Angular dependence of nonparabolicity factor of energy band structures

Nobuya Fujimoto, Akira Hiroki, and Shin Hiratoko
Graduate School of Science and Technology, Kyoto Institute of Technology
Kyoto, Japan
hiroki@kit.ac.jp

Abstract—**This paper describes an angular dependence of the nonparabolicity factor of energy band structures and the influence on the density of states (DOS). The angular dependence of the nonparabolicity factor is investigated using the silicon band structure data calculated by the first principle calculation. In order to investigate the influence of the angular dependence on DOS, we propose a macroscopic model to estimate the average nonparabolicity factor calculated from the information of the band structure in several directions. It is found that the angular dependence of the nonparabolicity factor is essential to model not only DOS but also E-k dispersion relations.**

Keywords- nonparabolicity factor, band structure, density of states, angular dependence

I. INTRODUCTION

Advanced devices, such as FinFETs and nanowire transistors, are required in low voltage (< 1V) operation [1]. In these devices, low energy carrier transport dominates the electric characteristics. To simulate the characteristics, it is essential to model not only the density of states (DOS) but also E-k dispersion relations because of the scattering rates, post-free-flight carrier energies, and post-scattering momentum selections [2]. Full band approach allows the accurate modeling and shows that the inclusion of the nonparabolicity of the energy band structures is essential [3], [4]. This approach, however, requires enormous computer resources. On the other hand, macroscopic models used in the DD and HD approaches have computational efficiency. These approaches need the physical macroscopic models, such as carrier concentration, mobility and impact ionization models. These macroscopic models include the average parameters, such as the intrinsic carrier concentration, the effective density of states and the nonparabolicity factor. However, the parameters used in the macroscopic models are little consistent with the microscopic parameters calculated from the E-k dispersion relations. An inconsistency between the intrinsic carrier concentration and effective masses has been carefully investigated [5] and the results have been used in the DD models [6].

In this paper, we investigate the angular dependence of the nonparabolicity factor of silicon energy bands. The angular dependence is estimated from the E-k dispersion relations calculated using the first principle program. A macroscopic model of the nonparabolicity factor is proposed, in which the factor is averaged over the several directions. To confirm the model accuracy, DOS calculated with the averaged factor is compared with the DOS data using the first principle program.

II. ANGULAR DEPENDENCE OF NONPARABOLICITY

The nonparabolicity of energy band structure has been modeled by Kane's dispersion relations [7]. In this paper, the dispersion relations is modified to consider the angular dependence by the following equation,

$$E\left[1+\alpha(\theta,\phi)E\right]=\frac{\hbar^2k^2}{2m^*(\theta,\phi)} \tag{1}$$

where E is the energy in the conduction band, α is the nonparabolicity factor, $\hbar$ is the reduced Plank constant, k is the wave vector, m^* is the effective mass. θ and ϕ are the polar angle and azimuthal angle in the polar coordinate system, respectively. The origin of the system is placed at the bottom of the valley. The coordinate axes are identical to the principal axes of the equivalent energy ellipsoidal. The effective mass $m^*(\theta,\phi)$ is defined as the limited value in the (θ,ϕ) direction in the limit of k to zero. The effective mass is obtained by using the least squares method in the range of $E \leq 0.05$ eV. The nonparabolicity factor $\alpha(\theta,\phi)$ is calculated to fit the band structure data calculated by the first principle calculation software, ecalj [8]. The nonparabolicity factor is obtained by using the least squares method in the range of $E \leq 0.5$ eV. The nonparabolicity factors and effective masses in the seven directions are shown in Table 1. The energy dispersion curves calculated by using the nonparabolicity factors and the effective masses are shown in Fig. 1 comparing with the usual macroscopic model ($\alpha = 0.5$ eV^{-1}) [9]. In Fig. 1, (a) $(\pi/2,0)$, (b) $(\pi/2,\pi/2)$ and (c) $(0,\phi)$ show E-k dispersion relations in principal directions, (d) $(\pi/2,\pi/4)$, (e) $(\pi/4,0)$, (f) $(\pi/4,\pi/2)$ and (g) $(\cos^{-1}(1/\sqrt{3}),\pi/4)$ show E-k dispersion relations in the middle directions of principal directions. In the principal directions, $(\pi/2,0)$, $(\pi/2,\pi/2)$ and $(0,\phi)$, the α values are small, which are close to the suggested value 0.2 eV^{-1} [2]. On the other hand, in the directions, $(\pi/4,\pi/2)$ and $(\cos^{-1}(1/\sqrt{3}),\pi/4)$, the nonparabolicity is significant. In $(\pi/4,\pi/2)$ direction, the difference of energy between $\alpha =$ 3.43 and 0.5 eV^{-1} is 0.18 eV at $k = 0.15 \times 2\pi/a$ m^{-1}. It is found that the angular dependence of the nonparabolicity factor is essential to simulate the carrier energy at post-free-flight.

III. MACROSCOPIC NONPARABOLICITY FACTOR MODEL

In order to investigate the relationship between the macroscopic and microscopic parameters, we consider the average values integrated over the constant energy surfaces in the wave vector space. The square of the wave vector length is calculated from (1).

$$k^2(E,\theta,\phi)=\frac{2}{\hbar^2}m^*(\theta,\phi)E[1+\alpha(\theta,\phi)E] \quad (2)$$

The average value of the square wave vector length is calculated by the following equation,

$$k^2=\frac{\int_\Omega k^2(E_0,\theta,\phi)dS}{\int_\Omega dS} \quad (3)$$

where E_0 is constant energy, dS is the infinitesimal area on the constant energy surface Ω. Substituting (2) into (3), the average value of the square wave vector length becomes,

$$k^2=\int_\Omega \frac{2}{\hbar^2}m^*(\theta,\phi)E_0[1+\alpha(\theta,\phi)E_0]dS\Big/\int_\Omega dS \,. \quad (4)$$

To investigate the angular dependence of nonparabolicity factor, the integral regions are divided into several directions,

$$k^2=\frac{1}{n}\sum_{i=1}^{n}\frac{2m^*(\theta_i,\phi_i)}{\hbar^2}E_0[1+\alpha(\theta_i,\phi_i)E_0] \quad (5)$$

where i runs over 1 to n which is the number of the divided area. We assume the effective mass and the nonparabolicity factor are constant in each area.

For the macroscopic parameters, the following Kane's dispersion relation is satisfied.

$$E(1+\alpha E)=\frac{\hbar^2k^2}{2m^*} \quad (6)$$

The square of the average wave vector length becomes,

$$k^2=\frac{2}{\hbar^2}m^*E(1+\alpha E). \quad (7)$$

From (5) and (7), we can get the relationship between the microscopic and macroscopic parameters,

$$\frac{2m^*}{\hbar^2}E_0(1+\alpha E_0)=\frac{1}{n}\sum_{i=1}^{n}\frac{2m^*(\theta_i,\phi_i)}{\hbar^2}E_0[1+\alpha(\theta_i,\phi_i)E_0]$$

$$\left[m^*-\frac{1}{n}\sum_{i=1}^{n}m^*(\theta_i,\phi_i)\right]E_0$$

$$+\left[m^*\alpha-\frac{1}{n}\sum_{i=1}^{n}m^*(\theta_i,\phi_i)\alpha(\theta_i,\phi_i)\right]E_0^2=0\,. \quad (8)$$

Assuming the above equation is satisfied on an arbitrary energy surface, we propose a macroscopic model which is averaged by the weighted microscopic nonparabolicity factors over the several directions, as the following equations.

$$m^*=\frac{1}{n}\sum_{i=1}^{n}m^*(\theta_i,\phi_i) \quad (9)$$

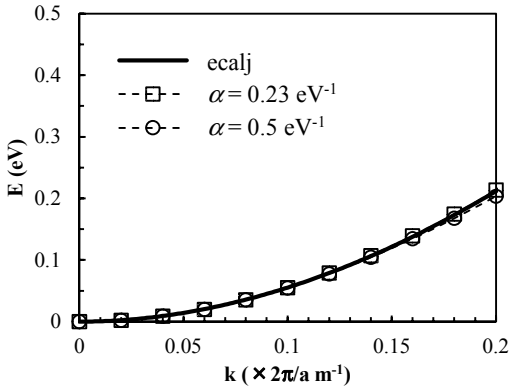
$$\alpha=\frac{\sum_{i=1}^{n}m^*(\theta_i,\phi_i)\alpha(\theta_i,\phi_i)}{\sum_{i=1}^{n}m^*(\theta_i,\phi_i)} \quad (10)$$

In n = 3, using only the values in the principal directions, (π/2,0), (π/2,π/2) and (0,ϕ), in Table 1, the average nonparabolicity factor is estimated to be 0.21 eV^{-1}. In n = 7, using the values in the seven directions in Table 1, the average factor is 0.54 eV^{-1}. The average nonparabolicity factor 0.21 eV^{-1} is much smaller than 0.5 eV^{-1} because the nonparabolicity factors in the principal directions, (π/2,0), (π/2,π/2) and (0,ϕ), are small. On the other hand, the average nonparabolicity factor 0.54 eV^{-1} is close to 0.5 eV^{-1} because the nonparabolicity factors in the directions, (π/4,π/2) and (cos^{-1}(1/√3),π/4), are significant.

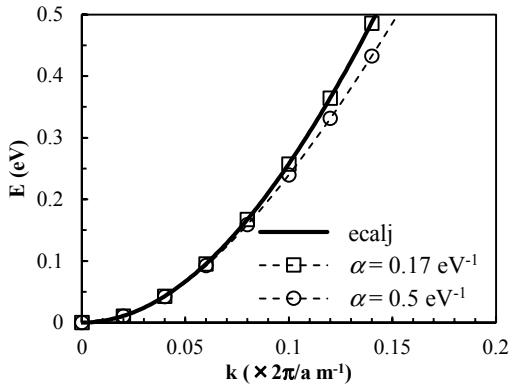
In order to verify the macroscopic model, the density of states is compared with the ecalj result. Using the average nonparabolicity factor, the density of states $D(E)$ is given by the following equation,

$$D(E)=4\pi g\left(\frac{2m_{dc}}{h^2}\right)^{3/2}(1+2\alpha E)\sqrt{E(1+\alpha E)} \quad (11)$$

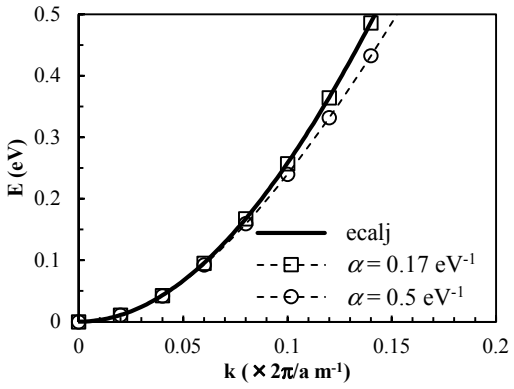
where g is the degeneracy, $m_{dc}=(m_l m_t^2)^{1/3}$ is the density of states effective mass, $m_l = m^*(\pi/2,0)$ and $m_t = m^*(\pi/2, \pi/2) = m^*(0,\phi)$ are the longitudinal effective mass and the transverse effective mass, respectively. Fig. 2 shows the density of states calculated by ecalj and (11). In Fig. 2, (a) show $D(E)$ in the range of $E \le 0.5$ eV and (b) show $D(E)$ in the range of $E \le 5$ eV. In n = 7, the density of states is more in agreement with ecalj than that of n = 3 in the range of $E \le 0.5$ eV. There are little discrepancy between the model with n = 7 and ecalj in the range of $E > 0.13$ eV due to the second conduction band. It is found that the angular dependence is essential to model the macroscopic nonparabolicity factor.



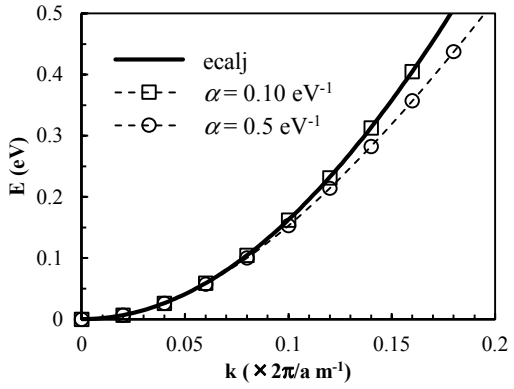
(a) (π/2,0) direction



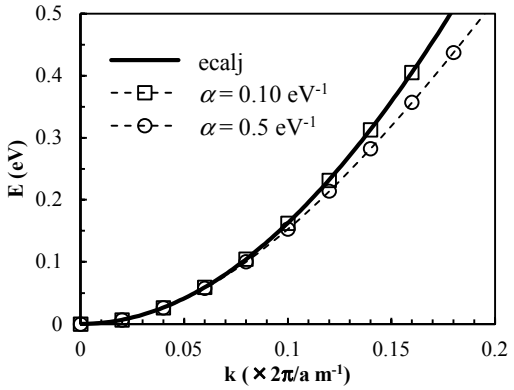
(b) (π/2,π/2) direction



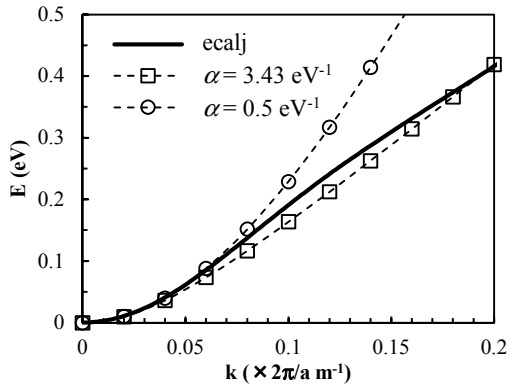
(c) (0,ϕ) direction



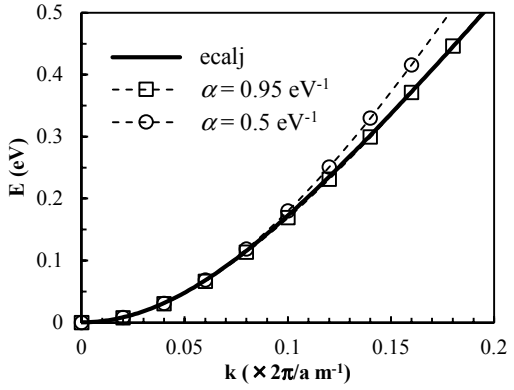
(d) (π/2,π/4) direction



(e) (π/4,0) direction



(f) (π/4,π/2) direction

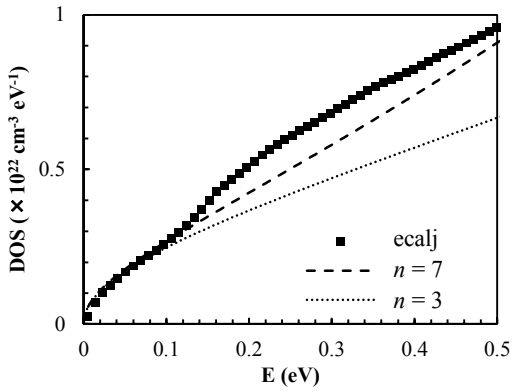


(g) (cos^{-1}(1/√3),π/4) direction

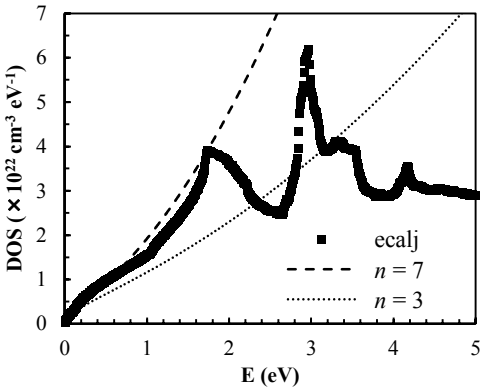
Figure 1. E-k dispersion relations for silicon band structure. (θ,ϕ) = (a) (π/2,0), (b) (π/2,π/2), (c) (0,ϕ), (d) (π/2,π/4), (e) (π/4,0), (f) (π/4,π/2) and (g) (cos^{-1}(1/√3),π/4) directions.

TABLE I. EFFECTIVE MASS AND NONPARABOLICITY FACTOR IN EACH DIRECTION

	θ = π/2 ϕ = 0 i = 1	π/2 π/2 2	0 ϕ 3	π/2 π/4 4	π/4 0 5	π/4 π/2 6	cos^{-1}(1/√3) π/4 7
m^*/m_0	0.91	0.19	0.19	0.31	0.31	0.20	0.26
α (eV^{-1})	0.23	0.17	0.17	0.10	0.10	3.43	0.95



(a) $E \leq 0.5$ eV



(b) $E \leq 5$ eV

Figure 2. Density of states calculated using the present model comparing with ecalj. (a) $E \leq 0.5$ eV and (b) $E \leq 5$ eV.

IV. CONCLUTION

We have investigated the angular dependence of the nonparabolicity factor of the silicon band structure and the influence of the angular dependence on the density of states. In the case of using only the information in the principal directions, $(\pi/2,0)$, $(\pi/2,\pi/2)$ and $(0,\phi)$, the average nonparabolicity factor is obtained 0.21 eV^{-1} which is much smaller than 0.5 eV^{-1} because the nonparabolicity factors in this three directions are small. On the other hand, in the case of using the information in the seven directions in Table 1, the average nonparabolicity factor is obtained 0.54 eV^{-1} which is close to 0.5 eV^{-1} because the nonparabolicity factors in the directions, $(\pi/4,\pi/2)$ and $(\cos^{-1}(1/\sqrt{3}),\pi/4)$, are significant.

REFERENCES

[1] Mark Bohr, Digest of International Electron Device Meeting 2011, December 2011.

[2] Xiaolin Wang, V. Chandramouli, Christine M. Maziar, and Al F. Tasch Jr., J. Appl. Phys., vol. 73, no. 7, pp. 3339-3347, April 1993.

[3] M. V. Fischetti and S. E. Laux, Pysical Review B, vol. 48, no. 4, pp. 2244-2274, July 1993.

[4] Seonghoon Jin, Massimo V. Fischetti, and Ting-wei Tang, J. Appl. Phys., vol. 102, no. 8, pp. 083715-1-083715-14, October 2007.

[5] M. A. Green, J. Appl. Phys., vol. 67, no. 6, pp. 2944-2954, March 1990.

[6] N. Shigyo, N. Konishi and H. Satake, Trans. IEICE, E75-C, p. 156, 1992.

[7] E. O. Kane, J. Phys. Chem. Solids, vol. 1, pp. 249-261, 1957.

[8] T. Kotani, J. Phys. Soc. Jpn., vol. 83, no. 9, pp. 094711-1-094711-11, 2014.

[9] C. Jacoboni, R. Minder, and G. Majni, J. Phys. Chem. Solids., vol. 36, pp. 1129-1133, 1975.