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Electron–phonon interactions in silicon: Mean free paths, related distributions and transport characteristics

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ABSTRACT

The mean free path (MFP) for electron–phonon interactions in pure silicon is an important characteristic needed both for low energy electron transport calculations using Boltzmann transport equation, and for Monte Carlo simulations. Full band calculations present a basic (though complicated) approach to the solution of the problem. Simpler approaches based on analytical presentation of the scattering rates have also been used; however they are valid for a restricted range of electron energies, below 2 eV. In this paper we introduce a hybrid method that utilizes the density of energy states calculated from the full band calculations for electron energies larger than 2 eV, allowing to extend the analytical approach for energies up to 5 eV, where the impact ionization becomes the dominant mechanism of electron interactions within bulk silicon. The resulting MFPs as function of electron energy and lattice temperature, together with the integral probability distribution for given energy losses by phonon emission (or energy gain by absorption of phonons) form the database for Monte Carlo calculations. Using this method, we calculate the electron diffusivity and mobility as function of the electron and lattice temperatures. These parameters are important for solution of the two temperature model, used for calculations of the track structure created by swift ions and nanosecond laser beams.

1. Introduction

The transport of low energy electrons (LEE) in semiconductor materials is an important area both for theoretical and experimental research, especially when these electrons are ejected by an intense femtosecond laser beam, or by swift ions from an ion source or of cosmic origin. It is important to note that the slowing down of LEE is dominated by electron-lattice interactions through electron–phonon scattering. Such interactions not only change the spectrum of the electrons, which is important for charge collection in electronic devices, but also influence the structure of the solid through heating by phonons. They lead to local phase changes and structural modifications in the solid, the so-called track effects (TE). The thermal origin of TE was the subject of numerous investigations during the last two decades [1–5 and references therein]. These works are based on the solution of two coupled differential equations for the electron and the solid temperatures, T_e and T_a, which change in time and space after the femtosecond release of LEE by ions and laser beams. This approach is named in the literature as the two temperature model (TTM), the mathematics of which is given by the coupled differential equations:

$$C_e(T_e)\frac{\partial T_e(r,t)}{\partial t} = \nabla\cdot[D_e(T_e)\,C_e(T_e)\nabla T_e(r,t)] - \frac{1}{\rho_e}g(T_e,T_a)\cdot[T_e(r,t)-T_a(r,t)] + S(r,t) \quad (1)$$

and

$$C_a(T_a)\frac{\partial T_a(r,t)}{\partial t} = \nabla\cdot[D_a(T_a)\,C_a(T_a)\,\nabla T_a(r,t)] + \frac{1}{\rho}g(T_e,T_a)\cdot[T_e(r,t)-T_a(r,t)] \quad (2)$$

where $D_e(T_e)$, $D_a(T_a)$ and $C_e(T_e)$, $C_a(T_a)$ are the electron and lattice diffusivity and electron and lattice specific heats, all being temperature dependent, g is the coupling parameter, which accomplishes the feedback of the lattice heating by electrons and ρ_e and ρ are the densities of the electron gas and solid respectively. The coupling parameter g is also temperature dependent as shown in [6], though often used as an adjustable constant to get agreement with experimental data [3]. There is an uncertainty of this parameter as can be seen by comparing its values for silicon: $g = 1.8\cdot10^{12}$ W/cm^3/K obtained in [3] by fitting to experimental data, and $g = 5\cdot10^{12}$ W/cm^3/K obtained in [7], where an attempt was made to use MC calculations in conjunction with TTM calculations. In fact, the latter value of g was also obtained by an adjustment procedure. The source term $S(r,t)$ is related to the energy delivered by a heavy ion or a laser beam to the electronic subsystem of the solid. In [8] it was noted

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that $S(r,t)$ cannot be approximated (as was done in the major works exploiting the TTM) in an analytic form as a product of two independent functions: of time and radial distance of the track. The accurate presentation of $S(r,t)$ should be obtained only in the full MC simulations.

Though the TTM was (and still is) widely used, its basic assumptions are questionable. Firstly it is assumed that the temperature of the solid starts to change (increase) *immediately* after the ejection of the electrons by the ion or the laser beam. In reality, the phonons will cause heating of the solid after a time delay, from hundreds of femtoseconds to picoseconds, during which the electron and lattice temperatures equilibrate. Therefore the coupling parameter should be time and space dependent. The latter dependence is due to the rapid decrease of the electron density in the lateral direction with respect to the ion (laser) track axis. The parameters entering in the above equation, namely the electron diffusivity D_e, the atomic diffusivity D_a, the coupling parameter $g(r,t)$ and the source term $S(r,t)$ need to be calculated *ab initio* in the frame of well-established models. Because the transport of electrons and their energy exchange with the lattice is a stochastic process, the most appropriate methods to be used are the solution of the Boltzmann transport equation or Monte Carlo simulations These methods have been used in numerous applications in the field of high intensity energy deposition by particles and laser beams at ultra-short time intervals, and the relaxation of the induced high density plasma (see for example [9,10 and references therein]). Recently, with the drastic growth of computer capabilities, the MC method appears to be preferable due to its simpler calculation algorithm and its easier handling of complicated boundary conditions in restricted space problems (such as nanometric dimensions of electronic devices). In the pioneering work of Jacoboni and Reggiani [11], the effectiveness of the MC method for solution of the major problems related to the LEE transport in matter was convincingly demonstrated. Nevertheless, in order to have a complete picture of the electron-solid interactions and its effects on the solid, one needs to use molecular dynamics (MD) calculations. Only recently are these hybrid schemes of calculations (MC + MD) beginning to be successfully exploited [12,13].

In this article we present a database for MC transport simulations of low energy ($\leq$5 eV) electron transport in pure silicon at 300 K, and calculate parameters such as the electron diffusivity D_e and mobility μ_e, used in the TTM mentioned above and for other purposes. The database is based on the non-parabolic band approximation intensively used by Pop and coauthors [14,15] for electron energies below 1.5 eV, which gives a density of states (DOS) that agrees with the full band DOS, and extension of this approach to electron energies up to 5 eV using the results of full band calculations of the IBM group [16,17]. The full database (for a wide range of lattice temperatures) contains all the characteristics needed for the implementation of the MC algorithm. We restrict ourselves only to the treatment of the electron–phonon interactions of acoustical and optical modes, and ignore the scattering of ionizing impurities (e.g. doping elements) [18], since we treat pure silicon only. Our approach does not consider the hole interactions, as well as impact ionization, an effect which is negligible for the LEE. For higher energies this effect was included in our previous work [19] and can be added in a straightforward manner into the calculation algorithm, as we show below in Section 3.1.

The MC procedure that can be used with this database is the ordinary event-by-event scheme and it was described and used by us in set of articles [20–22]. Distinctively for the LEE transport with electron–phonon interactions, each mode, acoustical or optical, has two options: emission (energy loss of the electron due to emission of phonons) or absorption (energy gain by the electron from the lattice through phonon absorption). Moreover each of these two processes is realized through transverse or longitudinal phonons. This will increase more than four times the amount of tabulated data compared to the case of electron transport of higher energy electrons. This, however, should not pose any difficulties to contemporary computers.

2. Theory

As stated above, we base our calculations on an analytical approach presented in Pop et al. [14,15 and references therein]. This model for the electron–phonon scattering process has some advantages over the previous models: (a) the intravalley acoustical phonon excitation is treated as an inelastic process, therefore having an angular distribution different from that of elastic scattering (no losses) and thus affecting the heat generation by acoustical phonons, and (b) it uses a dispersion relation for phonon frequency ω_q (different from the simple quadratic dependence on the wave number q), namely an isotropic relation $\omega_q = \omega_0 + v_s q + cq^2$. For acoustic phonons, v_s is the sound velocity in silicon, whose value depends on the branch (transverse or longitudinal) of the acoustic mode considered. The parameters v_s, ω_0 and c are given in Table 1 of [14]. Naturally for optical phonons $v_s = 0$.

2.1. Acoustical phonons

Acoustical phonons are the result of intravalley (within the same conduction-band valley) scattering. The basic formula for the scattering rate Γ_A of the acoustical phonons is [14]:

$$\Gamma_A = \frac{D_i m_e}{4\pi\rho\hbar^2 k_s}\int_{q_{min}}^{q_{max}} \frac{1}{\omega_q}\left(N_q + \frac{1}{2} \mp \frac{1}{2}\right) I_q^2 q^3 dq. \quad (3)$$

D_i (in eV) is the electron acoustic deformation potential, which depends on the acoustical phonon branches: longitudinal (LA) or transverse (TA), and has the values 6.39 eV and 3.01 eV respectively [14], $m_e = 2.98 \times 10^{-28}$ g is the effective electron mass in silicon, ρ is the mass density of silicon, and k_s is the electron wave vector after transformation to spherical space [14]. For an electron with kinetic energy E_e, $k_s = (2m_e E_e(1 + \alpha E_e))^{1/2}/\hbar$, where $\alpha = 0.5$ is the non-parabolicity parameter. $N_q = (\exp(\hbar\omega_q/k_B T - 1)^{-1}$, where k_B and T are the Boltzmann constant and the temperature respectively. The function I_q and the interval $[q_{min}, q_{max}]$ of allowed q-values based on the energy and momentum conservation are given in [14]. The top and the bottom signs in Eq. (3) represent the phonon absorption or emission events respectively. Using Eq. (3) one can calculate the mean free path (MFP) λ as $\lambda = (2E_e/m_e)^{1/2}/\Gamma_A$. It is also easy to obtain from Eq. (3) the normalized integral distributions for sampling the random value of q. For q selected from this distribution one calculates ω_q using the dispersion relation mentioned above as well as the energy of the acoustical phonon $E_{ph}^A = \hbar\omega_q$ for emission and absorption, both for LA and TA modes. For the selected q, one can also obtain the angle of the scattered electron with respect to its previous direction of movement for phonon absorption or emission using simple vectors operations. The new direction of the scattered electron will be different from the case of pure elastic scattering.

2.2. Optical phonons

The electron-optical phonon scattering is related to the intervalley process for equivalent *valleys of the same lattice axis (g-type scattering) or for the non-equivalent valleys for* the perpendicular lattice axes (f-type scattering). Even though $f1$, $g1$ and $g2$ modes are acoustical transitions they are treated here as optical. These phonons are of low energy and with a low probability for emission (absorption) and have practically the same angular distributions as