Transient Analysis of Impact Ionization Anisotropy using Realistic Band Structure for GaAs

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1. Introduction

Recently high electric field effects such as impact ionization(I.I.) play a very important role in hot carriers transport as device dimensions are fastly scaled down. The exact model of I.I. is, therefore, demanded on device simulation. Keldysh formula with the power exponent of 2 has been extensively used to describe impact ionization though its physical meaning is lost at high field. Since Keldysh formula based on parabolic band is not suitable to simulate high energy electron transport accurately, a exact energy band structure has to be obtained and accurate I.I. scattering model be presented to analyze I.I process.

We have previously presented energy dependent I.I. scattering model as a form of modified Keldysh formula [1] and investigate the energy dependence on I.I. scattering rate in the present study once again in detail. It has been presented that both I.I. threshold energy and scattering rate are highly anisotropic in the near threshold energy range. The I.I. coefficients are, however, isotropic in case that we calculate and use the modified Keldysh formula. The transient analysis have been, therefore, done using GaAs realistic band structure and Monte Carlo simulation for investigating whether anisotropy of I.I. for GaAs depends on time or not.

We calculate the distributions of group velocity, a number of I.I. events, anisotropic ratio and average energy during very short time of about 0.3ps elapsed after high electric field is applied along the <100>, <110> and <111> direction. Anisotropy of I.I. has been also analyzed in detail as distribution of electron related to I.I. process has been shown in the momentum space as a function of time.

2. Band structure and I.I.

A realistic band structure is necessary to investigate hot electron transport in a high electric field because analytical band structures largely differ from the realistic band especially in the high energy range , in which I.I. effect is very strong.

In the present study, the energy band structure of GaAs is calculated by the use of the local empirical pseudopotential method[2], in which the periodic part of the Bloch wave function is expanded with a basis set of reciprocal lattice vectors **G**. We have employed a set of 113**G** vectors for the expansion. Nonlocal corrections and spin-orbit splitting are not included since their effects are very small. We have extracted new local form factors and compared with experimental results[3] at important points such as Γ-, L- and X-valley.

The form factors determined by using the steepest descent method[4] are shown in Table I. V^s and V^a are symmetric and asymmetric form factor, respectively. Calculated energies with experimental results are shown in Table II. The good agreement of the calculated results to the reported experimental data on energy band gap demonstrates that the new derived realistic energy band structure is correct and yields accurate I.I. scattering rate for a full band Monte Carlo simulation. Figure 1 shows four conduction band and three valence band calculated in the present study for GaAs .

Table I. Empirical pseudopotential form factors in Ry.

V_3^s	V_8^s	V_{11}^s	V_3^a	V_4^a	V_{11}^a
-0.2350	0.0164	0.0500	0.0786	0.0526	0.0051

Table II. Comparison with the experimental[3] and calculated energies in eV.

State	Experimental	Calculated
Γ_{6c} - Γ_{8v}	1.42	1.42
L_{6c} - Γ_{8v}	1.71	1.71
X_{6c} - Γ_{8v}	1.90	1.91

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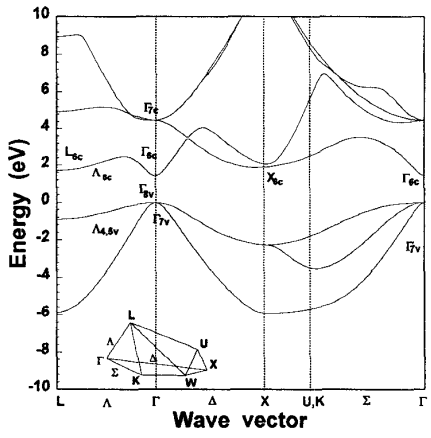

Fig. 1. Full band E-***k*** relationship for GaAs obtained from empirical pseudopotential method

The I.I. is a kind of an electron-electron interaction process occurred in semiconductor under high electric field. If a high energy electron in the conduction band(state 1) collides with an electron in the valence band(state 2), an electron-hole pair is generated, leaving two electrons in the conduction band(state 1' and 2') and a hole in the valence band(state 2). The I.I. rate is calculated from the Fermi's golden rule as follows:

$$S_{ii}(1) = \frac{1}{2}\sum_{2}\sum_{1'}\sum_{2'}\frac{2\pi}{\hbar}[|M_a|^2+|M_b|^2+|M_a-M_b|^2] \times\delta(E_1+E_2-E_{1'}-E_{2'}) . \quad (1)$$

M_a and M_b are matrix element of I.I. and delta function represents the energy conservation. The direct M_a and exchange M_b terms are

$$M_a = < \psi^*_{1'}(r_1)\ \psi^*_{2'}(r_2)|\frac{e^2}{4\pi\ \varepsilon\ (q,\omega)|r_1-r_2|}| \psi^*_1(r_1)\ \psi^*_2(r_2)> ,$$
$$M_b = < \psi^*_{2'}(r_1)\ \psi^*_{1'}(r_2)|\frac{e^2}{4\pi\ \varepsilon\ (q,\omega)|r_1-r_2|}| \psi^*_1(r_1)\ \psi^*_2(r_2)> , \quad (2)$$

where ψ is pseudowave function in the form of expanding with a basis set of reciprocal lattice vector. The $\varepsilon\ (q,\omega)$ is the wavevector and frequency dependent dielectric function[5].

Brillouin zone(BZ) is divided into cubic mesh for calculating I.I. rate, and the size of cubic mesh is $1/16(2\pi/a)$, where a is the lattice constant of GaAs. We use a tetrahedron method[6], in which each cubic is divided into six equal-volume-tetrahedron and each tetrahedron is integrated as the basic volume. The total number of tetrahedrons used for the integration is 98,304 and the total number of grid points used in the BZ is 17,585. Figure 2 shows equipotential curves of second conduction band energy and distribution of I.I. rates in 1/48 reduced Brillouin zone in case of k_z=0. I.I. donot nearly occur at X valley and I.I. rate is high at K direction, in which energy is high. We know I.I. rates very change along the direction as energy depends on direction in the momentum space and they depend on energy as shown in Fig. 2. We previously developed an I.I. model on the basis of a full realistic scheme and presented that modified Keldysh formula with the power exponent of 7.8 in range of $1.73eV \le E < 3.55eV$ and 5.6 in range of $E \ge 3.55eV$ shows very good agreement with experimental results in GaAs[1]. Threshold energy of modified Keldysh formula is 1.73eV. We use, therefore, the energy dependent I.I. rate calculated in the previous study for investigating I.I. anisotropy as a function of field direction.

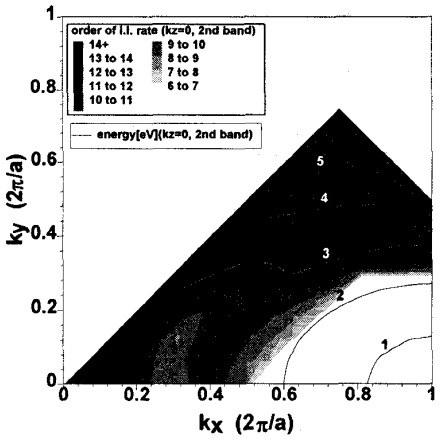

Fig. 2. Distribution of second conduction band energy and I.I. rate in Brillouin zone(k_z=0)

3. Monte Carlo simulation

Monte Carlo simulation is done for transient and steady state analysis of I.I. anisotropy. We use phonon scattering rates and phonon dispersion relation calculated in the previous study[1]. BZ is divided into (k_x, k_y, k_z)=$1/20(2\pi/a)$ and the total number of grid points is 33,861. The general full band Monte Carlo algorithm[7] is used, and a kind of scattering, energy state, free flight time etc. are determined by the random numbers.

Tagaki et al. reported firstly if an electric field is applied to different crystallographic directions, different I.I. characteristics are observed in Si[8]. We calculate I.I. coefficients at 4ps after electric fields are applied along the different directions in order to investigate I.I. characteristics for GaAs.

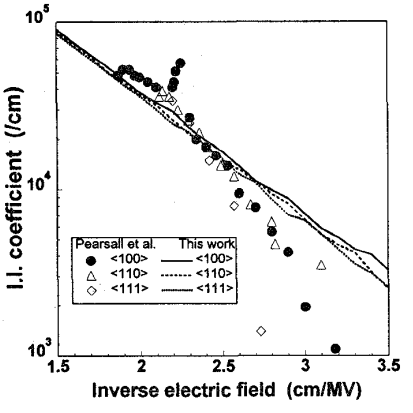

Fig. 3. I.I. coefficients at room temperature as a function of inverse electric field.

Figure 3 shows the calculated I.I. coefficients as a function of inverse electric field along the <100>, <110> and <111> direction and compares with experimental results[9]. The results show good agreement with the experimental data. Differences in I.I. coefficients for the electric field directions are, however, nearly not shown though I.I. rates depend on the directions such as Fig. 2. We investigate carrier transport during the very short time after the electric field is applied along the <100>, <110> and <111> direction, since we think I.I. anisotropy disappears after steady state.

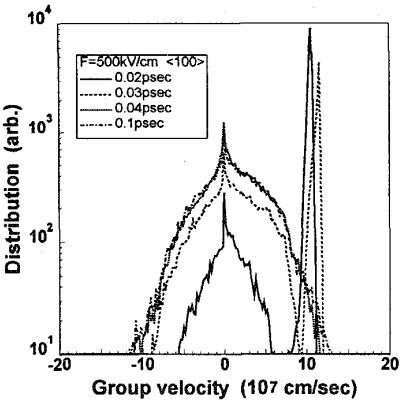

Fig. 4. Group velocity distributions at 0.02ps, 0.03ps, 0.04ps and 0.1ps after a 500kV/cm electric field is applied along the <100> direction

Firstly, the group velocity is calculated to analyze carrier transport until 0.1ps. Figure 4 shows distribution of group velocity at 0.02ps, 0.03ps, 0.04ps and 0.1ps after 500kV/cm electric field is applied along the <100> direction. At 0.02ps the right side peak of the group velocity distribution is due to light electrons in Γ valley, indicating ballistic transport. The light electrons, so called lucky electrons, contribute to velocity overshoot as you know. At 0.1ps, the distribution is close to the Maxwell-Boltzmann distribution, indicating the steady state condition.

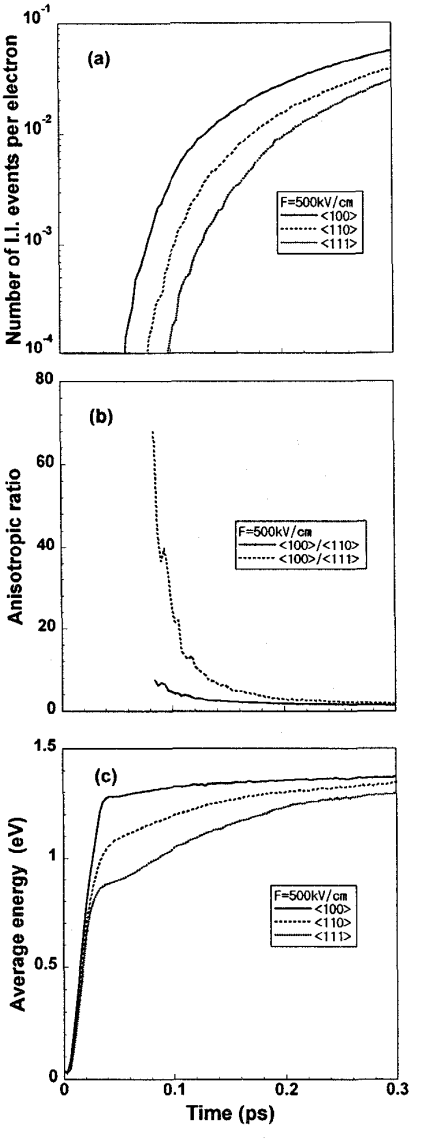

Fig. 5 (a) A number of impact ionization events, (b) anisotropic ratio and (c) average energy as a function of elapsed time after adding electric field of 500kV/cm along the <100>, <110> and <111> direction.

Figures 5(a), 5(b) and 5(c) show the number of I.I. events, anisotropic ratio and average energy as a function of elapsed time after adding electric field of 500kV/cm along the <100>, <110> and <111> direction.

The I.I. events is more frequent along the <100> direction than along the <110> and <111> directions. The I.I. shows anisotropy during transient time and anisotropy of <111> direction is stronger than one of <110> direction. Anisotropic property of I.I. is surely observed during the very short time after the electric field is applied, as shown in Fig. 5(a) and 5(b). We know anisotropic I.I. during the transit time is due to the different average energy and different I.I. rates according to the crystallographic direction.

Anisotropic properties of I.I. are strong before about 0.3ps since the difference for average energy along the directions is significant, but are vanished at steady state after about 0.3ps as average energy is nearly same regardless of field direction, as shown in Fig. 5(c).

In order to investigate this phenomenon in detail, we calculate and draw position of electrons that undergo I.I. in BZ at 0.02ps and 0.3ps after the 500kV/cm electric field is applied along the <100> and <111> directions, as shown in Fig. 6(a) and 6(b). At 0.02ps, I.I. has nearly not occurred as average energy is below 0.5eV, but lucky electrons obtain energy enough to occur I.I. during very short time, and occur I.I. after transition from Γ-valley to other region.

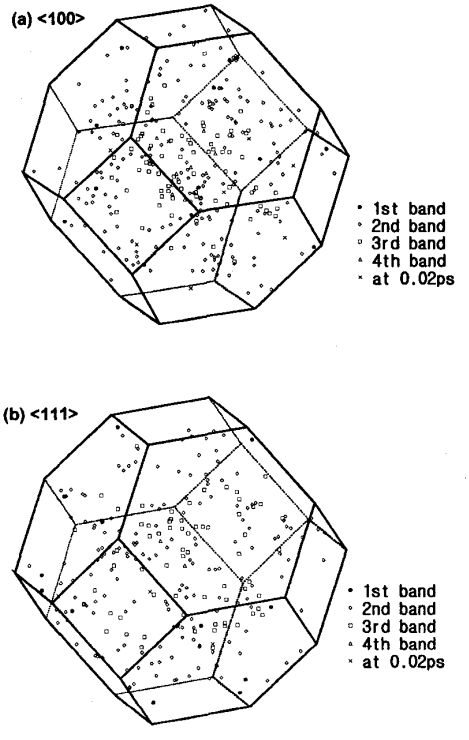

Fig. 6. Distribution of electron related to impact ionization processes in momentum space at 0.02ps(cross mark) and 0.3ps after the 500kV/cm electric field is applied along (a) <100> direction (b) <111> direction.

At 0.3ps, electrons of conduction band undergo I.I. at entire Brillouin zone regardless of applied electric field directions and a kind of band, as shown in Fig. 6(a) and 6(b). Anisotropy of I.I., therefore, disappears after time elapsed to steady state. That is the reason that impact ionization rate is anisotropic, but impact ionization coefficient do not show anisotropy in the Monte Carlo simulation.

4. Conclusions

We have investigated anisotropic properties for I.I. process of GaAs using Monte Carlo simulation and a realistic energy band structure. The realistic energy band structure is derived from the empirical pseudopotential method and I.I. scattering rates are calculated by the Fermi's golden rule. For observing anisotropic properties of I.I. coefficients, a Monte Carlo simulation has been done after electric fields are applied along the different directions.

Since we cannot, however, observe anisotropy for I.I. coefficients, carrier transport has been investigated during the very short time after electric field is applied. We calculate the distributions of group velocity, a number of I.I. events, anisotropic ratio and average energy during very short time of about 0.3ps elapsed after high electric field is applied along the <100>, <110> and <111> direction. A result of transient analysis for I.I. has presented that anisotropy of I.I. only arises during transient state and I.I. is isotropic under steady state. Anisotropic characteristics of impact ionization for GaAs which is presented in this paper, we think, can be used in carrying out a transient analysis for GaAs devices under high electric field.

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