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Temperature dependence of the Hall mobility of n-type 3C-SiC

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Abstract. The Hall mobility of n-type 3C-SiC has been calculated employing a set of hydrodynamic balance equations. The acoustic, polar optical, piezoelectric, and intervalley optical lattice scattering, as well as the ionized and neutral impurity scattering are considered in the transport study. The calculated Hall mobility is in good agreement with the experimental data from 70 K to 1000 K. The Hall factor is shown to be less than unity, due to the nonparabolicity of the energy bands.

1. Introduction

In the last few decades research on silicon carbide has remained an active field because of its many meritorious properties for high-temperature electronics and short-wavelength optical applications [1]. Recent success in heteroepitaxial growth of large-area single-crystal films of cubic silicon carbide (3C-SiC) has attracted additional interest in this promising wide-band-gap semiconductor [2]. For impurity control during crystal growth and the application of a material in practical devices, it is important to know several parameters such as the mobility, carrier concentration at different temperatures, and doping concentration required for the device in actual operation. Measurements of the Hall coefficient provide such information for semiconductor materials.

The Hall mobility of heteroepitaxial n-type 3C-SiC has been measured by several groups. To estimate the concentration of donors, N_D, the concentration of acceptors, N_A, and the ionization energy of donors, E_d, the data on the electron concentration as a function of temperature are analysed and contrasted with the carrier concentration n obtained from the Hall coefficient R_H by using $n = (R_H e)^{-1}$, where e is the electronic charge. Under the assumption that the shallow donors were not compensated ($n \sim \exp(-E_d/k_B T)$), where k_B is the Boltzmann constant and T is the lattice temperature, Sasaki *et al* [3] found E_d to be 40–50 meV. The electron Hall mobility changed with temperature as $\mu_H \sim T^{\beta}$ with β between -1.2 and -1.4. Yamanaka *et al* [4] employed the following formula to calculate the carrier concentration:

$$n = \frac{N_D}{1 + 2\exp\left[(E_F - E_D)/k_B T\right]} - N_A + N_V \exp\left[\frac{E_V - E_F}{k_B T}\right] \tag{1}$$

where N_V is the effective density of states in the valence band. E_F, E_D, and E_V are energies of the Fermi level, donor level, and the top of the valence band. They found the donor ionization energy E_d (=$E_C - E_D$) to be 18 meV (E_C is the bottom of the

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conduction band). However, the carrier concentration calculated using the above formula deviated greatly from the experimental data at temperatures below 70 K. Moreover, the Hall mobility calculated by considering the acoustic phonon and ionized impurity scatterings differs from the experimental results over the entire temperature range (10–1000 K). Suzuki *et al* [5] measured the Hall mobility in three n-type 3C-SiC samples at temperatures ranging from 70 K to 1000 K. They found that the mobility varied as $\mu_H \sim T^{-2.0 \text{ to } -2.2}$ above room temperature. A conventional theoretical model was used by Suzuki *et al* [6] to fit the temperature dependencies of the Hall mobility by considering the acoustic, polar optical, and piezoelectric lattice scatterings, as well as the ionized and neutral impurity scatterings. The calculated Hall mobility agreed with the experimental data for lightly doped samples, but was much larger than the experimental data at low temperature for heavily doped samples. Tachibana *et al* [7] conducted Hall measurements of n-type 3C-SiC at temperatures from 87 K to 1000 K, and employed a compensation model to analyse the carrier concentration versus temperature data. They found the compensation ratio (N_A/N_D) to be about 0.36, and the ionization energy of donors to be 14–21 meV.

Although the Hall mobility of 3C-SiC has been measured over the last ten years by many groups, there is still no consistent theory that can reasonably explain all of the available experimental data. Here we present a transport theory of Hall mobility in 3C-SiC based on a set of hydrodynamic balance equations [8]. In this, we use the compensation expression [9] for computing the carrier concentration as functions of temperature, donor concentration, and acceptor concentration. Furthermore, we show that the relation between the Hall coefficient and the carrier concentration should be modified because of the nonparabolicity of energy band of 3C-SiC. We compare our calculated results with experimental data, and demonstrate good agreement of our theory with most of the experiments.

2. Carrier concentration and the Hall mobility

For a nondegenerate, n-type semiconductor with a shallow donor, the carrier concentration can be determined using the equation [9]

$$\frac{n(n+N_A)}{N_D - N_A - n} = \frac{N_C}{g} \exp\left(\frac{-E_d}{k_B T}\right) \tag{2}$$

where g is the degeneracy factor (taken as 2). N_C is the effective density of states in the conduction band, and is given by

$$N_C = 2M\left(\frac{2\pi m_c k_B T}{h^2}\right)^{3/2} \tag{3}$$

in which M is the number of equivalent minima in the conduction band and m_c is the effective mass of electrons in the conduction band. Since 3C-SiC has the zinc-blende structure, and its conduction-band minimum is near X [10], then $M = 3$. The value of $m_c = 0.346m_0$.

Within the hydrodynamic balance equation approach [8], a set of frictional acceleration balance equations can be obtained for carriers under the influence of a crossed magnetic field and an electric field:

$$\frac{eE_x}{m^*_{xx}} + A_x = 0 \tag{4}$$

$$\frac{eE_y}{m^*_{yy}} - \frac{eBv_d}{m^*_{yy}}\gamma_{x,yy} = 0 \tag{5}$$

where $A_x = A_{ix} + A_{px}$ is the frictional acceleration due to impurity and phonon scattering. Its expression is given in reference [11]. E_x and E_y are the drift electric field and the Hall field, respectively, and $\boldsymbol{v}_d$ is the drift velocity:

$$\boldsymbol{v}_d = \frac{2}{n} \sum_{\boldsymbol{k}} \nabla_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) f(\bar{\varepsilon}(\boldsymbol{k}), T_e). \tag{6}$$

$1/m^*_{xx}$ and $1/m^*_{yy}$ are components of the ensemble-averaged inverse effective-mass tensor $\mathcal{K}$ along the x-direction and the y-direction, respectively, and

$$\mathcal{K} = \frac{2}{n} \sum_{\boldsymbol{k}} \nabla_{\boldsymbol{k}} \nabla_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) f(\bar{\varepsilon}(\boldsymbol{k}), T_e). \tag{7}$$

$\gamma_{x,yy}$ is a dimensionless parameter used to describe the motion of the centre of mass in a crossed magnetic field and electric field configuration, which is defined as

$$\gamma_{x,yy} = \frac{\langle (\partial\varepsilon/\partial k_x)(\partial^2\varepsilon/\partial k^2_{yy}) \rangle}{\langle \partial\varepsilon/\partial k_x \rangle \langle \partial^2\varepsilon/\partial k^2_{yy} \rangle} \tag{8}$$

where $\langle\ \rangle$ stands for the ensemble average:

$$\langle (\cdots) \rangle = \frac{2}{n} \sum_{\boldsymbol{k}} (\cdots) f(\bar{\varepsilon}(\boldsymbol{k}), T_e) \tag{9}$$

where

$$f(\bar{\varepsilon}(\boldsymbol{k}), T_e) = \frac{1}{\exp[(\bar{\varepsilon}(\boldsymbol{k}) - \mu)/K_B T_e] + 1} \tag{10}$$

is the Fermi function at electron temperature T_e. $\bar{\varepsilon}(\boldsymbol{k}) = \varepsilon(\boldsymbol{k} - \boldsymbol{p}_d)$ is the relative electron energy with the momentum of the centre of mass $\boldsymbol{p}_d$. The chemical potential (or the Fermi energy) μ is determined by the carrier concentration n:

$$n = 2 \sum_{\boldsymbol{k}} f(\varepsilon(\boldsymbol{k}), T_e) \tag{11}$$

where $\varepsilon(\boldsymbol{k})$ is the band energy of electrons, which is determined by the Kane relation [12]:

$$\frac{\hbar^2 k^2}{2m_c} = \varepsilon(\boldsymbol{k})(1 + \alpha\varepsilon(\boldsymbol{k})) \tag{12}$$

where $\alpha = 0.323$ eV^{-1} is the nonparabolic coefficient of 3C-SiC, arising from higher-lying conduction bands rather than from the valence bands [13].

From equations (4) and (5), the Hall mobility is obtained as

$$\mu_H = \frac{1}{B} \frac{E_y}{E_x} = -\frac{e v_d}{m^*_{xx} A_x} \gamma_{x,yy}. \tag{13}$$

3. Numerical results and discussion

In our numerical calculations, four modes of lattice scattering due to acoustic, piezoelectric scattering, polar optical and intervalley optical scattering, and two modes of impurity scattering due to ionized impurity and neutral impurity scattering are considered. To compare our results with the experimental data [6], we study three n-type 3C-SiC samples: (1) $N_D = 0.48 \times 10^{18}$ cm^{-3}, $N_A = 0.12 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (2) $N_D = 0.90 \times 10^{18}$ cm^{-3}, $N_A = 0.27 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (3) $N_D = 2.30 \times 10^{18}$ cm^{-3}, $N_A = 0.57 \times 10^{18}$ cm^{-3}, and $E_d = 14.4$ meV. The temperatures considered range from 70 K to 1000 K. The neutral impurity concentration was taken as $N_n = N_D - N_A - n$.

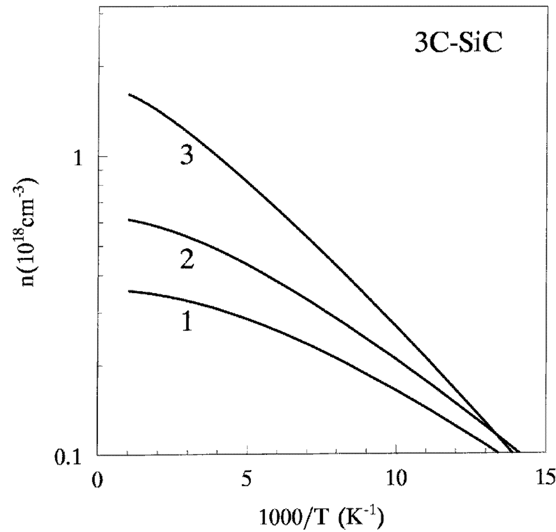

Figure 1. The carrier concentration of n-type 3C-SiC as a function of temperature for three samples: (1) $N_D = 0.48 \times 10^{18}$ cm^{-3}, $N_A = 0.12 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (2) $N_D = 0.90 \times 10^{18}$ cm^{-3}, $N_A = 0.27 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (3) $N_D = 2.30 \times 10^{18}$ cm^{-3}, $N_A = 0.57 \times 10^{18}$ cm^{-3}, and $E_d = 14.4$ meV.

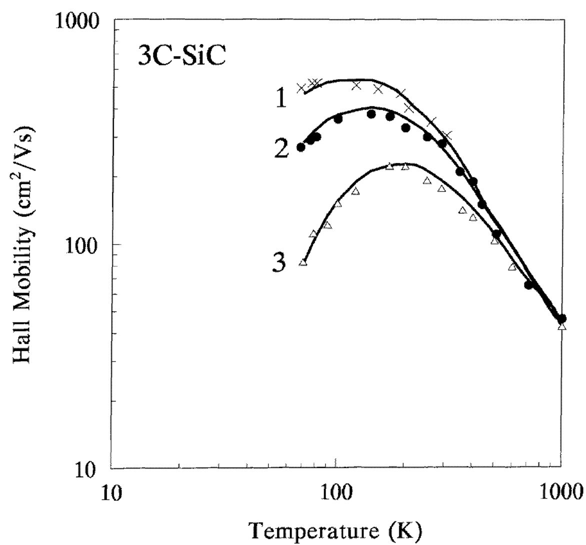

Figure 2. The Hall mobility of n-type 3C-SiC as a function of temperature for three samples: (1) $N_D = 0.48 \times 10^{18}$ cm^{-3}, $N_A = 0.12 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (2) $N_D = 0.90 \times 10^{18}$ cm^{-3}, $N_A = 0.27 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (3) $N_D = 2.30 \times 10^{18}$ cm^{-3}, $N_A = 0.57 \times 10^{18}$ cm^{-3}, and $E_d = 14.4$ meV. The experimental data (represented by crosses, dots, and triangles for samples 1, 2, and 3) are taken from reference [6].

The other parameters used in the calculation for Hall mobility are taken as the same as in reference [6].

The calculated carrier concentration n is illustrated in figure 1 as a function of temperature from 70 K to 1000 K. The numbers near the curves denote the different samples. According to the expression for the electron concentration (2), the carrier concentration increases linearly with increasing temperature at low temperature, and is nearly constant and given as $N_D - N_A$ (exhaustion region) at high enough temperature. This expression is known [6] to give a reasonable fit to the experimental values for temperature from 70 K to 1000 K.

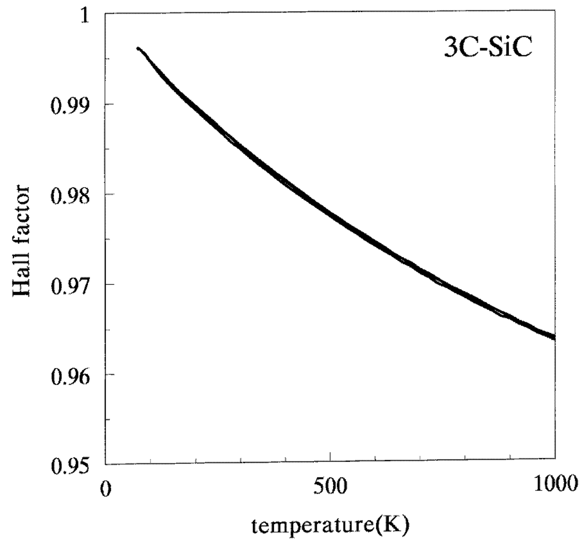

Figure 3. The Hall factor of n-type 3C-SiC as a function of temperature for three samples: (1) $N_D = 0.48 \times 10^{18}$ cm^{-3}, $N_A = 0.12 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (2) $N_D = 0.90 \times 10^{18}$ cm^{-3}, $N_A = 0.27 \times 10^{18}$ cm^{-3}, and $E_d = 18$ meV; (3) $N_D = 2.30 \times 10^{18}$ cm^{-3}, $N_A = 0.57 \times 10^{18}$ cm^{-3}, and $E_d = 14.4$ meV.

The Hall mobility is plotted in figure 2 as a function of temperature from 70 K to 1000 K for three different samples. The crosses, dots, and triangles denote the experimental values [6]. At low temperature, the Hall mobility increases with increasing temperature before reaching a maximum then decreasing with increasing temperature. The Hall mobilities for the three samples at low temperature are significantly different. Sample 1 has the highest Hall mobility. With increasing donor concentration and acceptor concentration, the Hall mobility decreases. The differences between the Hall mobilities of these three samples become small with increasing temperature and vanish at 1000 K. Our calculated Hall mobility is in good agreement with the experimental data for the whole temperature range. In the calculation we found that at low temperature the ionized impurity scattering played the dominant role in determining the Hall mobility, and at high temperature the Hall mobility was mainly determined by the polar optical and intervalley optical phonon scatterings. In the first two samples the donor ionization energy is taken as 18 meV and the impurity concentration is taken as $n_i = n + 2N_A$ [6]. As can be seen from the figure, the calculated Hall mobility is in good agreement with the experimental values. However, the calculated Hall mobility for the third sample would be much lower than the experimental value if the same value of E_d and the same expression for n_i as for the first two samples are used. For a better fit, we take $E_d = 14.4$ meV and $n_i = n + N_A$. By using these we found that the Hall mobility agrees well with the experimental data. It is known that the donor

ionization energy is a function of the donor concentration, and it decreases with increasing donor concentration for shallow acceptors in Si [14] and shallow donors in Ge [15]. Segall *et al* [16] suggested that the ionized energy of the donor for 3C-SiC decreased linearly with $N_d^{1/3}$. Furthermore, the decrease of the density of the ionized impurity indicates that the degree of complete ionization decreases with increasing concentrations of donors and acceptors.

In the balance equation approach, the Hall coefficient can be written as $R_H = \gamma_{x,yy}/ne$. So the Hall factor is just the dimensionless quantity, $\gamma_{x,yy}$, defined by equation (8). We plot it as a function of temperature in figure 3. The Hall factors for the three samples differ only slightly over the whole temperature range, but they are less than unity and decrease with increasing temperature. Although the energy band gap for 3C-SiC is as high as 3.0 eV, the nonparabolicity is as large as 0.323 eV^{-1} which results from the influences of the upper conduction bands. At high temperatures the electron states will deviate from the parabolic-band states, so the Hall factor must be different from that of a parabolic band for which the Hall factor is identically 1.

In conclusion, the Hall mobility of n-type 3C-SiC has been obtained on the basis of the combination of balance equations and a compensation model for carrier concentration, which gives better agreement with experiments than all previous theoretical studies. The Hall factor obtained for 3C-SiC is less than unity and decreases with increasing temperature. The Hall factors for the three samples considered are almost the same. This approach can also be used to obtain other sample parameters (the carrier concentration, mobility, impurity concentration, and compensation ratio) from the data from Hall measurements.

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References

[1] Morkoc H, Strite S, Gao B G, Lin M E, Sverdlov B and Burns M 1994 *J. Appl. Phys.* **76** 1363
[2] Edmond J A, Withrow S P, Wadlin W and Davis R F 1987 *Interfaces, Superlattices and Thin Films (Materials Research Society Proceedings 77)* ed J D Dow, I K Schuller and J Hilliard (Pittsburgh, PA: Materials Research Society) p 193
[3] Sasaki K, Sakuma E, Misawa S, Yoshida S and Gonda S 1984 *Appl. Phys. Lett.* **45** 72
[4] Yamanaka M, Daimon H, Sakuma E, Misawa S and Yoshida S 1987 *J. Appl. Phys.* **61** 509
[5] Suzuki A, Uemoto A, Shigeta M, Furukawa K and Nakajima S 1986 *Appl. Phys. Lett.* **49** 450
[6] Suzuki A, Ogura A, Furukawa K, Fujii Y, Shigeta M and Nakajima S 1988 *J. Appl. Phys.* **64** 2818
[7] Tachibana T, Kong H S, Wang Y C and Davis R F 1990 *J. Appl. Phys.* **67** 6376
[8] Lei X L and Weng X M 1994 *J. Phys.: Condens. Matter* **6** L461
[9] Blackmore J S 1962 *Semiconductor Statistics* (New York: Pergamon) p 117
[10] Choyke W J, Hamilton D R and Patrick L 1964 *Phys. Rev.* A **133** 1163
[11] Lei X L 1992 *Phys. Status Solidi* b **170** 519
[12] Kane E O 1957 *J. Phys. Chem. Solids* **1** 249
[13] Zhou J R, Vasileska D and Ferry D K 1993 *Solid State Electron.* **36** 1289
[14] Pearson G L and Bardeen J 1949 *Phys. Rev.* **75** 865
[15] Debye P P and Conwell E M 1954 *Phys. Rev.* **93** 693
[16] Segall B, Alterovitz S A, Haugland E J and Matus L G 1986 *Appl. Phys. Lett.* **49** 584