Monte Carlo study of $\beta$-$\text{Ga}_2\text{O}_3$ conductivity

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Abstract. Using semiclassical Monte Carlo simulations a conductivity of $\beta$-$\text{Ga}_2\text{O}_3$ is investigated considering a scattering of charge carriers on acoustical phonons, polar optical phonons and charged impurities. Modelling takes into account 12 IR active polar optical phonons modes. Dependence of mean collision frequency on energy of charge carriers is examined. The results are compared with the conclusions of other groups of researchers.

Gallium oxide in the last few years has attracted the attention of researchers in connection with the prospect of creating of high-voltage switching elements, ultraviolet LEDs, power electronics devices [1]. As it has been founded on the base of analysis of experiments on Hall effect, at temperatures in order of 100K a main contribution into the conductivity of this material makes a scattering of electrons on ionized impurities, whereas at room temperatures the conductivity is determined by scattering on lattice oscillation. Now there is no a general consensus on the relative contribution of different type scattering to the conductivity of gallium oxide. In [3-5] the electron-phonon interaction energy of $\beta$-modification of gallium oxide was modeled from the first principles and the current-voltage characteristics of this material at room temperatures were plotted. As for the mobility of the charge carriers, a value of about 100 cm$^2$/(V·s) was obtained, which is close to the experimentally observed value. In [6] an attempt to study the conductivity of this material using Monte Carlo simulation is made. The peculiarity of [6] is the accounting the electron scattering by eight modes of polar optical phonons, active in infra-red (IR) spectra, the scattering probabilities on which are attributed to a certain weights. Authors of [6] consider 8 phonon modes with symmetry $B_g$ polarized within the a-c plane and focused on electron movement in a-direction, values of electron-phonon coupling coefficients were taken from [3]. It is not clear from the text [6] from what considerations the weight of each mode is determined, it is noted only that because high-energy optical phonon modes can mask (screen) the effects of low-energy phonons, authors of [6] assigned zero weights for the low-energy optical phonon modes. In [7] electron-phonon interaction coefficients were approximated using the electron-phonon scattering energy calculated in [5], and all 12 IR-active modes of polar optical phonons were considered. Generally, coefficients of electron-phonon interaction for polar optical phonons are strongly direct-dependent and are inhered to distribution of coupled electric charges in a unit cell of crystal, so in [7] space averaging of these coefficients were performed. This average, as it is underscore in [7], can be performed because of approximately isotropic conductivity band of $\beta$-$\text{Ga}_2\text{O}_3$. The total probability of scattering by j mode of polar optical phonons is determined by the expression [7]:

$$P_j = \frac{1}{2} \int_{0}^{\infty} \frac{1}{\sigma_j(E) \sqrt{2\pi\tau_j(E)}} \exp\left(-\frac{x^2}{2\tau_j(E)}\right) dx$$
where $\rho = 5.88 \text{ g/cm}^3$ is a bulk density of the material, $\hbar \omega_j^0$ - energy of $j$ phonon mode, $v$ - electron velocity, $\varepsilon(p) = p^2 / (2m)$ - electron energy, $m = 0.28 m_e$ - electron effective mass in $\beta - \text{Ga}_2\text{O}_3$, $m_e$ - mass of free electron, $N(\omega_j) = 1 / (\exp(\hbar \omega_j / kT) - 1)$ is a phonon distribution function. Values of $\hbar \omega_j^0$ and $C_j$ are presented in [7]. Coefficients $C_j$ summarize information on coupled charge distribution and relative contribution of electron scattering on $j$ mode of polar optical phonons. Article [7] is devoted to examine how different types of electron scattering influence on conductivity of $\beta - \text{Ga}_2\text{O}_3$, authors of [7] make an attempt to determine mean relaxation time and use the relaxation time approximation (RTA) to explain transport properties of considering material. A special significance is taken by energy dependence of mean collision frequency associated with electron scattering on polar optical phonons, predicted in [7] – this process is significantly inelastic, so introduction mean relaxation time in this case require to taking into account a certain amount of assumptions. On the other hand, Monte Carlo simulations allow us to study kinetic phenomena without necessity to introduce of model collision integral, so this method can be used to independent checking of RTA. In this paper, it made an attempt to simulate the conductivity of $\beta$-gallium oxide by Monte Carlo method taking into account the scattering of charge carriers on polar optical phonons, acoustic phonons and charged impurities.

Full probability of electron scattering on acoustical phonons has a form

$$W^a(p) = \frac{D_a^2 kT m}{\pi \hbar^3 \rho v_s^2} p,$$

where $D_a = 6.9 \text{ eV}$ is a deformation potential constant of acoustic phonons [2] (it should be note, that in [7] value of deformation potential constant is assumed to be 16.6 eV), $v_s = 6.8 \cdot 10^5 \text{ cm/s}$ is a sound velocity [2], $T$ is an absolute temperature, $k$ is a Boltzmann constant.

Full probability of electron scattering on ionized impurities has a form

$$W^i(p) = \frac{16\pi n_i Z^2 e^4 r_0^2 m}{\varepsilon_a^2 \hbar^3} \frac{\sqrt{2mc(p)}}{1 + 8mc(p) r_0^2 / \hbar^2},$$

$\varepsilon_a = 11.4$ - static dielectric constant of gallium oxide, $Ze$ - charge of impurity, $n_i$ - impurity concentration, $r_0$ - Debye radius [8],

$$\frac{1}{r_0^2} = \frac{4\pi e^2}{\varepsilon_a kT} \left( n + \frac{(N_D - N_A - n)(N_A + n)}{N_D} \right),$$

where $N_D = 1.43 \cdot 10^{17} \text{ cm}^{-3}$ is a donor concentration, $N_A = 4.2 \cdot 10^{16} \text{ cm}^{-3}$ is an acceptor concentration [7], $n_{ji}$ is charged impurity concentration, $n_i = n + 2N_A$, the charge carrier concentration $n$ is calculated as follows [8]:

$$n = \frac{N_C}{2g} \exp \left( - \frac{E_D}{kT} \right) + \frac{N_A}{2} \left[ \frac{1}{2g} \left( N_C \exp \left( - \frac{E_D}{kT} \right) + gN_A \right)^2 + 4gN_C (N_D - N_A) \exp \left( - \frac{E_D}{kT} \right) \right],$$
\( E_D = 28.5 \text{meV} \) is an energy of donor ionization, \( g \) is a factor of degeneracy (we assume \( g = 2 \)), \( N_c = 2 \left( \frac{(2\pi mkT)}{(2\pi \hbar)^3} \right)^{3/2} \) - effective density of state in a conductivity band. The characteristic value of the charge carriers concentration is about \( 10^{17} \text{cm}^{-3} \).

Monte Carlo modeling was carried out by way which is described, for example, in our previous work [9]. We assume that between subsequent scatterings electron moves in according to classical equations of motion. A mean free time is evaluated from the equation:

\[
 r = \exp \left[ -\int_{0}^{t} W(p(t'))dt' \right],
\]

where \( r \) is a the random variate uniformly distributed on segment \([0, 1]\), \( W(p)\) is a collision probability summarized on all scattering mechanisms,

\[
 W(p) = W^\infty(p) + W^n(p) + \sum_{j} W^\infty_j(p) = \sum_{j} W_j(p).
\]

After determination of scattering moment we should choose scattering mechanism. We compare each scattering channel with a segment, whose length is equal to the probability of scattering, and arrange these segments one after another. Then one plays a random variable \( s \) uniformly distributed on the segment \([0, W(p)]\). We choose the scattering mechanism corresponding to the segment within the value of \( s \) is localized. Calculations for different electrons are performed independently, resulting values of electron velocity are averaged on ensemble and (in case of static conductivity modeling) on time.

The most interesting is to study the scattering of charge carriers on polar optical phonons. In [7] the dependence of the average collision frequency \( 1/\tau \) of electrons and polar optical phonons on the energy \( \varepsilon \) of charge carriers is studied. In [7] the expression for mean collision frequency has a form:

\[
 \frac{1}{\tau(\varepsilon)} = \sum_{j} C_j^2 \left\{ n(\omega_j) B^+ \left[ \sqrt{1 + \frac{\hbar \omega_j}{\varepsilon}} + \frac{\hbar \omega_j}{\varepsilon} \sinh^{-1} \left( \frac{\varepsilon}{\hbar \omega_j} \right) \right] + \left[ n(\omega_j) + 1 \right] B^- \left[ \sqrt{1 - \frac{\hbar \omega_j}{\varepsilon}} + \frac{\hbar \omega_j}{\varepsilon} \sinh^{-1} \left( \frac{\varepsilon}{\hbar \omega_j} - 1 \right) \right] \right\},
\]

where \( B^\pm \) is a Farvacque correction [10], \( f_0 \) is an equilibrium distribution function of electrons

\[
 B^\pm = \pm \frac{f_0(\varepsilon \pm \hbar \omega_j) - f(\varepsilon)}{\hbar \omega_j \left( \frac{d f_0}{d \varepsilon} / \frac{d f}{d \varepsilon} \right)}.
\]

Generally, the Farvacque correction allows us to specify the description of the substantially inelastic scattering of electrons on optical phonons using the approximation of constant relaxation time. Knowledge of the energy dependence of the average relaxation time allows us to draw conclusions about the contribution of this scattering type to the conductivity. The dependence of the average collision frequency on the energy of the charge carriers obtained from the simulation for temperatures of 100 K and 300 K is shown on figure 1, a comparison of the dependence of the average collision frequency obtained from the simulation and plotted using the formula (8), taking into account the Farvacque correction and without this correction, is presented on figure 2 (in last case we assume \( B^\pm = 1 \)).
Figure 1. Dependence of mean collision frequency on electron energy at $T = 300$ K and $T = 100$ K (scattering on polar optical phonons only).

Figure 2. Dependence of mean collision frequency on electron energy at $T = 300$ K. Curve 1 is plotted using (8) with $B^z = 1$, curve 2 is plotted using (8), (9), taking into account a Farvacque correction, curve 3 is fitted by data of Monte Carlo simulations, taking into account scattering of charge carriers on polar optical phonons only, curve 4 is fitted by data of Monte Carlo simulations, taking into account scattering of charge carriers on polar optical, acoustical phonons and charged impurities.
Expression (9) for mean collision frequency can be verified immediately using Monte Carlo approximation in the following way. If on some time step the collision is fixed, we should save in array a number of the time step, energy of electron before collision, number of scattering mode. After the end of modeling we calculates time \( \tau \) between each two consecutive collisions, collects records on electron collisions on different scatters in different lists (we consider acoustic phonons, charged impurities, 12 polar optical modes with phonon adsorption and 12 polar optical modes with phonon emission). Next, for each mode we divide energy interval from 0 to \( E_{\text{max}} \) into \( M \) bins and collects collisions with electron energy \( \varepsilon_j < \varepsilon(p) \leq \varepsilon_{j+1} \) into \( j \) list, \( j \in [0, M-1] \). Then we calculate \( \langle 1/\tau \rangle_j \) for each bin \( j \) in a list corresponded to a certain collision mode \( i \), whereupon we calculate \( \langle 1/\tau \rangle \), averaged on all collision modes taking into account relative weight of each mode (relation of collisions, corresponded to \( j \) bin of \( i \) mode to sum of collisions of \( j \) bin on all modes). Dependencies, obtained in this way, are presented on figure 1 and figure 2.

From figure 2 it can be seen that the dependence of mean collision frequency, taking into account scattering on optical phonons (curve 3), obtained from simulations, has form, similar to form of the dependence calculated by the formula (8) (curve 2) at energies more the 0.05 eV, which confirms that application of the Farvacque correction is a good approximation to determine mean scattering frequency in material with predominance of inelastic scattering processes. Taking into account elastic scattering mechanisms (scattering on acoustical phonons and charged impurities) lead to increase of mean collision frequency at small energy of electron (curve 4 on figure 2).

The dependence of the direct current density on the electric field strength applied to the sample is shown on figure 3. At a temperature of 300 K, the dependence of the current density on the electric field strength is approximately linear. The obtained values of mobility (about 100 \( \text{cm}^2/\text{V} \cdot \text{s} \)) are close to those presented in other experimental and theoretical works. A nonlinear form of current-voltage characteristic at temperatures of about 100 K can be explained in the following way. Scattering probability on charged impurities has a sharp maximum near \( \varepsilon = 0 \), then at \( \varepsilon \geq 0.01 \text{ eV} \) it slowly decreases. But in energy interval from 0 to 0.02 eV total scattering probability with adsorption of polar optical phonons rises steeply. At temperature of 100 K (\( kT \sim 0.009 \text{ eV} \)) at \( E \sim 50 \cdot 10^3 \text{ V/cm} \) an addition to electron energy is about 0.006 eV, so heating up of electron gas by electric field leads to activate scattering on optical phonons and increasing of total scattering probability and, correspondingly, decreasing of mean velocity. At temperature of 300 K a greater part of electrons has energy enough to activate polar optical modes, so heating up of electron gas under the influence of electric field don’t lead to significant change of total scattering probability.

Thus, using the parameters of electron-phonon interaction obtained from quantum chemical modeling in [3-5] and the approximation of these data obtained in [7], a semiclassical Monte Carlo simulation of the conductivity of \( \beta \)-modification of gallium oxide was carried out, taking into account the scattering of current carriers on polar optical phonons, acoustic phonons and charged impurities. The dependence of the average collision frequency on the energy of the charge carriers was studied, and the results were compared with calculations based on explicit formulas.
Figure 3. Dependence of direct current density on the electric field strength at temperatures $T = 100\,\text{K}$, $T = 200\,\text{K}$, $T = 300\,\text{K}$.

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