Thermal effect mechanism of magnetoresistance in p-type diamond films*

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Based on the analysis and the discussion of the influence of thermal ionization energy and various scatterings on magnetoresistance(MR) of p-type diamond films, a revised model of valence band split-off over temperature is put forward, and a corresponding calculation formula is given for the MR of p-type diamond films (Corbino discs). It is shown that the theoretical calculation that the MR of diamond films changes with temperature is consistent with the experiment. The influence of Fermi energy level on MR of diamond films is discussed. Additionally, the thermal effect mechanism of MR in p-type diamond films is also explored.

Keywords: diamond film, magnetoresistance, valence-band split-off
PACC: 7530V, 8120V, 7125

1. Introduction

Diamond has aroused great interest in the past decades due to its outstanding physical and chemical properties, i.e., high hardness, high stiffness, high thermal conductivity at room temperature, excellent chemically corrosion and radiation resistance, low thermal expansion, wide transparency region from ultraviolet to infrared light, wide band gap for high temperature semiconductor, etc. This indicates that diamond films have technological applications in tribology,[1] radiation detector material,[2] magnetosensor material,[3] biology,[4] electronics such as diamond transistors operating at $T > 700$ K,[5,6] and the metal–insulator transition with the appearance of a superconducting state.[7,8] Oriented heteroepitaxial high quality p-type diamond films with little secondary nucleation have been successfully prepared by microwave plasma chemical vapour deposition (CVD) on mirror-polished single-crystalline (001) silicon substrates with a negative bias, and the electronic properties of these epitaxial diamond films are more excellent than those of the polycrystalline diamond films by a common CVD.[9−11] Since the 90 s of the 20th century, theoretical and experimental studies on magnetoresistive effect of diamond films have been widely conducted,[12−16] because the heteroepitaxial diamond films have a significant magnetoresistive effect. The studies of the epitaxial B-doped diamond films have indicated that the magnetoresistive effect of the materials are closely dependent on B-doped concentration, the hole mobility, the ambient temperature, magnetic field intensity, and the geometric shape of the samples. Furthermore, the experimental studies[12] have indicated that the magnetoresistance (MR) of p-type diamond films with Corbino disk structure at a magnetic field intensity of 5 T decreases from 0.85 to 0.18 when the temperature increases from 300 to 500 K. In addition, our previous researches[15,16] have shown a theoretical description of the magnetoresistive effect in diamond films by solving the Boltzmann transport equation in the relaxation time approximation.

In the present article, a revised theoretical model of valence band split-off over temperature is proposed, based on the experimental results and the influence of thermal ionization energy and various scatterings on MR of p-type diamond films. The values of MR of the diamond films under different ambience temperatures are theoretically calculated, and simultaneously the influence of Fermi level on MR is also discussed. Finally, a reasonable thermal effect mechanism is employed to explain MR value in a p-type diamond film.

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2. Revised model of valence-band split-off over ambience temperature

MR is one of the intrinsic properties of materials. It can change the electronic resistance of the materials under an externally applied magnetic field. For the boron (B) atoms doped semiconductor materials such as Si and Ge, the thermal ionization energies for acceptors B atoms are 45 meV and 10.4 meV, respectively. These values are much close to the thermal energy ($k_{\rm B}T \sim 26$ meV) at room temperature. This indicates that the thermal ionization energy for acceptor B in Si or Ge has a significant influence on conductivity. However, the thermal ionization energy shows a slight change from 26 meV to 43 meV with temperature increasing from 300 K to 500 K, and this change is much less than that of thermal ionization energy for acceptor B in diamond films (0.36 eV). Therefore, the MR of p-type diamond films dramatically decreases with temperature increasing,[12] which cannot result from the thermal ionization of acceptor B.

In general, the conductance is closely dependent on ionized impurity scattering, lattice scattering, defect scatterings (the scatterings of point defects, dislocations, interfaces, grain boundaries, *etc.*), and it is sensitive to the change of temperature. However, it is quite difficult to give a theoretical relation among the conductance, the scatterings, and the temperature, owing to the complexity of the scattering mechanism. Then, we cannot build a relation between MR and temperature by using those various scatterings. For the relatively small radius (25 μm) and big grain size(2–4 μm), defect scatterings in Corbino disc diamond films can be neglected.[15] Because thermal ionized B atoms in the films are very few in number, we can also approximately view a B-doped diamond film as a non-polar neutral doped crystal, with neglecting ionized impurity scattering and optical wave scattering. Additionally, in the long acoustic wave approximation, the change of the theoretical value of the MR is only 0.07 when the temperature increases from 300 K to 500 K. So the significant change of the MR cannot result mainly from the acoustical scattering.

As we know, the valence bands of p-type diamond films are composed of light-hole band, heavy-hole band, and split-off band. The energy level interval between the split-off band and the top of the valence band is only 0.006 eV. The light-hole and the heavy-hole bands are degenerate if the effect of the internal stress is not taken into consideration. There exists an apparent lattice mismatch between the heteroepitaxial diamond film (0.3567 nm) and the Si substrate (0.5430 nm). Furthermore, there is a big difference between the coefficients of thermal expansion of diamond ($0.08 \times 10^{-6}/^{\circ}$C) and Si ($2.6 \times 10^{-6}/^{\circ}$C), and the valence-band split off can change with temperature. For the small valence-band split-off, a linear relation between the temperature and the energy level interval of valence-band split-off is assumed to be

$$\Delta\varepsilon = a(T - T_0), \tag{1}$$

where a and T_0 are the undetermined parameter. Using subscripts (1, 2, 3) to mark the light-hole band, the heavy-hole band, and the split-off band, respectively, the ratios of the hole-density distributions can be expressed as

$$p_{12} = \frac{p_1}{p_2} = \left(\frac{m_1^*}{m_2^*}\right)^{3/2} \cdot \exp\left[\frac{a}{kT}(T - T_0)\right], \tag{2}$$

$$p_{32} = \frac{p_3}{p_2} = \left(\frac{m_3^*}{m_2^*}\right)^{3/2} \cdot \exp\left(-\frac{\Delta}{kT}\right). \tag{3}$$

Under the condition of Maxwell–Boltzmann statistics and spherical energy band surfaces, the conductivity components of Corbino disc diamond films can be written as[15]

$$\sigma_{\rm rr} = 2pe\mu_{\rm L}\varphi(\kappa)K(\beta,\gamma), \tag{4}$$

$$\sigma_{\varphi{\rm r}} = -\sqrt{\pi}pe\mu_{\rm L}\gamma^{1/2}\eta(\kappa)L(\beta,\gamma), \tag{5}$$

where p is the hole concentration; $\mu_{\rm L}$ is the hole mobility; $\varphi(\kappa) = 1 - 3/8\kappa$; $\eta(x) = 1 - 9/16\kappa$, with κ being a parameter that is related to the film thickness and the relaxation time; β is a slow function of energy and defined as the degree of impurity scattering (pure lattice scattering $\beta = 0$);

$$K(\beta,\gamma) = \int_0^\infty \frac{\alpha^3 {\rm e}^{-\alpha}(\alpha^2+\beta)}{(\alpha^2+\beta)^2 + \gamma\alpha^3}{\rm d}\alpha; \tag{6}$$

$$L(\beta,\gamma) = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\alpha^{9/2}{\rm e}^{-\alpha}}{(\alpha^2+\beta^2) + \gamma\alpha^3}{\rm d}\alpha; \tag{7}$$

$$\gamma = \frac{9\pi}{16}(\mu_{\rm L}B)^2; \quad \alpha = (E_{\rm v} - E)/kT. \tag{8}$$

Considering a parallel connection model for the conductivity of light-hole band, heavy-hole band and split-off band, the conductivity can be expressed as

$$\sigma_{\rm r}(\gamma,T) = \sum_{i=1}^{3}\sigma_{\rm rr}(i), \quad \sigma_\varphi(\gamma,T) = \sum_{i=1}^{3}\sigma_{\varphi{\rm r}}(i), \tag{9}$$

$$\sigma_{\rm c}(\gamma,T) = \sqrt{\sigma_{\rm r}^2(\gamma,T) + \sigma_\varphi^2(\gamma,T)}. \tag{10}$$

Then, the transverse MR can be obtained as

$$\frac{\Delta\rho}{\rho_0} = \frac{\sigma_{\rm c}(0,T)}{\sigma_{\rm c}(\gamma,T)} - 1 = \frac{2A(0,T)}{\sqrt{4A^2(\gamma,T)+\pi\cdot\gamma_2 B^2(\gamma,T)}} - 1, \quad (11)$$

$$A(\gamma,T) = \sum_{i=1}^{3} p_{i2}(T)\cdot\mu_{i2}\cdot\varphi(\kappa_i)\cdot K(\beta_i,\gamma_i), \quad (12)$$

$$B(\gamma,T) = \sum_{i=1}^{3} p_{i2}(T)\cdot\mu_{i2}^2\cdot\eta(\kappa_i)\cdot L(\beta_i,\gamma_i), \quad (13)$$

where $\mu_{i2} = \mu_{\rm Li}/\mu_{\rm L2}$ is the relative rate of the hole mobility, and the expression $p_{i2}(T) = p_i/p_2$ is given by Eqs. (2) and (3).

3. Results and discussion

Equations (11)–(13) express the magnetoresistive effect of Corbino disc diamond films by the revised model of valence band split-off at ambient temperature. The values of the parameters are theoretically calculated, and shown in Tables 1 and 2. Thus, just as shown in Fig. 1, if we give appropriate parameters ($\alpha = 3\times10^{-23}$ J$\cdot$K^{-1} and $T_0 = 280$ K), the numerical calculation value is in good agreement with the experimental result in a range of 300–500 K. Specifically, the theoretical value is slightly higher than the experimental result in a middle temperature range, while it is lower than in the remaining ranges. The error possibly results from the scattering fluctuation due to the changing temperature. The meaning of using the revised model of valence-band split-off at ambience temperature is very clear. When the temperature goes up, the upward shift of the light-hole band causes more hole carriers to participate in electric conduction, thereby inducing the decrease of the MR.

Table 1. Ratios of hole concentration.

ratio	p_1/p_2	p_3/p_2
calculated value	0.19	0.28

Table 2. Parameters $\mu_{\rm L}$, β, κ, m^*.

parameters	band 1	band 2	band 3
$\mu_{\rm L}/({\rm cm^2\cdot V^{-1}\cdot s^{-1}})$	3900	195	1365
β	0.001	0.0001	0.0003
κ	9.2	60.7	17.3
m^*	$0.7m_0$	$2.12m_0$	$1.06m_0$

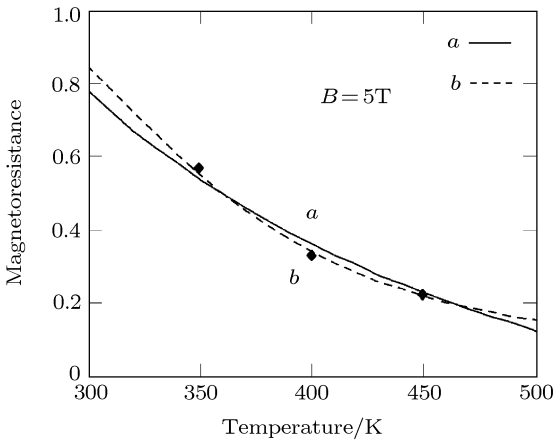


Fig. 1. Comparison between calculation result (curve a) and experiment result (curve b).

In order to further understand the thermal effect mechanism of MR in p-type diamond films, we need take the variation of the Fermi energy level into account. Assuming light hole and heavy hole to have different Fermi energy levels, the ratio of the hole-density distributions for a certain energy level interval of valence-band split-off ($\Delta_1 = E_{\rm v1} - E_{\rm v2}$) can be written as

$$p_{12} = \left(\frac{m_1^*}{m_2^*}\right)^{3/2}\exp\left[\frac{(E_{v1}-E_{v2})-(E_{f1}-E_{f2})}{kT}\right] = \left(\frac{m_1^*}{m_2^*}\right)^{3/2}\exp\left(\frac{\Delta\varepsilon}{kT}\right). \quad (14)$$

Here, the Fermi energy level formulas of light hole and heavy hole can be described as

$$E_{\rm f1} = \frac{1}{2}(E_{\rm v1}+E_{\rm a}) - \frac{1}{2}kT\ln\left(\frac{N_{\rm a}}{N_{\rm v1}}\right), \quad (15)$$

and

$$E_{\rm f2} = \frac{1}{2}(E_{\rm v2}+E_{\rm a}) - \frac{1}{2}kT\ln\left(\frac{N_{\rm a}}{N_{\rm v2}}\right), \quad (16)$$

where $E_{\rm a}$ is the energy level of the accepter; $E_{\rm v}$ is the energy level of the valence band; $N_{\rm a}$ is the impurity density; $N_{\rm v1}$ and $N_{\rm v2}$ are, respectively, the effective state densities of light holes and heavy holes, and given as

$$N_{\rm v1} = \frac{2(2\pi m_1^* kT)^{3/2}}{h^3},$$

and

$$N_{\rm v2} = \frac{2(2\pi m_2^* kT)^{3/2}}{h^3}. \quad (17)$$

Substituting Eqs. (15) and (16) into Eq. (1) yields

$$\Delta\varepsilon = \Delta_1 - (E_{\rm f1}-E_{\rm f2}) = -\frac{3}{4}k\ln\left(\frac{m_1^*}{m_2^*}\right)\left[T - \frac{2(E_{\rm v1}-E_{\rm v2})}{3k\ln(m_1^*/m_2^*)}\right]$$

$$= a(T - T_0), \tag{18}$$

where

$$a = -\frac{3}{4}k\ln(m_1^*/m_2^*), \tag{19}$$

$$T_0 = \frac{2(E_{\rm v1} - E_{\rm v2})}{3k\ln(m_1^*/m_2^*)}. \tag{20}$$

From Eqs. (18)–(20), we can see that the form of Fermi energy level varying with temperature is equivalent to that of the model of revised valence-band split-off produced by temperature mathematically. Substitute the effective masses of the light hole ($m_1^* = 0.7m_0$) and the heavy hole ($m_2^* = 2.18m_0$) into Eq. (19), then we will have $a = 1.18 \times 10^{-23}$J$\cdot$ K^{-1}, which is slightly lower than the experimental value 3×10^{-23} J $\cdot$ K^{-1}, but both are of the same order of magnitude. If $\Delta_1 = 0.02$ eV, then, $T_0 = 135$ K, which is also comparable to the experimental value (280 K). Consequently, there are presumably two main reasons for thermal effect mechanism of MR in p-type diamond films. One is that the valence band split-off is dependent on temperature, the other is that Fermi energy level changes with temperature, namely, $\Delta\varepsilon$ in Eq. (1) may result from the variations of valence band split-off and Fermi energy level with temperature.

4. Conclusions

We put forward a revised model of valence band split-off over temperature and give a corresponding calculation formula to express the magnetoresistive effect of Corbino disc diamond films, based on the analysis and the discussion of the influence of thermal ionization energy and various scatterings on MR of p-type diamond films. The theoretical calculation values of the MR that changes with temperature are in good agreement with the experimental data. The influence of Fermi energy level on MR of diamond films is also discussed. Finally, two main reasons for thermal effect mechanism of MR in p-type diamond films are given, namely, one is that the valence band split-off is dependent on the temperature, and the other is that Fermi energy level changes with temperature.

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