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Effects of model approximations for electron, hole, and photon transport in swift heavy ion tracks

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ABSTRACT

The event-by-event Monte Carlo code, TREKIS, was recently developed to describe excitation of the electron subsystems of solids in the nanometric vicinity of a trajectory of a nonrelativistic swift heavy ion (SHI) decelerated in the electronic stopping regime. The complex dielectric function (CDF) formalism was applied in the used cross sections to account for collective response of a matter to excitation. Using this model we investigate effects of the basic assumptions on the modeled kinetics of the electronic subsystem which ultimately determine parameters of an excited material in an SHI track.

In particular, (a) effects of different momentum dependencies of the CDF on scattering of projectiles on the electron subsystem are investigated. The 'effective one-band' approximation for target electrons produces good coincidence of the calculated electron mean free paths with those obtained in experiments in metals. (b) Effects of collective response of a lattice appeared to dominate in randomization of electron motion. We study how sensitive these effects are to the target temperature. We also compare results of applications of different model forms of (quasi-) elastic cross sections in simulations of the ion track kinetics, e.g. those calculated taking into account optical phonons in the CDF form vs. Mott's atomic cross sections. (c) It is demonstrated that the kinetics of valence holes significantly affects redistribution of the excess electronic energy in the vicinity of an SHI trajectory as well as its conversion into lattice excitation in dielectrics and semiconductors. (d) It is also shown that induced transport of photons originated from radiative decay of core holes brings the excess energy faster and farther away from the track core, however, the amount of this energy is relatively small.

1. Introduction

In this paper we analyze model assumptions used in the Monte-Carlo (MC) codes describing electron kinetics in highly excited systems. We perform our analysis on example of the recently developed code modeling Time Resolved Electron Kinetics in swift-heavy-ion Irradiated Solids (TREKIS) [1]. The model describes excitation of a solid by a nonrelativistic swift heavy ion (SHI) decelerated in the electronic stopping regime as well as further spreading of generated electrons and holes and their interaction with matter in the vicinity of the ion trajectory.

The present work extends the original model [1] by a detailed analysis of solid state effects on scattering processes of appearing electrons, valence holes, and photons generated in an ion track by decay of core holes. Focusing on the energies of swift heavy ions near the Bragg peak, we investigate how these processes affect temporal and spatial evolution of the electron ensemble and its interaction with the atomic subsystem of a material.

The MC method uses cross sections of interactions of a projectile with an ensemble of scattering centers. Due to spatial and temporal correlations, these scattering cross sections depend on collective response of the electronic and atomic subsystems of a solid target to perturbations caused by a projectile.

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Cross sections of interaction of a projectile with a solid can be calculated precisely from the first-principle models that take into account the band structure of a target and other collective effects [2–4]. But such techniques require great computational resources and are difficult to combine with other codes. Thus, approximate methods prevail so far in calculations of charged particle cross sections in solids [5–9]. An analysis of effects of different model forms of the cross sections (or the mean free paths, MFP) of inelastic and elastic scattering of electrons and holes, evaluated by different methods, is necessary to select the most important channels of the relaxation kinetics of the extremely excited electron subsystem in SHI tracks.

Also, a study of the cross sections of interaction of a particle with a solid has a practical interest, because they are widely used for interpretation of experiments dealing with propagation of electrons in materials, e.g. Auger electron spectroscopy [10], X-ray photoemission spectroscopy [11], low-energy electron diffraction and Bremsstrahlung isochromat spectroscopy [9], etc.

In particular, within the first Born approximation (the first order of the perturbation theory of the kinetic energy of a projectile), effects of collective response of a condensed target can be taken into consideration expressing the scattering cross sections in terms of the Dynamic Structure Factor (DSF) [12]. The fluctuation-dissipation theorem links the DSF to the Complex Dielectric Function (CDF) of a material [13–15].

The CDF of a material can be calculated using theoretical or semi-empirical models [4,16,17]. One of the well-known approaches was developed in [9,18,19] using the Lindhard-type dielectric function within the random phase approximation, and was later replaced by Mermin dielectric function [20], extended further by the so-called full-conserving dielectric function [21].

It is important that the dependencies of the CDF on the transferred energy can be obtained from the experimental optical data. Ritchie and Howie [8] demonstrated that these data can be very well fitted when CDF is approximated by a set of artificial Drude-like oscillators. Such CDFs are often used for calculations of electron mean free paths (MFPs) [22,23], as well as in many other applications [5,6,8,9], in particular for quantitative evaluation of various effects in electron spectroscopy [24].

The CDF from the optical data provides appropriate cross sections but, unfortunately, does not contain the dependence on the momentum transferred during a collision, because in the optical limit the wave vector transferred to the scattering system is equal to zero ($\boldsymbol{q} = 0$) within the dipole approximation. We use additional assumptions about the dispersion dependencies of the artificial oscillators [25] ($\boldsymbol{q}(E)$, see below) to model the dependence on momentum of the CDF fitted from the optical data: free-particle, single-pole approximation [18], momentum dependence proposed by Ritchie et al. [8], and the effective one-band approximation [26].

This forms the problem of an accuracy of the introduced approximations to be studied. We investigate this effect of application of different dispersion dependencies of the artificial oscillators used for fitting of CDF obtained in optical experiments. We compare the calculated mean free paths of electrons calculated under different assumptions about the dispersion law $\boldsymbol{q}(E)$ in different materials with those from experiments and other simulations. We also investigate effect of the model forms of the dispersion laws in the applied CDF on transient spatial distributions of electrons and valence holes densities in SHI tracks.

The elastic scattering of electrons and valence holes generated in a track governs transfer of the excess electronic energy into the lattice resulting in its excitation [27]. Throughout this paper, the term 'elastic scattering' refers to scattering events with exchange of the kinetic energy only, without transfer into potential energy via inducing excitation or ionization events. Sometimes in the literature such processes are referred to as 'quasi-elastic' to emphasize that the energy of the incident particle is changing in the course of collision, albeit this energy change is small [28–30]. Such loss of energy in 'elastic' scattering events is taken into account in TREKIS [1].

Further relaxation of the excess lattice energy can cause transformations of the material structure in a track. Causing large changes of the momentum of an incident particle, this kind of electron and valence hole scattering thereby considerably influences their transport. This effect was demonstrated in experiments where LiF crystals were irradiated with gold ions at cryogenic and room temperatures [31,32]. A lack of phonons participating in scattering events at cryogenic lattice temperatures results in twice as large diffusion ranges of valence holes before their self-trapping.

In this paper we investigate effects of two limit forms of the elastic cross sections on electrons-to-lattice energy transfer rate, and spatial spreading of electronic excitations: (a) the cross sections corresponding to the optical phonons branch of the CDF restored from the experimental photo-absorption data [33], and (b) Mott's atomic cross sections with modified Molier's screening parameter [34].

Already within tens of femtoseconds after the projectile passage, appearing valence holes accumulate noticeable part of the excess electronic energy generated in a track [35,36]. We demonstrated that the kinetics of valence holes significantly affects redistribution of this energy in the vicinity of an SHI trajectory, as well as its conversion into a lattice excitation in dielectrics and semiconductors [36]. It was shown that valence holes provide the lattice with even more energy than generated free electrons in the track core, thus affecting strongly the kinetics of structure changes in an SHI track [36].

An effect of radiative decays of core holes in SHI tracks is also studied. Core-hole relaxation is dominated by the Auger decay for the excitation regimes studied here; nevertheless radiative decays are possible and thus their influence on the energy transport in tracks can affect the track kinetics. Photoemission by radiative decays is incorporated into TREKIS code [1] to analyze the effect of photon transport in SHI tracks. It is demonstrated quantitatively that even though photons can bring energy far from the track core, this effect is small due to small probabilities of radiative decays for the analyzed range of SHI energies.

2. Scattering cross sections

Within the assumed first Born approximation, when the kinetic energy of a projectile is much larger than the potential energy of its interaction [37], a cross section of scattering of an incident particle on a spatially and dynamically coupled system of scattering centers can be split into a product of the cross section of scattering on a single (isolated) scattering center and the Dynamic Structure Factor (DSF) [12]. DSF describes the collective response of a target to excitation. For scattering of charged particles, the DSF can be expressed in terms of the loss function of a target (imaginary part of the Complex Dielectric Function (CDF), $\varepsilon(\omega,q)$) via the fluctuation-dissipation theorem [13–15]. This results in the following form of the differential cross section, σ, of a charged particle interacting with a coupled system of charged scattering centers in the isotropic case assumed within MC models:

$$\frac{d^2\sigma}{d(\hbar\omega)d(\hbar q)} = \frac{2(Z_e(v,q)e)^2}{n_{sc}\pi\hbar^2 v^2}\frac{1}{\hbar q}\left(1-e^{-\frac{\hbar\omega}{k_B T}}\right)^{-1}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega,q)}\right], \quad (1)$$

where e is the electron charge; $\hbar\omega$ is the transferred energy and $\hbar$ is the Planck's constant; k_B is the Boltzmann constant, and T is the temperature of the sample; n_{sc} is the density of scattering centers.

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