Kinetic Equation Method and Monte Carlo Method for Charge Carriers Dynamics Description in Diamond

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Abstract: In this work charge carriers mobility in diamond, calculated by two means – by kinetic equation method and by Monte Carlo method – is analyzed. Temperature of diamond crystal less than 300 K and low concentration of impurities are considered, therefore carriers are scattered preliminary by acoustic phonons. Electron-phonon interaction is taken in deformation potential approximation. Phonon emission and adsorption rates are calculated and Monte-Carlo method is used to obtain carriers mobility. The mobility is compared with that obtained by kinetic equation method in our previous work. The results are important for the treatment of electrical experiments in pure monocrystalline diamonds.

1 INTRODUCTION

At temperatures below 300 K and sufficiently low concentration of impurities and defects, the charge carriers mobility in diamond is restricted substantionally by scattering at acoustic phonons. Over the years, the carrier mobility in diamond has been measured many times as a function of temperature for different types of this material (Prelas et al., 1998; Nesladek et al., 2008; Isberg et al., 2002; Pernegger et al., 2005; Pomorski et al., 2007). Nevertheless, the temperature range below 80 K in pure diamond crystals has hardly been studied. Even latest works with mobility studies deal with rather impure samples, for example in (Jansen et al., 2013) the order-of-magnitude estimate for the concentration of neutral impurities was about 10^{17} cm^{-3}, what leads to mainly impurity mechanism of scattering at temperatures lower than 100 K and so impedes high carriers mobility. In view of good prospects of diamond for design of electronic devices with unique properties (Sussmann, 2009; Isberg et al., 2012), particularly ionizing radiation detectors, increasingly pure diamond single crystals will be produced, carriers mobility at low temperatures will be sooner or later measured in them, and the interpretation of these experiments will be an urgent problem.

Generally, the mobility is calculated within the quasielastic approach, but this approach gives bad accuracy in diamond due to high velocity of sound (Baturin, 2010; Belousov, Soloviev, Chernousov, 2013). In these works the inelasticity was taken into account by utilizing a not simplified collision integral in the right part of kinetic equation in two-moment approximation and in 0-dimensional or 1-dimensional cases. The solution was based on the numerical integration of the kinetic equation. If necessary, this approach can easily be modified to take into consideration a self-consistent electric field, created by charge carriers. On the other hand, this approach does not take into account quadrupole and higher moments of distribution function, what leads to discrepancies from exact solution. In order to estimate the error of calculation, it is reasonably to compare it with the results of Monte-Carlo method simulation, what is implemented in this work. Monte-Carlo method is favourable to analyze kinetic processes with low concentration of charge carriers, i.e., without self-consistent field, but its advantage is possibility to conventionally solve 2- and 3-dimensional problems.

2 FORMULATION OF THE PROBLEM

2.1 Physical Model

In this work a model from (Baturin et al., 2010; Belousov, Soloviev, Chernousov, 2013) of diamond

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radiation detector consisting of thin plate, which facets are covered by metal electrodes, linked to power supply (fig. 1), is considered.

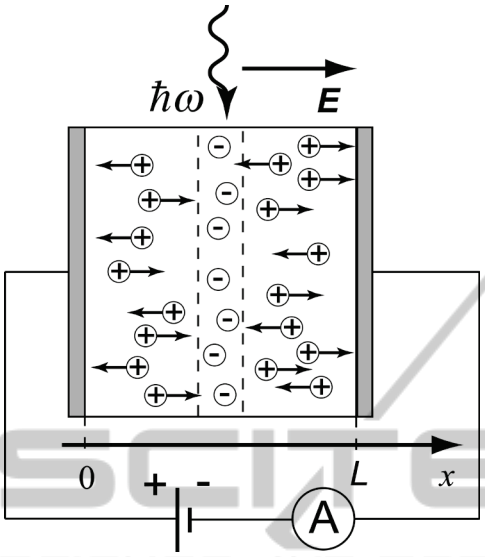

Figure 1. Physical model of diamond ionizing-radiation detector.

The plate sizes are taken much larger than its thickness – this allows to treat the system as one-dimensional in the direction perpendicular to the plates. Ionizing radiation creates electron-hole pairs and ionize impurities. As in previous studies, to fix the idea, the diamond is assumed to be doped with boron atoms (acceptor, binding energy of a hole is 0.37 eV), the non-equilibrium carriers are generated in a certain layer of the plate by laser radiation, ionizing the impurities and the case of completely permeable electrode-diamond contacts is considered (the charge carrier, coming to the contact, disappears). Charge carriers, moving into the sample, induce electric current in an external circuit (Shockley-Ramo theorem). Parameters of ionizing radiation can be determined from the pattern of current versus time dependency and from the charge traversed in an external circuit.

The concentration of impurities which generate carriers, is assumed to be constant and independent of how many carriers have been captured on them by the given point of time.

2.2 Mathematical Model

In a pure monocrystalline diamond at temperatures below 300 K, the main mechanism of charge carrier scattering is scattering by acoustic phonons. Following (Baturin et al., 2006; Varfolomeev, Gorelkin, Soloviev, 2013), the probabilities of absorption Ω^- and emission Ω^+ of phonon by charge carrier in deformation potential approximation are respectively:

$$\Omega^- = \pi \frac{\Xi^2 q}{Mc} \overline{n}_q \delta\left(\frac{\hbar^2 q^2}{2m} - \hbar cq + \frac{\hbar^2 (\boldsymbol{kq})}{m} \right), \quad (1)$$

$$\Omega^+ = \pi \frac{\Xi^2 q}{Mc} (\overline{n}_q + 1) \delta\left(\frac{\hbar^2 q^2}{2m} + \hbar cq - \frac{\hbar^2 (\boldsymbol{kq})}{m} \right), \quad (2)$$

where Ξ is a deformation potential constant, $\overline{n}_q = 1 \Big/ \left(\exp\left(\frac{\hbar sq}{k_B T} \right) - 1 \right)$ is the average number of phonons with the wave vector q, M is the mass of the crystal, m is the effective mass of the carrier, s is the speed of sound in the crystal, T is the temperature of the crystal, k_B is the Boltzmann constant, $\hbar$ is the Planck constant, $\hbar qs$ is the energy of the phonon, $\varepsilon = \hbar^2 k^2 / 2m$ is the energy of the carrier with wave vector $\boldsymbol{k}$.

Hence the frequency of the emission $\nu_e(k)$ and absorption $\nu_a(k)$ of phonons by the carrier can be found:

$$\nu_e(k) = \int \Omega^+ \frac{Vd^3\boldsymbol{q}}{(2\pi)^3} = \Psi \int_0^{\max(0,\, 2k - 2ms/\hbar)} (\overline{n}_q + 1) q^2 dq, \quad (3)$$

$$\nu_a(k) = \int \Omega^- \frac{Vd^3\boldsymbol{q}}{(2\pi)^3} = \Psi \int_{\max(0,\, 2ms/\hbar - 2k)}^{2k + 2ms/\hbar} \overline{n}_q q^2 dq, \quad (4)$$

here, $\Psi = \frac{\Xi^2}{4\pi\rho s} \frac{m}{\hbar^2 k}$, ρ is the density of diamond.

The total frequency (of carrier-phonon processes and recombination) for carrier equals

$$\nu(k) = \nu_e(k) + \nu_a(k) + \nu_{cap}(k), \quad (5)$$

where $\nu_{cap}(k)$ is the frequency of carrier capture by traps (if any).

In addition, carrier can get to the plate coating and leave the volume of the plate.

2.3 Monte-Carlo Method Usage

In our case, the use of Monte Carlo simulation consists in manifold independent simulation of carrier dynamics. Carriers are generated probabilistically in accordance with a specified density of sources of carriers situated within the sample. There are two competing processes – the generation of new particles by the source and their

capture by traps or leaving the sample. In the course of time, a dynamic equilibrium between these processes establishes (the number of "departures" equals the number of "arrivals" in a unit of time), and the average velocity of the carriers yields the value of the mobility. Clearly, the average speed of the carriers will give the less fluctuations over time and hence the more accurate value of mobility, the more particles there are in the sample in "stationary state".

Any period of time of the free motion of the carrier ends with one of the processes: emission of a phonon, absorption of a phonon, capture of the carrier by the trap or leaving the volume of the sample.

The mean free time can be found by means of expression (5) for total frequency and by the instrumentality of random number generator (Mihailov, Voitishek, 2006):

$$\tau = -\frac{1}{\nu(k)}\ln(1-r) \tag{6}$$

where r is a random number with uniform distribution on the interval [0,1].

The shift of the carrier along x axis during the mean free time is calculated:

$$\Delta x = \frac{\hbar k_x}{m}\tau + \frac{eE}{m}\frac{\tau^2}{2}, \tag{7}$$

after that the test is done whether the carrier has leaved the volume of the sample. If it has, than it disappears and the program creates another carrier, and so on until the necessary number of generated carriers is obtained (100000 particles in our calculation).

If the carrier hasn't gone from the volume of the sample, a process that aborted carrier's motion in electric field is drawn. When there aren't any traps in the sample, these processes can only be emission and absorption of a phonon. Obviously, in this case probabilities of emission or absorption are respectively

$$p^+ = \frac{\nu_e(k)}{\nu_e(k)+\nu_a(k)} \text{ and } p^- = \frac{\nu_a(k)}{\nu_e(k)+\nu_a(k)} \tag{8}$$

The magnitude of wave vector of absorbed or emitted phonon is drawn with the use of cumulative distribution function for emission (absorption) of phonon with given wave vector:

$$F_e(k,q) = \frac{\int_0^{L_{11}(q)} \left(\overline{n}_{q'}+1\right) q'^2 dq'}{\int_0^{L_{12}(q)} \left(\overline{n}_{q'}+1\right) q'^2 dq'}, \tag{9}$$

where

$$L_{12}(q) = \max\left(0,\, 2k - 2ms/\hbar\right), \tag{10}$$

$$L_{11}(q) = \max\left(0,\, \min\left(L_{12}(q), q\right)\right), \tag{11}$$

$$F_a(k,q) = \frac{\int_{L_{20}(q)}^{L_{21}(q)} \overline{n}_{q'} q'^2 dq'}{\int_{L_{20}(q)}^{L_{22}(q)} \overline{n}_{q'} q'^2 dq'}, \tag{12}$$

where

$$L_{20}(q) = \max\left(0,\, 2ms/\hbar - 2k\right), \tag{13}$$

$$L_{21}(q) = 2k + 2ms/\hbar, \tag{14}$$

$$L_{22}(q) = \max\left(\min\left(L_{21}(q), q\right), L_{20}(q)\right) \tag{15}$$

Statistical sampling of q is conducted by conventional formulae $q = F_e^{-1}(k,r)$ for emission and $q = F_a^{-1}(k,r)$ for absorption of phonon (inversion of the function is done for the second argument). Scattering angle χ is found explicitly from conservation laws and from the magnitude of phonon wave vector, for emission process by formulae

$$\cos\chi = \frac{k^2 - q\left(\frac{ms}{\hbar} + \frac{q}{2}\right)}{k\sqrt{k^2 - \frac{2msq}{\hbar}}}, \tag{16}$$

for absorption process by formulae

$$\cos\chi = \frac{k^2 - q\left(\frac{q}{2} - \frac{ms}{\hbar}\right)}{k\sqrt{k^2 + \frac{2msq}{\hbar}}} \tag{17}$$

Azimuthal angle of a new direction of carrier movement relative to initial direction is calculated as random number, uniformly distributed on the interval $[0; 2\pi]$.

2.4 Results of Simulation

Figure 2 shows the results of Monte Carlo simulation in comparison with the results obtained

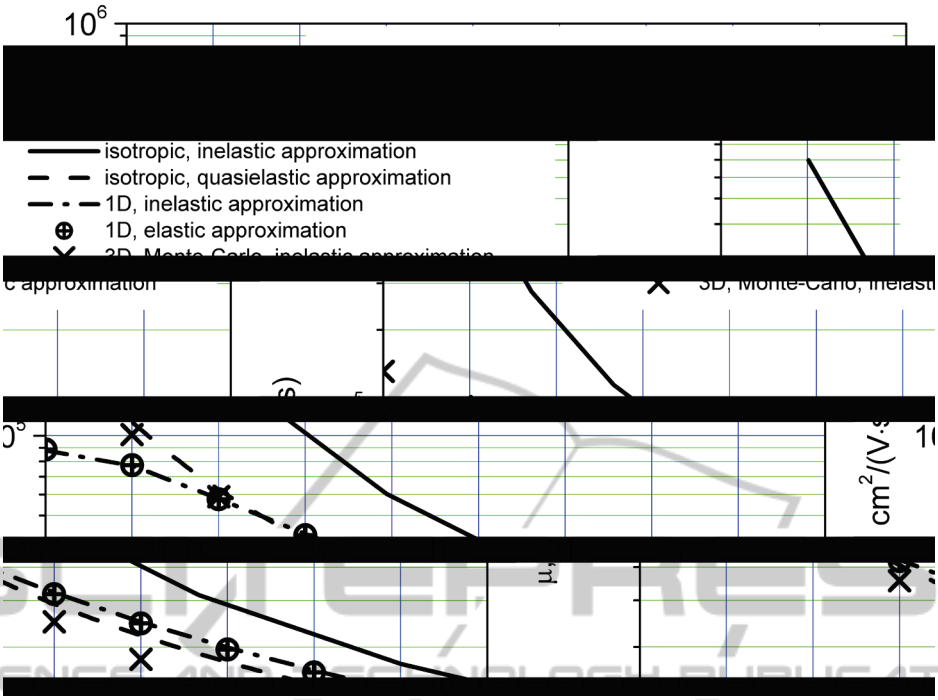

Figure 2: Results of Monte Carlo simulation in comparison with the mobility obtained by the kinetic equation method.

by the kinetic equation method (Baturin et al., 2010; Belousov, Soloviev, Chernousov, 2013). The kinetic equation method was taken in two-moment approximation (Baturin et al., 2010) in isotropic and one-dimensional versions, in quasi-elastic and inelastic approximations.

Among these variants of the kinetic equation the one-dimensional inelastic approximation seems to be the most accurate. On the other hand, the Monte Carlo method for the physical and mathematical models described above should provide even more accurate results because it is not simplified by two-term approximation. Comparison of different variants of the kinetic equation with the "exact" results obtained by the Monte Carlo method can be used to assess the accuracy of the method of kinetic equation. The value of mobility obtained by the Monte-Carlo method at 90 K should be considered as an overshoot due to a not large enough number of particles accumulated. For the one-dimensional inelastic approximation in the method of kinetic equation almost equilibrium mobility values are less than the Monte Carlo values at $T < 30$ K and more than it at $T > 30$ K. The relative difference between these mobilities is significant, up to 50%. Interestingly enough that more rough version of the kinetic equation method in the quasi-elastic isotropic approximation gives mobility values closer to the "exact" ones than the one-dimensional inelastic variant, with the relative difference from “exact” mobility up to 30%.

3 CONCLUSIONS

A comparison of the charge carriers mobilities calculated using kinetic equation and using the Monte Carlo method in diamond crystal at temperatures less than 100 K and the absence of impurities was performed. Carrier scattering is mainly caused by acoustic phonons, the electron-phonon interaction being taken in the deformation potential approximation.

Results obtained by kinetic equation method in two-moment approximation give a qualitatively correct result, but, apparently, are not suitable for an accurate enough quantitative description. The values of mobility in the quasi-elastic approximation (“law of 3/2”) at T > 20 K differ from those obtained by the Monte Carlo method no more than 30%. The one-dimensional inelastic approximation in the method of kinetic equation gives a result which differs from the Monte Carlo method no more than 50%. At the same time it should be noted that the kinetic equation method allows qualitative estimates in the presence of the self-consistent field created by charge carriers, what is complicated in the case of the use of more precise Monte Carlo method.

The obtained results yield assessments of the accuracy of various approximations used for the simulation of kinetic processes in diamond. This is important both for choosing the correct method of simulation of radiation detectors and other electronic devices based on diamond, and for more accurate definition of diamond charge carriers parameters by experimental data.

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