NUCLEAR THEORY, Vol. 30 (2011)
eds. A. Georgieva, N. Minkov, Heron Press, Sofia

Modeling of Electronic Excitation and Dynamics in Swift Heavy Ion Irradiated Semiconductors

T. Apostolova[1], **M.V. Ivanov**[1], **C. Kozhuharov**[2]

[1]Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
[2]GSI, Planckstr.1, 64291 Darmstadt, Germany

Abstract. High energy particle interactions within semiconductor materials play an important part in detector reliability and hardness insurance. In this paper, we consider a bulk GaAs semiconductor doped with electron concentration and establish a Boltzmann scattering equation for the description of the relative scattering motion of electrons interacting with a swift heavy ion by including the electron impurity and phonon scattering processes modified by the interaction with the ion projectile as well as the Coulomb scattering between two electrons. The thermodynamics of hot electrons is studied by calculating the non-equilibrium electron distribution. Numerical results are given for the average electron kinetic energy as a function of both the impact parameter of the ion projectile and its charge number.

1 Introduction

The past half century has seen an explosive growth of the discipline that is characterized by the deposition of localized high energy densities in solid matter due to very dense electronic excitation by means of either by photons (associated with femtosecond pulse laser) or energetic ions (produced *e.g.*in particle accelerators) via ion-electron collisions leading to the formation of dense electron-hole plasma. The possibility for investigation of solids in highly non-equilibrium state is related to the creation of ultrashort and highly localized excitations of electronic system of solids, which arise during solid irradiation by ions with energies above 0.1 MeV/amu and masses $M > 50$ amu. The electron energy loss of such a swift heavy ion (SHI) reaches several keV/nm, constituting the major part of its total energy loss, while the loss due to elastic collisions with the target atoms is of secondary importance. The modification of the solid structure in a narrow region (track) along SHI trajectory occurs indirectly, following the electronic excitation decay. The track (only a few nanometers in diameter [1]) exhibits a modified structure that depends on the type of the irradiated material, *i.e.*conductor, semiconductor or a dielectric and, at a lesser extent, on irradiation conditions, embedded into undamaged matrix.

Material modification and damage induced by electronic excitation is of maximum relevance for radiation-matter interaction in inorganic, organic, and even biological materials. The modification of materials induced by SHI irradiation provides flexible and often unique methods to achieve desired performances in a variety of areas, going from physics to medicine. Irradiation of dielectric and semiconductor solids with swift ions, *i.e.*, operating in the electronic stopping power regime when the deposited excitation energy is above a given threshold value, gives rise to numerous changes in the material's physical and chemical properties, part of which has proven to be detrimental, and part of which is beneficial for technological applications and is being used as an alternative to nuclear collision damage and implantation to induce structural modifications [2–4] and produce devices, *e.g.*, for optoelectronics and photonics [5, 6]. Charged particle beams can offer an improved dose conformation to the target volume as compared with photon radiotherapy, with better sparing of normal tissue structures close to the target.

Investigations of heavy-ion-induced damage processes in solids were started in the 1950s using fission fragments from radioactive sources. It is a curious fact that ion-induced damage effects in minerals were found long before the discovery of radioactivity. In 1815 Berzelius observed thermoluminescence in gadolinite caused by the α-decay of U and Th traces [7]. As early as the 19th century, also inadvertently, Baumhauer etched tracks of fission fragments in apatite [8]. The ionization caused by swift heavy charged particles can be very extensive depending on the energy, charge and mass of the ionizing particle and the properties of the traversed medium. These studies were mainly stimulated by the need of developing materials for nuclear reactors [9]. Along the path of a charged particle, a damaged zone (latent track) with an approximate cylindrical geometry enriched with free chemical radicals and other chemical species is then created. Elastic energy loss of ions becomes only about a few per cent (2-10%) from the total ion energy, and the energy loss of ions is practically almost transferred to target exclusively by electronic excitation or ionization of the electron system of the target atoms. Since the ion track has another electrical, chemical and structural properties than the bulk target due to the large electronic excitations it can be registered. The occurrence of individual latent tracks of fission fragments was discovered in a LiF crystal by Young (1958) [10]. One year later, Silk and Barnes (1959) reported the identification of damaged regions in mica caused by heavy charged particles through the use of the transmission electron microscope [11]. Fleischer *et al.*(1965), [12] extensively studied this method, and applied the elaboration of the etching technique to mica as well as other materials such as minerals, plastics and glasses. Nowadays, track damage is analyzed using a large spectrum of different experimental techniques [13, 14].

Historically there has been a discrepancy between the solid state theory and heavy ion (fast charged particle) incident on matter models leading to an obstacle to the understanding of the nature of induced elementary excitations and radiation defects. The concepts of electronic energy losses are based on the clas-

sical ideas which mainly exploit the mechanisms of Coulomb interactions. The earliest works which are still quoted are those by J.J. Thomson [15], E. Rutherford [16] and N. Bohr [17].

The physics of the processes in the ion track formed in matter after a heavy ion passage carries essentially quantum character. An attempt should be made to eliminate this discrepancy and define main connection points between the solid state theory and the processes in the ion track.

The problem of energy losses was formulated by N. Bohr [18]. By considering the simple problem of energy transfer to a free electron by a fast heavy particle and exploring the effects of a binding force on the electron, the classical Bohr formula for energy loss was obtained in the 1915 paper.

Bohr's formula gives a reasonable description of the energy loss of relatively slow alpha particles and heavier nuclei. But for electrons, mesons, protons, and even fast alpha particles, it overestimates the energy loss considerably. The reason is that for the lighter particles quantum- mechanical modifications cause a breakdown of the classical result. The important quantum effects are discreteness of the possible energy transfers, and limitations due to the wave nature of the particles and the uncertainty principle. Bohr's formula was corrected by M. Bethe [19] on the basis of quantum theory. The next appreciable step has been done by F. Bloch [20] when he considered the stopping of fast ions.

Bloch evaluated the differences between the classical (Bohr) and quantum-mechanical (Bethe) approaches for particles with velocities much larger than the target electrons.

Thus Bloch found the bridging formulation between the classical Bohr impact-parameter approach, and the quantized Bethe momentum transfer approach to energy loss.

Fano published various extensions of Bethe's and Bloch's work which summarized most of the theoretical work in the prior fifty years [21]. He described a relativistic version of the Bethe-Bloch energy loss formula where two additional corrective terms are included, the Shell Correction term, $C/Z2$, and the Density Effect correction term, $\delta/2$ [22]. The shell correction term corrects the assumption that the ion velocity is much larger than the target electron velocity. The term is usually calculated by detailed accounting of the particle's interaction with each electronic orbit in various elements. This term contributes up to a 6% correction to stopping powers. This density effect term corrects for polarization effects in the target, which reduces the stopping power since the ion's electromagnetic fields may not be at the assumed free-space values, but reduced by the dielectric constant of the target medium. There have been many corrections proposed to improve on Fano's theoretical approximations. Traditionally, this is done by expanding this equation in powers of Z (charge number of the ion), that can be used to add additional corrections to the ion and target interaction.

Some principal ideas arose with the concept of excited quantum plasma in crystals when the energy losses were connected with the plasma vibrations [23–25]. The further development of the theory of energy losses was presented

in [26–28]. Following the classical papers of Lindhard [29], the energy loss of particles in materials could be separated into interactions with the electronic system (ionization) and with the system of the lattice. In fact, the physics is more complicated, due both to the possible excitations of these systems, and to their mutual interaction (electron – phonon). The processes of energy transport in materials are governed by phonon-phonon scattering and by phonon-electron interactions. Additional corrections to the theory of the energy loss were given in [30–32]. The variation of the energy loss as a function of incoming's particle velocity is generally divided into three regions. At low velocities the main mechanism of energy loss is particle's (elastic) scattering on the atoms placed in their sites in the lattice. At high velocities, the projectile loses energy mainly by the ionization of individual target atoms, and Bohr and Bethe-Bloch theories give a good description of the processes. The intermediate energy region could be characterized by the presence of both mechanisms, but a complete theory does not exist yet. A detailed discussion on this subject, as well as on the development of understanding related to phenomena associated with the energy loss could be found, *e.g.*, in Sigmund's papers [33]. Theories of Firsov [34] and Lindhard-Scharff [35] based on the statistical model of the atom and on the electron-gas model of metals predict a velocity-proportional behavior of the rate of electronic energy loss in the intermediate region, in agreement with experiments within 20% accuracy. In the works reviewed above the impinging charged particle is assumed to interact with the target only through electromagnetic forces and in one way or another Thomas-Fermi-like potentials and quasi-classical approach to the electronic subsystem of solids are used. The results for energy loss given by these theories practically differ by modifications of the expressions under well-known logarithm of the original Bethe-Bloch formula plus additional correction terms described above. Only collision processes within the track volume (i.e., inside) without taking into account the possible excitations of the matter outside were considered. The next step in the theoretical description is connected with the analysis of many-cascade processes within the tracks and the introduction of concept of δ-electron interactions accompanying ion passages [36,37]. Another classification of the phenomena related to the energy loss of projectiles and energy transport in the target regards individual versus collective effects. An important example is related to plasmons, quantized collective oscillations of valence electrons [38]. The full Coulomb interaction could be replaced by a screened interaction, and the long range component which is neglected re-emerges in the form of an additional collective oscillation, this last corresponding to compression waves in the electron gas [39]. The case of collective excitations is important, because for low momentum transfers (*i.e.*distant collisions according to Bohr's terminology) the projectile interacts simultaneously with many atoms, and the perturbed atoms will react with projectile's field affecting its interaction with any other atom of the medium. This way, energy is directly transferred far from the trajectory of the incoming particle. The plasmon is characterized by a significant amount of energy and a little momentum, and

its creation is possible in a binary process too, in accordance with constraints of energy and momentum conservation.

A model of the ion explosion as a probable mechanism of acoustical excitations in a solid caused by Coulomb repulsion of suddenly ionized atoms within the track volume leading to the "acoustical shock" was proposed in [40]. The so-called "thermal spike" model [41] was further developed in the works of Toulemonde *et al.* [42] for the description of heavy ion track damage creation in metals end oxides on the basis of existing short-living plasma state in the track volume. However, the processes of creation of radiation defect as well the critical values of energy loss (*e.g.*, for single point defects, etchings or latent track formations) have not been elucidated yet. Most importantly, a general model of radiation damage processes based on the mechanisms of elementary excitations does not exist.

In the modern era the practice of experimental particle physics usually requires the use of extremely large and costly composite detectors. The new generation of high energy experiments at colliders will use silicon tracking detectors in a heavier way than in the past. High particle production rate requires a high granularity and fast detector response.

For example, the ATLAS Inner Detector [`http://atlas.ch/`] combines high-resolution detectors at the inner radii with continuous tracking elements at the outer radii, all contained in the Central Solenoid, which provides a nominal field of 2 T. The very high cost for the silicon instrumented tracker has led to the request that the detectors should be fully operational for at least *10 years* and hence it has to be guaranteed that the detectors will have a sufficiently high radiation tolerance. Also it is assumed that the dismounting and mounting of the detectors for diagnostic and repair procedures comprises a very expensive and labor-consuming procedure. At the microscopic level the radiation damage suffered by the detectors can be divided in two different classes: effects which are due to surface damage and those which are due to bulk damage.

Knowledge of high energy particle interactions within semiconductor materials plays an important part in detector reliability and hardness insurance. To achieve microscopic understanding of the fast ion irradiation of materials used for detectors that is a vast and extremely complicated field we restrict ourselves to describing the damage produced in GaAs semiconductor when irradiated with swift heavy ions (coming from a given experimental radiation environment) by utilizing something we have already described, *i.e.*GaAs material irradiated with femotosecond laser pulse (by a photon beam).

Our intention in this paper is, among other things, to initiate ideas on how to set up appropriate experiments, which would follow conditions imposed by numerical simulations and to present the possibilities of the numerical simulations for the deposited energy distribution on microscopic or submicroscopic levels.

It has been shown in the literature that at energies above about 1 MeV/u, in some crystals the elastic collisions between the projectile and the target atoms can be neglected and therefore the interaction of high-energy ions could be char-

acterized by almost pure electronic excitation of target atoms. The primary ionization and excitation processes and the following electron cascades are shown experimentally to occur within a very short time of 10^{-17} to 10^{-14} s that is much shorter than the time necessary to create defects via lattice relaxation (10^{-17} to 10^{-14} s). It has been demonstrated that the energy deposited by heavy ions passing through or near the device structure, produces in very short time high density plasma of electrons along the particle trajectory. This plasma thermalizes in about 1 ps and the associated electron–hole pairs can be collected by a drift (applied dc field) or diffusion in a few hundreds of picoseconds. The rapidly passing ion projectile that has reached its equilibrium charge state may only have minor fluctuations of its internal state and will move with constant velocity along a straight-line trajectory until deep inside the solid. Thus, the projectile ion acts as a well defined and virtually instantaneous source of strongly localized electronic excitation [43].

As mentioned above, after investigating the electron dynamics in semiconductors on a femto-second time scale in such physical processes as irradiation by an intense ultra-short laser pulse we adapt the technique to the passage of a highly charged ion. We choose the same time scales of interaction.

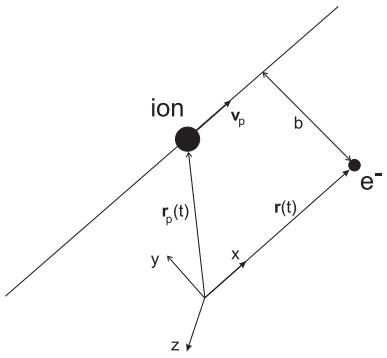
Previously in the case of ultra-short pulsed laser interaction with GaAs semiconductor, we demonstrate that when the motion of electrons is separated into center-of mass and relative motions, the incident electromagnetic field is found to be coupled only to the center-of-mass motion but not to the relative motion of electrons [44]. This generates an oscillating drift velocity in the center-of mass motion, but the time-average value of this drift velocity remains zero. The oscillating drift velocity, however, affects the electron-phonon and electron-impurity interactions. The thermodynamics of electrons is determined by the relative motion of electrons that includes the scattering of electrons with impurities, phonons, and other electrons [45]. When the incident electromagnetic laser field is spatially uniform, electrons in bulk GaAs cannot directly absorb incident photons through an intraband transition. Because both impurity atoms and lattice ions do not move with the electron center-of-mass, electrons inside a drifting system feel that impurities and ions are oscillating against them due to the Galilean principle of relative motion. This leads to impurity and phonon-assisted photon absorption in the system. The relative scattering motion of electrons can be very well described by a Boltzmann scattering equation (Boltzmann transport equation without a drift term) [46]. The effect of an incident optical field is reflected in the impurity- and phonon-assisted photon absorption through modifying the scattering of electrons with impurities and phonons. This drives the distribution of electrons away from the thermal equilibrium distribution to a non-equilibrium one. At the same time, the electron temperature increases with the strength of the incident electromagnetic field, creating hot electrons. In previous paper we have established a Boltzmann scattering equation for an accurate description of the relative scattering motion of electrons interacting with an intense optical field by including both the impurity- and phonon-assisted photon

absorption processes as well as the Coulomb scattering between two electrons.

2 Theoretical Approach

In this paper, we consider a bulk GaAs semiconductor doped with electron concentration to form a 3D electron gas and establish a Boltzmann scattering equation for the description of the relative scattering motion of electrons interacting with a swift heavy ion by including both the impurity- and phonon-assisted interaction with the ion potential as well as the Coulomb scattering between two electrons. The potential created by the ion projectile turns out to be only time dependent due to a choice of the coordinate system and electrons cannot directly couple to it without the assistance from phonons and impurities. We study the thermodynamics of hot electrons by calculating the average kinetic energy (effective electron temperature) as a function of both the impact parameter of the ion projectile and its charge number. Numerical results are given for the distribution of electrons and the dependence of electron temperature on the projectile impact parameter and charge number.

For projectile with constant-velocity $v/c < 0.1$, we consider only constant-velocity, straight-line trajectories. In terms of three-dimensional Cartesian coordinates, we define the reaction to occur in the $x-y$ plane with the beam directed along $\vec{e}_x$ and the impact parameter b along $\vec{e}_y$ defining the straight-line trajectory to be



We first separate the dynamics of a many-electron system into a center of-mass motion plus a relative motion under the influence of the ion projectile. The equation for the center-of-mass motion of electrons is built after a quantum-statistical average is taken (to obtain a classical frictional force). The relative motion of electrons is studied by using the Boltzmann scattering equation including anisotropic scattering of electrons with phonons and impurities beyond the relaxation-time approximation. In the presence of the time dependent only potential of the ion projectile

$$V_p\left(\vec{r},t\right) = -\frac{Z_p e^2}{4\pi\varepsilon_0\left|\vec{r}-\vec{r}_p(t)\right|} \tag{1}$$

with $\vec{r}_p(t) = (v_p t, b, 0)$, where v_p is the velocity of projectile and b is the impact parameter [47] the Hamiltonian of an *interacting* three-dimensional electron gas can be written as

$$H = \frac{1}{2m^*}\sum_i \hat{\vec{p}_i}^{\,2} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r}_i-\vec{r}_j|} - \sum_i \frac{Ze^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r}_i-\vec{r}_p|} + \sum_{i,a} U^{imp}(\vec{r}_i-\vec{R}_a) + \sum_{i,l}\vec{u}_l.\vec{\nabla}_{\vec{r}_i}U^{imp}(\vec{r}_i-\vec{R}_l) \quad (2)$$

where $i = 1, 2, ...N_e$ is the index of N_e electrons, $a = 1, 2, ...N_a$, is the index for N_a impurity atoms, $l = 1, 2, ...N_l$ is the index for N_l lattice ions, $\vec{r}_i$ is the position vector for the ith electron, $\vec{R}_a$ and $\vec{R}_l$, are the position vectors of impurity atoms and lattice ions, $\vec{u}_l$, represents the ion displacement from the thermal equilibrium position, m^* is the effective mass of electrons, and ε_r is the relative dielectric constant of the host material. The single-electron momentum operator is $\hat{\vec{p}}_i = -i\hbar\vec{\nabla}_{\vec{r}_i}$ and both the impurity potential $U^{imp}\left(\vec{r}_i - \vec{R}_a\right)$ and the ion potential $U^{ion}\left(\vec{r}_i - \vec{R}_l\right)$ are included. The center-of-mass momentum and position vectors are defined by

$$\hat{\vec{P}}^C = \sum_{i=1}^{N_e}\hat{\vec{p}}_i,\ \vec{R}^C = \frac{1}{N_e}\sum_{i=1}^{N_e}\hat{\vec{r}}_i,\ \text{where } \hat{\vec{p}}'_i = \hat{\vec{p}}_i - \frac{1}{N_e}\hat{\vec{P}}^C,\ \vec{r}'_i = \vec{r}_i - \vec{R}^C.$$

By using the center-of-mass and relative momentum and position vectors defined above, we can separate the total Hamiltonian, including the Hamiltonians of electrons and phonons, into one center-of-mass Hamiltonian H_{cm} and another relative Hamiltonian H_{rel}, given by

$$\hat{H}_{CM} = \frac{(\hat{\vec{P}}^C)^2}{2N_e m^*} \quad (3)$$

$$\hat{H}_{rel} = \sum_{\vec{k},\sigma}\varepsilon_k \hat{a}^\dagger_{\vec{k}\sigma}\hat{a}_{\vec{k}\sigma} + \sum_{\vec{q},\lambda}\hbar\omega_{q\lambda}\hat{b}^\dagger_{\vec{q}\lambda}\hat{b}_{\vec{q}\lambda} + \frac{1}{2}\sum_{\vec{k},\vec{k}',\sigma,\sigma'}\sum_{\vec{q}}\frac{e^2}{\varepsilon_0\varepsilon_r q^2\nu}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}^\dagger_{\vec{k}'-\vec{q}\sigma'}\hat{a}_{\vec{k}'\sigma'}\hat{a}_{\vec{k}\sigma} + \sum_{\vec{k},\sigma}\sum_{\vec{q},\lambda}C_{q\lambda}(\hat{b}_{\vec{q}\lambda} + \hat{b}^\dagger_{-\vec{q}\lambda})e^{i\vec{q}.\vec{R}^C}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} + \sum_{\vec{k},\sigma}\sum_{\vec{q},a}U^{imp}(q)e^{i\vec{q}.(\vec{R}^C-\vec{R}_a)}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} \quad (4)$$

where, V is the volume of the system, $\hbar\omega_{q\lambda}$ is the phonon energy with wave number q for mode λ (totally three modes), $\varepsilon_k = \hbar^2k^2/2m^*$ is the kinetic energy of electrons with wave number k, and the index $\sigma = \pm 1$ is for up and down spin states for electrons; $\hat{a}^\dagger_{\vec{k}\sigma}$ $\left(\hat{a}_{\vec{k}\sigma}\right)$ represent the creation (annihilation) operator of electrons and $\hat{b}^\dagger_{\vec{q}\lambda}$ $\left(\hat{b}_{\vec{q}\lambda}\right)$ denote the creation (annihilation) operator of phonons. $U^{imp}(q)$ is the Fourier transform of the impurity potential

$$\left|U^{(im)}(q)\right| = \frac{Ze^2}{\varepsilon_0\varepsilon_r\left(q^2+Q_s^2\right)},$$

where Z is the charge number of an ionized impurity atom and $Q_s^2 = \left(e^2/\varepsilon_0\varepsilon_r\right) \times \left(m^*/\pi^2\hbar^2\right)\left(3\pi^2\sigma_{3D}\right)^{1/3}$ and $C_{q\lambda}$ is the electron-phonon coupling constant and for polar optical phonons is given by:

$$|C_{q\lambda}|^2 = \left(\frac{\hbar\omega_{LO}}{2V}\right)\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)\frac{e^2}{\varepsilon_0\left(q^2+Q_s^2\right)}$$

where ω_{LO} is the frequency of dominant longitudinal-optical (LO) phonon modes at high temperatures, ε_∞ and ε_s are the high-frequency and static dielectric constants of GaAs. For acoustic phonon scattering, in the deformation potential approximation: $|C_{q\lambda}|^2 = \left(\frac{\hbar\omega_{ql}}{2\rho c_l^2 V}\right)\left(D^2 + \frac{1}{32q^2}\left(eh_{14}\right)^2\right)\left(\frac{q^2}{q^2+Q_s^2}\right)^2$, $|C_{qt}|^2 = \left(\frac{\hbar\omega_{qt}}{2\rho c_t^2 V}\right)\frac{13}{64q^2}\left(eh_{14}\right)^2\left(\frac{q^2}{q^2+Q_s^2}\right)^2$, where $\lambda = l, t$ corresponds to one longitudinal and two transverse acoustic-phonon modes, c_l and c_t are the sound velocities for these modes, ρ is the ion mass density, D is the deformation potential coefficient, and h_{14} is the piezoelectric constant. Applying the Debye model to low-energy acoustic phonons, we get $\omega_{q\lambda} = c_\lambda q$ with $\lambda = l, t$.

We use the Boltzmann scattering equation without the drift term to describe the relative scattering motion with phonons given by

$$\frac{\partial}{\partial t}n_{\vec{k}}^e = W_k^{(in)(\alpha)}\left(1 - n_{\vec{k}}^e\right) - W_k^{(out)(\alpha)}n_{\vec{k}}^e \quad \alpha = (im), (ph), (c) \qquad (5)$$

The scattering rates $W_k^{(in)(\alpha)}$ and $W_k^{(out)(\alpha)}$ are obtained after solving the Schrodinger equation for the single electron wave-function in the presence of the ion potential Eq. (1). The modification of electron-phonon scattering results from the electrons interacting with the ion potential through phonon scattering. The free-carrier absorption of photons occurs only close to the Fermi surface if the Fermi energy of electrons is much larger than (*i.e.*, degenerate electrons) the electron temperature and phonon energies.

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \frac{\vec{p}^{\,2}}{2m^*}\psi\left(\vec{r},t\right) + V_p\left(\vec{r},t\right)\psi\left(\vec{r},t\right) \qquad (6)$$

The solution of the above equation is sought in the form: $\psi\left(\vec{r},t\right) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}f(t)$ and we obtain $f(t) = f(0)e^{\frac{i}{\hbar}c\ln(t+\sqrt{t^2+a^2})}e^{-\frac{i}{\hbar}c\ln(a)}$, where $a = \frac{b}{v_p}$; $c = \frac{Z_p e^2}{4\pi\varepsilon_0 v_p}$, Z_p being the charge number of the ion projectile.

By expanding the power of the exponential

$$c\ln(t+\sqrt{t^2+a^2}) = c\ln a + c\frac{t}{a} - c\frac{t^3}{6a^3} + c\frac{3t^5}{40a^5} - ..... \qquad (7)$$

and keeping only the first two terms, the electron scattering-in/scattering-out

rates due to phonons, including phonon-assisted photon absorption are obtained

$$W_k^{(in)(ph)} = \frac{2\pi}{\hbar}\sum_{\vec{q}\,\lambda}\left|C_{\vec{q}\,\lambda}\right|^2\left[n_{\vec{k}-\vec{q}}N^{ph}_{\vec{q}\,\lambda}\,\delta\left(E_{\vec{k}}-E_{\vec{k}-\vec{q}}-\hbar\omega_{\vec{q}\,\lambda}-\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right.$$
$$\left.+n_{\vec{k}+\vec{q}}\left(N^{ph}_{\vec{q}\,\lambda}+1\right)\delta\left(E_{\vec{k}}-E_{\vec{k}+\vec{q}}+\hbar\omega_{\vec{q}\,\lambda}+\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right] \tag{8}$$

$$W_k^{(out)(ph)} = \frac{2\pi}{\hbar}\sum_{\vec{q}\,\lambda}\left|C_{\vec{q}\,\lambda}\right|^2\left[\left(1-n_{\vec{k}+\vec{q}}\right)N^{ph}_{\vec{q}\,\lambda}\,\delta\left(E_{\vec{k}+\vec{q}}-E_{\vec{k}}-\hbar\omega_{\vec{q}\,\lambda}-\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right.$$
$$\left.+\left(1-n_{\vec{k}-\vec{q}}\right)\left(N^{ph}_{\vec{q}\,\lambda}+1\right)\delta\left(E_{\vec{k}-\vec{q}}-E_{\vec{k}}+\hbar\omega_{\vec{q}\,\lambda}+\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right] \tag{9}$$

The expansion we use and the approximation we make (7) allows us to obtain the scattering rates in analogy to the ones obtained in the case of interaction of GaAs semiconductor with an incident electromagnetic field of a pulsed laser.

The electron scattering-in (scattering-out) rates due to impurity atoms are given by:

$$W_k^{(in)(im)} = \frac{2\pi}{\hbar}N_I\sum_{\vec{q}}\left|U^{(im)}(q)\right|^2\left[n_{\vec{k}-\vec{q}}\delta\left(E_{\vec{k}}-E_{\vec{k}-\vec{q}}-\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right.$$
$$\left.+\,n_{\vec{k}+\vec{q}}\delta\left(E_{\vec{k}}-E_{\vec{k}+\vec{q}}+\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right] \tag{10}$$

$$W_k^{(out)(im)} = \frac{2\pi}{\hbar}N_I\sum_{\vec{q}}\left|U^{(im)}(q)\right|^2\left[\left(1-n_{\vec{k}+\vec{q}}\right)\delta\left(E_{\vec{k}+\vec{q}}-E_{\vec{k}}-\hbar\omega_{\vec{q}\,\lambda}-\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right.$$
$$\left.+\left(1-n_{\vec{k}-\vec{q}}\right)\delta\left(E_{\vec{k}-\vec{q}}-E_{\vec{k}}+\hbar\omega_{\vec{q}\,\lambda}+\frac{Z_p e^2}{b4\pi\varepsilon_0}\right)\right] \tag{11}$$

where $n_I = N_I/V$ is the impurity concentration with sample volume V.

The electron scattering-in/scattering-out rates due to the Coulomb interaction between electrons not affected by the ion potential are given by

$$W_k^{(in)(c)} = \frac{2\pi}{\hbar}\sum_{\vec{k}',\,\vec{q}}\left|V^{(c)}(q)\right|^2\left(1-n_{\vec{k}'}\right)n_{\vec{k}-\vec{q}}n_{\vec{k}'+\vec{q}}\,\delta\left(E_{\vec{k}}-E_{\vec{k}'}-E_{\vec{k}-\vec{q}}-E_{\vec{k}'+\vec{q}}\right) \tag{12}$$

$$W_k^{(in)(c)} = \frac{2\pi}{\hbar}\sum_{\vec{k}',\,\vec{q}}\left|V^{(c)}(q)\right|^2 n_{\vec{k}'}\left(1-n_{\vec{k}-\vec{q}}\right)\left(1-n_{\vec{k}'+\vec{q}}\right)\delta\left(E_{\vec{k}-\vec{q}}-E_{\vec{k}'+\vec{q}}-E_{\vec{k}}-E_{\vec{k}'}\right) \tag{13}$$

with $\left|V^{(c)}(q)\right| = \frac{e^2}{\varepsilon_0 \varepsilon_r (q^2+Q_s^2)V}$ Coulomb scattering of electrons is a relative motion between electrons. As a result, the external ion potential does not directly couple to it.

3 Results and Discussion

In the numerical calculations, GaAs is the host material. For GaAs we have taken parameters as follows: $m^* = 0.067m_0$ with free-electron mass m_0, $\sigma_{3D} = 1 \times 10^{18}$ cm^{-3}, $\hbar\omega_{LO} = 36$ meV, $\varepsilon_r = 12$, $\varepsilon_s = 13$, $\rho = 5.3$ g/cm^3, $c_l = 5.14\times10^5$ cm/s, $c_t = 3.04\times10^5$ cm/s, $D = -9.3$ eV, $h_{14} = 1.2\times10^7$ V/cm and $T = 300$ K. Other parameters, such as the impact parameter b and the charge number Z, will be given directly in the figure captions. In the numerical calculations below, we will only show results for steady-state cases. In our numerical calculation, we have employed the finite-difference method for solving the evolution of the distribution of conduction electrons under the ion potential. The time step Δt is taken to be 0.5 fs. The steady-state electron distribution is obtained by ensuring the relative change of the results at two successive times smaller than 10^{-6}. For discrete states of electrons, we have taken a total of eighty-one points for electron wave number k with $\Delta k = 0.05\left(3\pi^2\sigma_{3D}\right)^{1/3}$. With this precision, we find that the dominant peaks in Figure 1 can be resolved. We expect the curves in Figure 1 will be smoother if a higher precision is taken. Figure 1 displays a comparison between calculated non-equilibrium electron distributions n_k with the effect of pair scattering and the thermal-equilibrium Fermi-Dirac distribution of electrons (dash-dotted curve) at $T = 300$ K, for the same charge number Z of the projectile and different impact parameters. The

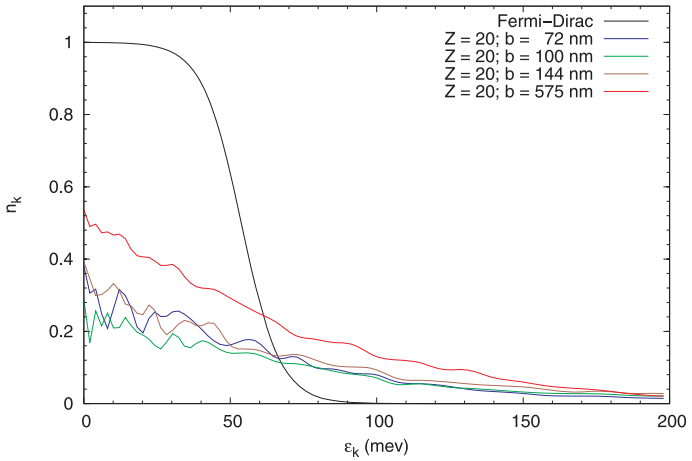


Figure 1. Calculated electron distribution function for bulk GaAs as a function of electron kinetic energy $T = 300$ K.

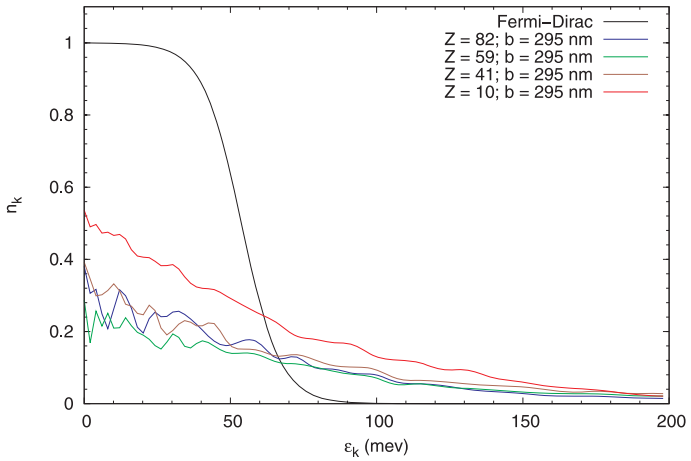


Figure 2. Calculated electron distribution function for bulk GaAs as a function of electron kinetic energy $T = 300$ K.

impurity- and phonon-assisted electron scattering processes in the presence of the projectile potential create multiple small peaks (dashed curve) on the high-energy tail (above 54 meV) of the Fermi-Dirac distribution. Figure 2 displays a comparison between calculated non-equilibrium electron distributions n_k with the effect of pair scattering and the thermal-equilibrium Fermi-Dirac distribution of electrons (dash-dotted curve) at $T = 300$ K, for different charge numbers Z of the projectile and the same impact parameter. Figure 3 is similar to Figure 1 but

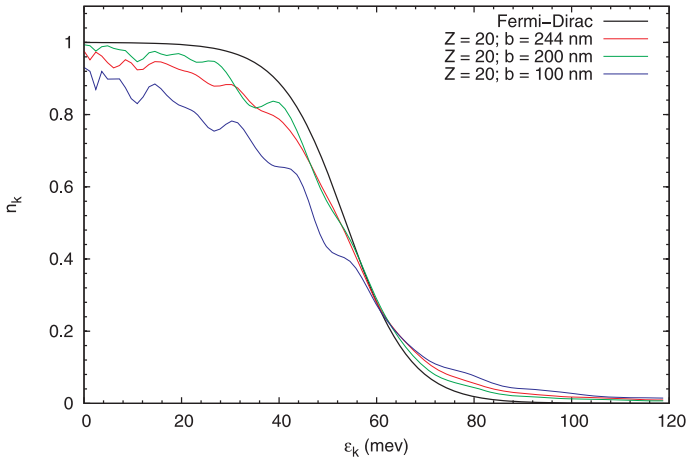


Figure 3. Calculated electron distribution function for bulk GaAs as a function of electron kinetic energy $T = 77$ K.

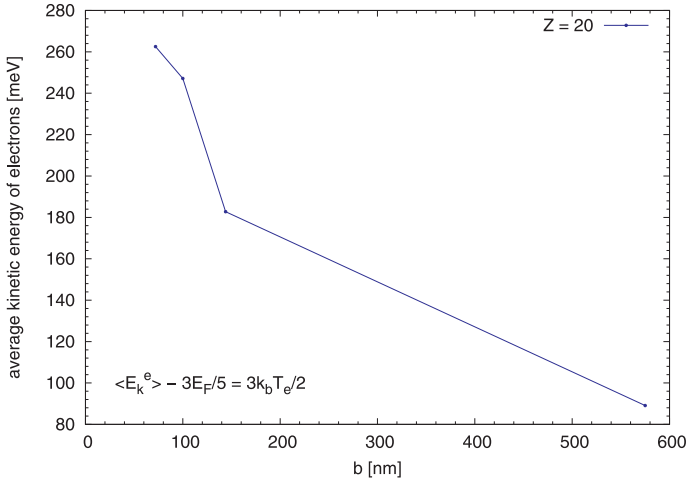


Figure 4. Average electron kinetic energy as a function of impact parameter for $T = 300$ K.

for $T = 77$ K. Figure 4 shows the average electron kinetic energy as a function of impact parameter and Figure 5 displays the average electron kinetic energy as a function of ion charge number Z.

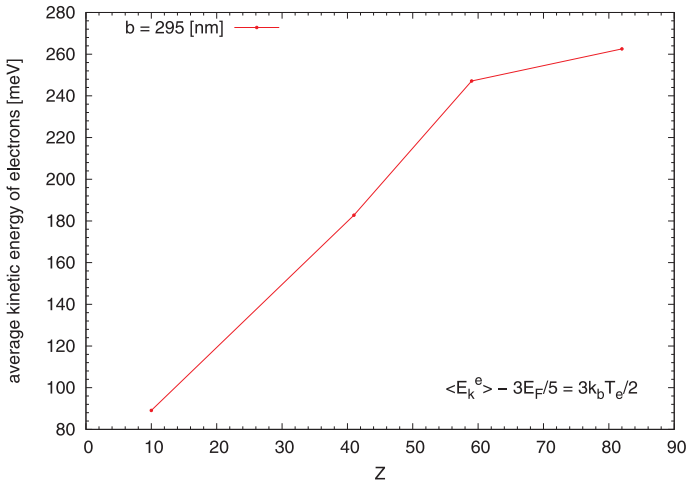


Figure 5. Average electron kinetic energy as a function of the ion projectile charge number.

4 Conclusions

In this paper the relative dynamics of conduction electrons in swift heavy ion irradiated semiconductors was studied by using generalized Boltzmann scattering equation including scattering of electrons with phonons and impurities beyond the relaxation-time approximation. The effect of an "incident" ion potential is reflected in modifying the scattering of electrons with impurities and phonons. This drives the distribution of electrons away from the thermal equilibrium distribution to a non-equilibrium one. At the same time, the electron average kinetic energy increases with the "strength" of the ion potential (depending on the magnitude of impact parameter and the charge number of the ion projectile in the approximation that has been made), creating hot electrons.

References

[1] R. Spohr, In *Ion Tracks, Michrotechnology: Basic Principles and Applications*, edited by K. Bethge Vieweg, Braunschweig (1990).

[2] G. G. Bentini, M. Bianconi, M. Chiarini, L. Correra, C. Sada, P. Mazzoldi, N. Argiolas, M. Bazzan, and R. Guzzi, *J. Appl. Phys.* **92** (2002) 6477.

[3] J. Olivares, G. García, F. Agulló-López, F. Agulló-Rueda, A. Kling, and J. C. Soares, *Appl. Phys. A: Mater. Sci.Process.* **81** (2005) 1465.

[4] F. Agulló-López, G. García, and J. Olivares, *J. Appl. Phys.* **97** (2005) 093514.

[5] J. Olivares, A. García-Navarro, G. García, A. Méndez, and F. Agulló-López, *Appl. Phys. Lett.* **89** (2006) 071923.

[6] A. García-Navarro, J. Olivares, G. García, F. Agulló-López, S. García-Blanco, C. Merchant, and J. S. Aitchison, *Nucl. Instrum. Methods Phys. Res. B* **249** (2006) 177.

[7] J. Berzelius, *Afhandl. Fys. Kem. Min.* 4 (1815) 217.

[8] H. Baumhauer, "Die Resultate der Atzmethode", Leipzig, (1894).

[9] F. Seitz, *Phys. Today* **5** (1952) 6.

[10] D.A. Young, *Nature* **182** (1958) 375.

[11] E.C.H. Silk, R.S. Barnes, *Philos. Mag.* **4** (1959) 970.

[12] R.L. Fleischer, P.B. Price, R.M. Walker, *Nuclear Tracks in Solids: Principles and Applications*, University of California, Berkeley (1975).

[13] Proceedings of 4th International Conference on Swift Heavy Ions in Matter, *Nucl. Instr. and Meth. B* **146** (1998).

[14] Proceedings of 11th International Conference on Radiation Effects in Insulators, *Nucl. Instr. and Meth. B* **191** (2002).

[15] J. J. Thomson, "Conduction of Electricity through Gases", Cambridge University Press (1903). J. J. Thomson, *Phil. Mag.* 6-23 (1912) 449.

[16] E. Rutherford, *Phil. Mag.* **21** (1911) 212; ibid **21** (1911) 699.

[17] N. Bohr, *Phil. Mag.* **25** (1913) 10.

[18] N. Bohr, *Phil. Mag.* **25** (1913) 10–31; N. Bohr, *Phil. Mag.* **30** (1915) 581–612.

[19] H. Bethe, *Ann. Phys.* **5** (1930) 325–400.

[20] Bloch, F. *Z.Phys.* **l6** (1933) 285.

[21] U. Fano, *Ann. Rev. Nucl. Sci.* **13** (1963) 1. This extended work is based on earlier papers: U. Fano, *Phys. Rev.* **72** (1947) 26; U. Fano, *Phys. Rev.* **102** (1956) 385; U. Fano, *Phys. Rev.* **103** (1956) 1202.

[22] U. Fano, *Ann. Rev. Nucl. Sci.* **13** (1963) 67.
[23] Tonk, L. and Lingmuir, I. *Phys.Rev.* **33** (1929) 195.
[24] Vlasov, A.A. *Zh. Eksp.Teor.Fiz.* **8** (1938) 291 (in Russian).
[25] Bohm, D. and Pines, D. *Phys.Rev.* **92** (1953) 609.
[26] Ahiezer, A.I. and Sitenko, A.G. *Zh.Eksp.Teor.Fiz.* **23** (1952) l61 (in Russian).
[27] Neufeld , J. and Ritchie, R. *Phys.Rev.* **98** (1955) 1632.
[28] Larkin, A.I. *Zh.Eksp.Teor.Fiz.* **37** (1959) 264 (in Russian).
[29] Lindhard, J. *Mat.Fys.Med.,Dan.Vid.Selsk.* **28** (1954) No. 8.
[30] Fermi, E. and Teller, E. *Phys.Rev.* **72** (1947) 399.
[31] Lindhard, J. and Winter, A. *Mat.Fys.Med.Dan.Vid.Selsk.* **34** (1964) No. 4.
[32] Trubnikov, B.A. and Yavlinski, Yu.N. *Zh.Eksp.Teor.Fiz.* **48** (1965) 253 (in Russian).
[33] P. Sigmund, *Mat. Fys. Medd. Dan. Vid. Sesk.* **40** (1978) 1–36; P. Sigmund, *Phys. Scripta.* 28 (1983) 257-267.
[34] J. Lindhard and M. Scharff, *Phys. Rev.* **124** (1961) 128; J. Lindhard, V. Nielsen, M. Scharff, P.V. Thomsen, *Mat.Phys. Medd. Dan. Vid. Sesk.* **33** (1963) 1–42.
[35] O.B. Firsov, *Sov. Phys. JETP* **9** (1959) 1076.
[36] Kobetich, E.J. and Katz, R. *Phys.Rev.* **170** (1968) 391.
[37] Kobetich, E.J. and Katz, R. *Phys.Rev.* **170** (1968) 405.
[38] Fred J. Currell (ed), *The Physics of Multiply and Highly Charged Ions*, Vol. **2**, Interactions with matter, Kluwer Academic Publishers (2003).
[39] O. Madelung, *Introduction to Solid-State Theory* (Springer Series in Solid State Sciences, Vol **2**) 1978.
[40] Fleischer , R.L, Price , P.B., Walker, R.M. *Phys.Rev.* **136** (1965) 3645.
[41] Seitz, F. and Koehler, J.S. (1956) *Sol.Stat.Phys., Vol.**2***. Ed. F.Seitz and D.Turnbull. Acad. Press, N.-Y., p. 307.
[42] Toulemonde, M., Paumier, E., Dufour, C. *Rad. Eff. and Def. in Solids* **126** (1993) 201.
[43] K. Schwartz *et al.*, *Phys. Rev. B* **58** (1998) 11232; G. Schiwietz *et al.*, *NIMB* **225** (2004) 4.
[44] C. S. Ting *et al.*, *Phys. Rev. B* **14** (1976) 4439; X. L. Lei and C. S. Ting, *Phys. Rev. B* **32** (1985) 1112; D. H. Huang, T. Apostolova, P.M. Alsing and D. A. Cardimona, *Phys. Rev. B* **69** (2004) 075214.
[45] A. Kaiser *et al.*, *Phys. Rev. B* **61** (2000) 11437; T. Apostolova *et al.*, *Phys. Rev. B* **66** (2002) 075208.
[46] D. H. Huang, T. Apostolova, P.M. Alsing and D. A. Cardimona, *Phys. Rev. B* **69** (2004) 075214.
[47] L. Plagne *et al.*, *Phys. Rev. B* **61** (2000) 033201; J. C. Wells, *et al.*, *Phys. Rev. B* **54** (1996) 593.