better neutralized than the charge of the first quasi-monoenergetic bunch and this bunch survives much longer time.

Due to Coulomb repulsion, the particles at the head of the bunch are accelerated forward while the particles at the back of the bunch are accelerated backward with respect to the bunch. This can be best seen in the phase space plot in Figure 4.39 panel d). This effect manifests itself in the double-energy spectrum shown in Figure 4.40 panel b). However, cooling of hot electrons already prevents further acceleration in this time and it suppresses significant Coulomb explosion of the bunch. Therefore, energy distribution of light ions does not evolve significantly after this time and the quasi-monoenergetic spectrum is preserved in the approximately same form.

The temporal evolution of energy distribution of deuterons plotted in Figure 4.41 is similar to the one plotted for protons in Figure 4.40. The parameters of PIC simulation are the same with the exception of the light ion mass which is two times higher here. In Figure 4.40
4.3. ACCELERATION OF IONS FROM THE REAR SURFACE OF THIN FOIL TARGET

(a) Early stage of deuteron acceleration  (b) Later stage of deuteron acceleration

**Figure 4.41:** Temporal evolution of the deuteron energy distribution taken from PIC simulation with the same parameters as in Figure 4.38. Only deuterons behind the initial target surface located at 13.3 µm are included.

and Figure 4.41 the same arbitrary units are used. Therefore, one can conclude that the number of accelerated deuterons is lower than the number of accelerated protons. However, it is interesting that the quasi-monoenergetic peak in the distribution of deuterons is shifted toward higher energy. In fact, the energy of monoenergetic deuterons is almost exactly two times the energy of protons. Consequently, both species of particles have nearly the same velocity. This is not surprising as the velocity of light monoenergetic ions is fully determined by the velocity of bunch of heavy ions which is the same in both cases.

Finally, we present the temporal evolution of proton energy distribution for the case of heterogeneous target in Figure 4.42. In this PIC simulation, 7 µm-thick aluminum foil is covered by a 100 nm low density \(3 \times 10^{21} \text{ cm}^{-3}\) layer of protons on the rear side. The target is irradiated by 50 fs laser pulse with the peak intensity \(4 \times 10^{19} \text{ W/cm}^2\). Here, the first monoenergetic peak of protons is created during first 150 fs. After this time, the peak is dispersed very quickly and the distribution of protons becomes almost homogeneous. However, the tail of the proton bunch is caught up by highly ionized aluminum ions in later time. The Coulomb repulsion between the light and heavy ions produces electric field which works as a piston. This creates the quasi-monoenergetic peak in the proton energy distribution again.

In summary, we have demonstrated that the electric field ionization on the target rear side has a profound effect on acceleration of light ions from the multiple-species targets. Nevertheless, PIC simulations with constant ionization can be utilized with sufficient accuracy if the proper charge is assigned to ions on the target rear side.
The process of formation of the quasi-monoenergetic peak in the energy distribution of light ions has been studied. Explanation of the mechanism leading to the peak formation has been found by Dr. Brantov and Prof. Tikhonchuk and confirmed also in our PIC simulations with variable ionization. Three distinct mechanisms of formation of quasi-monoenergetic distribution of light ions have been identified and described. Particularly, it has been demonstrated that fast heavy ions push forward the light ions and shape their energy distribution. Central energy of the peak in the distribution of light ions is thus fully determined by the heavy ions and their ionization state. The above described mechanism is efficient in the case of both homogeneous and heterogeneous targets and we believe that it is able to explain the quasi-monoenergetic spectrum of light ions observed in experiments [83, 234, 235].
5 SUMMARY AND CONCLUSIONS

At this point we return back to the introductory part of this work and remind what has been stated there. Generation and amplification of ultrashort laser pulses is just a few decades old topic. However, the progress made in this field of science since its beginning is enormous. Not only for this reason but alike due to potency in a wide range of new applications with possible impact to many other fields of science, generation of ultrashort laser pulses and the phenomena related to their interactions with matter are attracting attention of ever rising part of scientific community. No doubt that this field of science will stand behind the birth of new inventions in future and thus extend its consequences even into our everyday life.

A wide variety of nonlinear mutually interconnected processes is involved in the interaction of ultrashort laser pulses with matter. Experimental measurements generally provide only spatially, temporally and/or spectrally integrated diagnostics of the interaction and a detailed theoretical analysis is impossible without crude simplifications. Here, computer simulations offer a helping hand as they are able to resolve complex systems of equations describing the nonlinear physical processes involved in the interaction through the use of special techniques. Nevertheless, the temporal and spatial scale and resolution as well as the range of processes taken into account in the simulation are still strictly limited by the available computational performance.

In the presented thesis, numerical simulations based on the Particle-in-Cell method are applied to study interactions of ultrashort high intensity laser pulses with solid density targets and the phenomena closely related to this interaction. We attempt to stay in touch with the state of the art development in the field of short pulse high intensity lasers and address questions which are of prime importance in the context of contemporary short pulse laser solid target interaction experiments via computer simulations. For this reason, most of the simulations are performed in accordance with certain recent experiments. On the other hand, even though the presented results are calculated for a particular set of parameters the theory provided for explanation is mostly generalizable. Thus, when drawing the conclusions we endeavor to put them into the context of other experiments as well. Accordingly, we believe that our work does not only explicate the situation of these particular experiments but it can also be valuable for designing future experimental studies.

The thesis is organized in order to provide an introduction to the generation and amplification of ultrashort laser pulses and their interaction with matter, to review the theory relevant in this context, to give details about our simulation technique, and finally to present and discuss the most important results obtained. Generation and amplification of short laser pulses
and formation of the preplasma on the target surface are briefly described in the beginning of Chapter 2. This introduction is important to define the range of initial conditions of interactions studied further. Absorption processes of short high intensity laser pulses during the interaction with solid targets are reviewed next. Particular attention is paid to the description of processes resulting in acceleration of hot electrons as these electrons and the processes related to their acceleration and transport are the main subject of our work. At the end of Chapter 2 the most important applications associated with the population of hot electrons are mentioned.

Various theoretical approaches utilized to describe interaction of laser radiation with matter are introduced in the beginning of Chapter 3. Particle-in-Cell method is one of the most suitable models in the context of short pulse high intensity laser pulses. The code LPIC++ [12] based on this method and utilized throughout the rest of this work is described here with special punctuality. This Particle-in-Cell code has been enhanced by including additional physical processes relevant in the context of short pulse laser solid target interaction. Namely, electric field and collisional ionization have been implemented and the algorithm of elastic electron collisions has been revised. Theoretical description of these processes is therefore provided in details. As there are occasionally some discrepancies in the notation and mathematical formulation of these theories in recent publications we often return back to the works that laid the principles of the present-day theories on which our approach is based. We believe that both the theory as well as the implementation procedure are covered in sufficient details so that this part of work can also serve as a 'cookbook' for extension of other Particle-in-Cell simulation codes.

Our results are presented and discussed in Chapter 4. In the respective order we demonstrate the impact of variable plasma ionization on the energy and angular distributions of hot electrons in Section 4.1.1 and Section 4.1.2, the transport of a high-current hot electron beam in dielectric target in Section 4.2 and the acceleration of ions from the rear surface of laser irradiated thin foil targets in Section 4.3. Next, the most important conclusions drawn in the individual parts of Chapter 4 are briefly summarized.

In Section 4.1.1 it is found that the efficiency of resonant absorption and hot electron acceleration is significantly influenced by variable plasma ionization if the preplasma has a relatively long and slowly decreasing undercritical part of the density profile. Using additional simulation code based on hydrodynamic approach it is also demonstrated that such preplasma density profile is realistic and may be produced due to long lasting irradiation of the target surface with low intensity amplified spontaneous emission prepulse. Such prepulses are very frequent in current experiments with high intensity short laser pulses.

Simulations presented in Section 4.1.1 have been performed in accordance with experiments studying K-α emission from laser irradiated thin metallic foils [199]. These experiments have
been carried out by the team of Dr. Zhavoronkov in Max-Born Institute in Berlin. Our results are in reasonable agreement with both the experimentally measured K-α emission as well as the hot electron energy distribution deduced from the measurements of bremsstrahlung radiation, and we believe that our simulations successfully explain experimental observations. This part of work resulted in joint publications with Dr. Zhavoronkov [1,237] and several poster contributions at international conferences.

Impact of variable plasma ionization on the angular distribution of hot electrons has been studied in the Section 4.1.2. It has been demonstrated that electrons released from inner ionic shells around the peak of the laser pulse often appear significantly displaced from other free electrons in the momentum phase space. This may happen because the electric field of the laser wave is not harmonic in the undercritical plasma in front of the target due to reflection from the critical surface. Free electrons may have non-negligible momentum in the maxima of the individual laser cycles while at the same time electric field ionization efficiently injects new electrons with nearly zero energy into the interaction region.

Our theory demonstrates that the newborn electrons, which are significantly displaced in the momentum phase space from other free electrons, preserve some given momentum parallel to the target surface and upon acceleration by the laser field their angle of ejection from the interaction region is significantly different from the ejection angle of the initially free electrons. This effect applies particularly to relativistic laser pulses and it has been demonstrated that it strongly depends on the target material, laser wave polarization and angle of laser incidence. We find a significant effect of variable plasma ionization on the divergence of laser accelerated hot electron beam for particular target materials and laser irradiation conditions. Certain preliminary results of this work have been presented at the international conference (EPS 2006) and the entire work is being prepared for submission to an international journal.

Propagation of high-current hot electron beam in a cold dielectric target has been described in Section 4.2. Strong quasistatic electric field is induced at the beam’s head due to the noncompensated space-charge of the beam. This field ionizes the matter and produces a seed population of free electrons. Free electrons are then accelerated toward the beam and form the neutralizing return current. However, they also ionize the matter collisional which reduces the resistivity. The rest of the beam subsequently propagates similarly like in plasma.

Electric field is formed by the highest energy beam electrons at the head of the beam in the ionization front. It is found that this field predominantly influences propagation of the beam. It determines not only the beam propagation velocity and the distribution shape but it has also the dominant effect on the beam energy losses. High-current hot electron beam may propagates efficiently in cold dielectric target only until the highest energy electrons in the beam are depleted. For dense hot electron beams two-stream instability between the stream of hot electrons and the return current may arise behind the ionization front. This
instability is responsible for additional beam energy losses. Simulations of high-current hot
electron beam propagation in cold dielectric target have been performed in collaboration with
Prof. Tikhonchuk and PhD student Debayle from University of Bordeaux. Our colleagues from
Bordeaux have developed analytical theory covering hot electron beam propagation. Presented
numerical simulations are complementary with their theory and a good agreement between both
models is demonstrated. This work resulted in joint publication \cite{2} and has been presented at
several international conferences in both poster and oral forms.

Finally, acceleration of ions from the rear side of laser irradiated thin foil targets composed
of multiple species is presented in Section 4.3. We demonstrate that acceleration of light ions
is predominantly influenced by the ionization state of heavy ions, which may be very high
in the strong electrostatic field formed at the rear surface of the target. Particularly, the
highly ionized heavy ions are responsible for shaping the energy distribution of light ions and
formation of a quasi-monoenergetic peak. The process of quasi-monoenergetic peak formation
in the distribution of light ions works with similar efficiency in homogeneous targets, where
light ions are distributed in the target volume uniformly, and in heterogeneous targets, where
light ions are present only in a thin contamination layer on the target surface. This work
has been done in collaboration with Prof. Tikhonchuk and Dr. Brantov from the University
of Bordeaux. Our colleagues from Bordeaux have explained the formation process of the
quasi-monoenergetic distribution of light ions, which has been subsequently confirmed also in
our simulations. Our study is particularly intended to explain recent experiments with laser
irradiated water and heavy water droplets, however we believe that the same explanation can
be applied to other experiments as well. The work resulted in a joint publication \cite{3} with our
colleagues from Bordeaux and the experimental group from the Max Born Institute in Berlin.

I believe that the presented simulations bring new and interesting information about the
importance of ionization process in the short pulse laser solid target interactions. Hopefully, our
contribution in this field will be useful and it will find acceptance in the community of laser plasma
scientists. Hereafter, I would like to continue in the theoretical study of short pulse laser target
interactions and particularly in the study of the charged particle acceleration and transport.
I am convinced that this will be one of the leading trends in modern science and that the
range of applications of short high intensity laser pulses will increase with further development
of experimental techniques and devices as well as deeper theoretical understanding. I expect
a strong progress in the direction of multidimensional simulations and the so called hybrid
models in the area of numerical simulations of laser plasma interaction. Finally, I hope to
develop model of high-current hot electron beam transport in gas in the nearest future. This
topic is also interesting in the context of recent experiments related to the concept of Fast
Ignition of Inertial Confinement Fusion targets.
List of publications

Publications in peer reviewed journals


Poster presentations at international conferences


Oral presentations at international conferences

Summer schools and scientific missions


- December 2005 (3 months): Short term scientific mission in CELIA laboratory (Centre Lasers Intenses et Applications) at the University of Bordeaux, France. Collaboration with Prof. V. T. Tikhonchuk.
Bibliography


[130] H. R. Reiss, “Effect of an intense electromagnetic-field on a weakly bound system,” 


List of Figures

2.1 Schematic diagram of the CPA laser system .......................... 7
2.2 Typical temporal profile of the CPA laser pulse ....................... 9
2.3 Preplasma density profile, temperature and average ion charge .......... 12
2.4 Propagation and reflection of obliquely incident laser wave .............. 14
2.5 Free electron trajectory in the field of relativistic laser wave .......... 21
2.6 K-α emission from laser irradiated solid target ........................ 25
2.7 Target normal sheath acceleration of ions ............................. 27
2.8 Fast Ignition of ICF target ......................................... 29

3.1 PIC algorithm workflow ............................................. 34
3.2 Boost frame transformation used for oblique incidence ................. 37
3.3 Illustration of ATI, NSI and HHG .................................. 40
3.4 Ionization processes - MPI, tunneling and BSI ......................... 41
3.5 Comparison of tunneling ionization rates ............................. 47
3.6 Range of applicability of electric field ionization models ............... 49
3.7 Distant, close, and radiative collisions .............................. 53
3.8 Collisional ionization cross sections and frequencies for aluminum .... 57
3.9 Relativistic electron impact ionization cross section .................. 59
3.10 Mean square deflection due to elastic collisions ...................... 64
3.11 Temporal evolution of test particle distribution in the bath of field particles .. 65
3.12 Collision with charged particles within the Debye sphere ............ 66

4.1 Sectioning of results according to location where the processes under consideration take place .......................... 78
4.2 Preplasma density profile calculated by the code Ehybrid .......................... 83
4.3 Hot electron distributions calculated by PIC code ................................. 85
4.4 Electron density, electric field and mean ion charge during PIC simulation with ionization ................................................. 87
4.5 Electron phase space in PIC simulation with Ehybrid profile ................. 89
4.6 Time when hot electrons cross the rear boundary of the simulation box and hot electron energy distributions for various laser intensities .................. 91
4.7 K-α emission against target foil thickness ............................................. 92
4.8 Temporal and spatial profiles of K-α pulses ......................................... 93
4.9 Illustration of the laser target interaction geometry .............................. 96
4.10 Ejection angles of accelerated electrons ............................................. 97
4.11 Hot electron ejection angle in the case of normal laser pulse incidence ..... 99
4.12 Phase space of free electrons oscillating in the laser field ..................... 100
4.13 Demonstration of phase space when new electron is released .............. 102
4.14 Velocity and momentum phase space - titanium ............................... 103
4.15 Velocity and momentum phase space - aluminum .............................. 104
4.16 Velocity and momentum phase space - aluminum, circular polarization .... 105
4.17 Comparison of hot electron energy and angular distributions ............... 106
4.18 Newborn electron out of phase with free electrons - oblique incidence .... 108
4.19 Constant of electron motion and ejection angle in the case of oblique laser pulse incidence .................................................. 109
4.20 Velocity and momentum phase space - titanium, oblique incidence ...... 110
4.21 Comparison of hot electron energy and angular distributions - oblique incidence .................................................. 111
4.22 Illustration of the hot electron beam propagation model ...................... 118
4.23 Collisional and electric field ionization rates ..................................... 120
4.24 Demonstration of the ionization process .......................................... 125
4.25 Comparison of electric fields and cold electron densities .................... 126
4.26 Two-stream instability ................................................. 127
4.27 Average velocity and energy of cold electrons ................. 128
4.28 Cold electron energy distributions ............................... 129
4.29 Temporal evolution of average beam and plasma parameters . 131
4.30 Temporal evolution of the beam velocity distribution ........... 132
4.31 Temporal evolution of the beam current density ................. 133
4.32 Distribution of the beam electrons in the phase space .......... 134
4.33 Beam energy losses .................................................. 135
4.34 Snapshot of the PIC simulation box - simulation setup ........... 143
4.35 Snapshot of the electric field and electron and ion densities on the rear side of Al foil .................................................. 144
4.36 Energy distributions of protons accelerated from Al/hydrogen foil targets .......................................................... 145
4.38 Snapshots of the rear surface of water targets .................... 148
4.39 Phase space of protons accelerated from water targets ........... 150
4.40 Temporal evolution of proton energy distribution ................. 151
4.41 Temporal evolution of deuteron energy distribution ............... 152
4.42 Temporal evolution of proton energy distribution - heterogeneous target .................................................. 153
List of Tables

2.1 List of the most important laser absorption processes ........................................... 15
3.1 Constants used in the BEB model for aluminum ..................................................... 57
3.2 Short review of existing PIC simulation codes with variable ionization ................. 75
4.1 Hot electron beam parameters ............................................................................. 116