Impacts of Band Structures and Scattering Processes on High-field Carrier Transport in Wide Bandgap Semiconductors

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Abstract

In this talk, the results of our work on the impact of band structures and scattering processes on the high-field carrier transport properties of wide-bandgap semiconductors will be presented. Using a tunable band structure model, Monte Carlo simulation is performed to obtain transport characteristics including the impact ionization coefficients and the drift-velocities. It is shown that the smaller Brillouin zone width significantly reduces the impact ionization coefficients. The study also revealed that the impact ionization coefficient may show a positive temperature dependence when the Bloch oscillation occurs.

I. Introduction

Wide-bandgap semiconductors such as silicon carbide (SiC), gallium nitride (GaN), gallium oxide, and diamond have been attracting attention as materials suitable for power device applications toward an energy-saving and carbon-neutral society. Those materials have high breakdown electric field, which enables the simultaneous achievement of low resistivity and high blocking voltage. The high breakdown field of wide-bandgap semiconductors is usually considered to be attributed to their large bandgap (E_g). This is because that the main cause of the high-field breakdown is the avalanche multiplication of carriers through the impact ionization and it can occur when the carrier energy exceeds E_g. However, phenomena have been reported that cannot be explained only by this naïve scenario. For example, the electron impact ionization coefficient of 4H-SiC along the $\langle 0001\rangle$ direction is known to be much smaller than that along the $\langle 11\bar{2}0\rangle$ direction [1], [2] and the hole impact ionization coefficient [3]–[6], despite the common E_g for these cases. The electron impact ionization coefficient of 4H-SiC along the $\langle 0001\rangle$ direction is also smaller than a recently reported electron impact ionization coefficient of GaN [7], which has larger E_g. This suggests significant impacts of the band structure parameters such as the Brillouin zone (BZ) width and band-edge effective mass other than E_g. To clarify those issues, we conducted theoretical study on high-field transport characteristics by performing Monte Carlo simulation utilizing a tunable band structure model [8], [9].

II. Model

We employ a tunable band structure model with a dispersion:

$$E(\boldsymbol{k}) = \bigcup_{n=1}^{N} E_n(\boldsymbol{k}), \quad (1)$$

$$E_n(\boldsymbol{k}) = (n-1)\Delta E + \sum_{i=x,y,z} 2t_i[1-\cos(k_i a_i)]. \quad (2)$$

Here, $\boldsymbol{k} = (k_x, k_y, k_z)$ is the wavevector, n is the band index, N is the total number of bands considered, ΔE is the energy interval between adjacent bands, and a_i is the lattice period along the i-direction. The transfer energy, t_i, is given by the band-edge effective mass m_i as $t_i = (\hbar/a_i)^2/(2m_i)$ $(i = x, y, z)$. m_i is set to be $0.3\,m_0$. We assume an electric field, F, along the x-direction, and a_x is treated as a variable when investigating the impacts of the BZ width, $G_x = 2\pi/a_x$, along the k_x direction. Specifically, three values of $0.25\,\mathrm{nm}$, $0.5\,\mathrm{nm}$ and $1\,\mathrm{nm}$ are considered as a_x, while $a_y = a_z = 0.5\,\mathrm{nm}$ are fixed. For $a_x = 0.5\,\mathrm{nm}$, we set $N = 10$ and $\Delta E = 1\,\mathrm{eV}$. For other values of $a_x = 0.25\,\mathrm{nm}$ and $1\,\mathrm{nm}$, N and ΔE are set so as that both the total number of states and the total band width coincide with those of $a_x = 0.5\,\mathrm{nm}$.

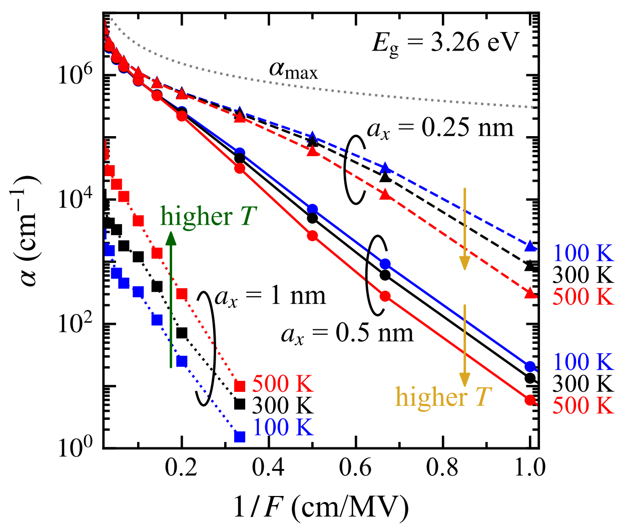

Fig. 1. Inverse electric field dependence of the impact ionization coefficients α with different BZ widths of $G_x = 2\pi/a_x$ for $E_g = 3.26\,\text{eV}$. Results for $T = 100, 300, 500\,\text{K}$ are shown by blue, black, and red symbols, respectively. α for $G_x = 2\pi/(1\,\text{nm})$ increases with T, while others decrease at higher T. The gray dotted line is the maximum impact ionization coefficient of $\alpha_{\max} = eF/E_g$.

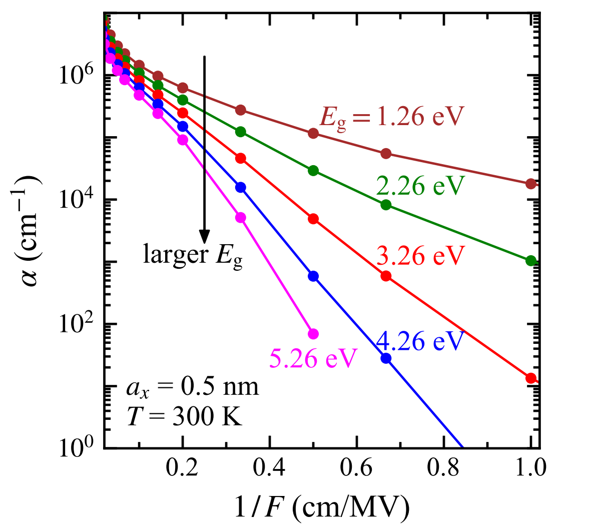

Fig. 2. Impact ionization coefficients α as a function of inverse electric field for different E_g. $a_x = 0.5\,\text{nm}$ and $T = 300\,\text{K}$.

We consider elastic acoustic and inelastic non-polar optical phonon scatterings. We assume that the scattering rates are proportional to the final density-of-states. In addition to the phonon scatterings, we take account of the impact ionization using the impact ionization rates with the form give by

$$W_{\text{ii}}(E) = a[(E - E_g)/E_0]^b, \quad (E > E_g), \qquad (3)$$

with $a = 1.11 \times 10^{13}\,\text{s}^{-1}$, $b = 3.38$, and $E_0 = 3.26\,\text{eV}$.

We perform a full-band Monte Carlo simulation to calculate the drift velocity, v_d, and the impact ionization coefficient of electrons, α, assuming the above-mentioned band structures and scattering mechanisms including impact ionization.

III. Results and Discussion

Figure 1 shows the impact ionization coefficient of electrons, α, as a function of the inverse electric field, F^{-1}. We see that α is larger for a larger BZ width $G_x = 2\pi/a_x$ (or smaller a_x). This can be attributed basically to the larger average group velocity along the x-direction. In addition, a smaller BZ width such as $G_x = 2\pi/(1\,\text{nm})$ leads to easier occurrence of Bloch oscillations, which suppress the energy gain from the electric field and result in smaller α. As for the temperature dependence, α for $G_x = 2\pi/(0.25\,\text{nm})$ and $2\pi/(0.5\,\text{nm})$ decreases at higher temperatures due to enhanced phonon scatterings. On the contrary, α for $G_x = 2\pi/(1\,\text{nm})$ increases with temperature. The positive temperature dependence is related to Bloch oscillations.

In Fig. 2, E_g dependence of α is presented. As expected, the increase of E_g leads to smaller α. However, even the increase of E_g from $3.26\,\text{eV}$ to $5.26\,\text{eV}$ does not outperform the impacts of decrease of G_x from $2\pi/(0.5\,\text{nm})$ to $2\pi/(1\,\text{nm})$ (see Fig. 1). This indicates that the impacts of E_g on α is not so significant as those of the BZ width and group velocity, which may be an important aspect when discussing the material dependence of impact ionization coefficients.

In the talk, effects of scattering processes on the drift-velocities and the impact ionization coefficients will also be presented.

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