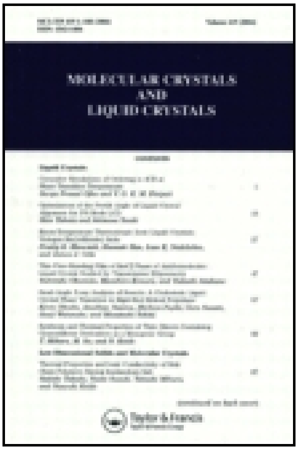

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Electronic and Transport Properties of Boronated Graphite — 3D-Weak Localization Effect —

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Electronic and Transport Properties of Boronated Graphite – 3D-Weak Localization Effect –

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Boronated graphite sample with B_4C contents of few wt% exhibit characteristic of 3D-weak localization at low temperatures and in weak magnetic field region. A boron atom supplies one hole and the Fermi surface with $E_F = -0.4$ eV (1 wt% sample) is composed of the two hole bands E_{1-} and E_{2-} and the electron Fermi surface disappears. E_{1-} band (majority hole) plays a dominant role in the 3D-weak localization. Kawabata theory is extended to the SWMcC-band and the present theory well explains the resistivity, magnetoresistance and Hall effect behaviors.

Keywords: Boronated graphite; 3D-weak localization; resistivity; magnetoresistance; Hall effect

INTRODUCTION

In 1985 Koike et al performed a detailed study on the resistivity and magnetoresistance in grafoil and Ceylon graphite samples[1]. These specimens exhibit the anomalous behaviors represented by

$$\text{(i)}\quad \delta\rho \equiv \rho(T) - \rho(0) = -aT^{1/2}\,(a > 0):\quad T \ll 1\,\mathrm{K}, \tag{1}$$

$$\text{(ii)}\quad \Delta\rho/\rho_0 \equiv \{\rho(B) - \rho_0\}/\rho_0 = -bB^{1/2}\,(b > 0):\quad B \ll 0.1\ \mathrm{Tesla}. \tag{2}$$

The above results were fairly well explained in terms of localization, electron-electron interaction and ellipsoid band in the 3D-weak localization regime. In this article we employed the boronated graphite samples with nominal B_4C contents of 1.0, 2.5 and 5.0 wt%. These samples were obtained by Ceylon natural graphite powder with B_4C powder by heat treatment at 2200°C for 1 hour under pressure of 19.8 MPa[2]. The behaviors represented by Eqs. (1) and (2) were also observed in our samples as shown in Figs. 1 and 2.

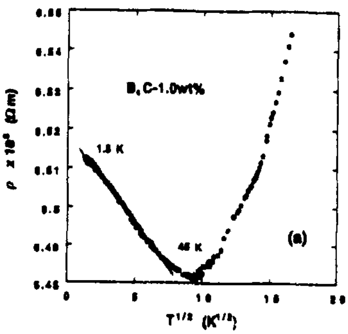

FIGURE 1. ρ vs $T^{1/2}$ curves for boronated sample.

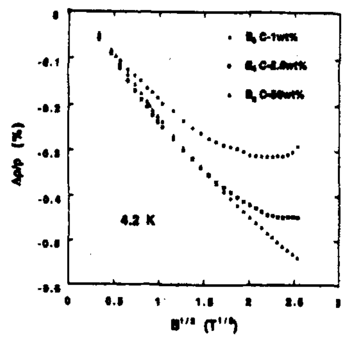

FIGURE 2. $\Delta\rho(B)/\rho_0$ vs $B^{1/2}$ plots for three boronated samples at 4.2 K.

As was discussed by Kawabata[3] Eqs. (1) and (2) are the characteristic resulted from the three-dimensional weak localization (3D-WL). It is worthy of note that the anomaly takes place at high temperature and in stronger magnetic field region in comparison with the case in ref. [1]. In the following we can explain the observed results in terms of the extended Kawabata theory to the SWMcC-band[4].

WEAK LOCALIZATION IN BORONATED GRAPHITE

Boron atoms substitute into graphite lattice with a maximum solubility of 2.35 wt% at 2350°C[5], and a boron atom supplies one hole. Therefore, the boronated graphite with B_4C contents of ~wt% becomes a metal composed of two hole bands E_1 and E_2 and the electron Fermi surface disappears. Figure 3 illustrates the schematic picture of the Fermi surface. ϕ_0 is the angle defined by $E_F = E_2(\phi_0)$, $E_2(\phi) = \Delta - 2\gamma_1\cos\phi + 2\gamma_5\cos^2\phi$ [4] and E_F = - 0.4 eV is evaluated from the Hall coefficient for B_4C 1 wt% specimen.

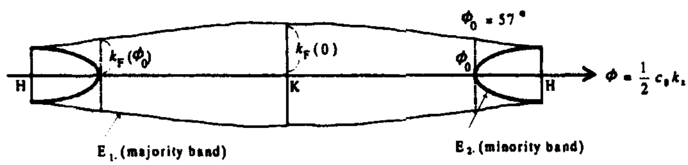

FIGURE 3. Schematic picture of the Fermi surface with B_4C-1wt%, ϕ_0 denotes the crossing point of E_F and E_2 band. (E_F = - 0.4 eV)

In the following the expressions for $\delta\rho/\rho(0)$ and $\Delta\rho(B)/\rho_0$ are given. Hall coefficient R_H at 4.2 K decreases with magnetic field intensity B and it takes a constant value for $B > 4$ T (see Fig. 4, B_4C contents of 1 wt%). This can be explained as follows. Since $(\omega_c\tau)^2_{min.} \gg 1$ for $B > 4$ T while $(\omega_c\tau)^2_{maj.} < 1$ for $B > 4$ T, the minority carrier contribution to R_H is negligible, where ω_c is the cyclotron frequency and τ the in-plane relaxation time. We obtain n_h(maj.) = 3.90×10^{26} /m^3, n_h(min.) = 3.0×10^{25} /m^3 and E_F = - 0.4 eV.

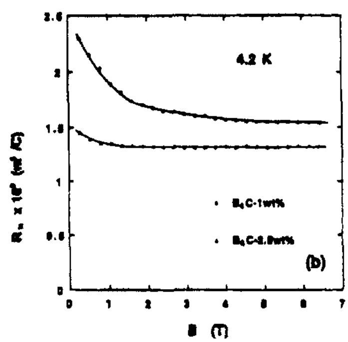

FIGURE 4. Hall coefficient of two boronated specimens plotted as a function of magnetic field at 4.2 K.

By extending the Kawabata theory to the SWMcC-band, we obtain the quantum correction $\delta\rho$ due to the 3D-WL as

$$\frac{\delta\rho}{\rho_0} = -\frac{2\sqrt{2}}{\pi^4 \hbar g(E_F)} \frac{1}{\sqrt{\overline{l}\,\overline{l_\varepsilon}}} \frac{1}{\sqrt{\overline{D_a}\,\overline{D_c}}}, \tag{3}$$

$$\overline{D_a} = \frac{1}{2}\overline{v_a^2 \tau}, \quad \overline{D_c} = \overline{v_c^2 \tau}, \quad \mathbf{v} = (\mathbf{v}_a, v_c),$$

$\overline{l} = \overline{v_a \tau}$: average mean free path for the elastic scattering, (4)

$\overline{l_\varepsilon} = \overline{v_a \tau_\varepsilon}$: average mean free path for the inelastic scattering,

$g(E_F)$: density of the state at E_F,

and $\overline{l} \ll \overline{l_\varepsilon}$, where l_ε or τ_ε is associated with the scattering process due to the out-of-plane vibrations. In Eq. (3) $\overline{l_\varepsilon}$ is the only T-dependent quantity, which is proportional to T^{-1} [6], then we have $\delta\rho/\rho_0 \propto T^{1/2}$ at low temperatures (see : Fig.1). The quantities except l or τ in eq. (3) can be theoretically evaluated. By using the observed value of $\delta\rho/\rho_0 = -4.6\times10^{-3}$ at 40 K we obtain $\rho_0 = 2.3\times10^{-6}$ Ωm which is the same order magnitude as the measured one. Corresponding value of $\overline{l}$ to the above ρ_0 value is 50 Å. The measured resistivity takes a nearly constant value over the range of 4.2 K–300K and $\rho = 6.5\times10^{-6}$ Ωm for B_4C-1wt% sample. As is shown in Fig. 1, ρ increases with T for T > 80 K. In this region the interactions with the out-of-plane vibrations and in-plane vibrations in Bloch equation play the important role.

Next the negative magnetoresistance term represented by eq. (2) is calculated in the following. By extending the Kawabata theory to the graphite band we obtain

$$\frac{\Delta\rho(B)}{\rho_0} = -\rho_0 \frac{e^2 F}{4\pi^2 \hbar l_B A}, \quad F = 0.6, \quad A = \sqrt{2\,\overline{v_c^2}/\overline{v_a^2}}, \tag{5}$$

and l_B denotes the magnetic length given by $\sqrt{\hbar/eB}$. A = 0.24 is obtained by using the SWMcC-band $(\Delta\rho(B)/\rho_0)_{calc.}$ = - 0.25% for B = 0.4 T while the experimental data is – 0.12 %. Equation (5) is valid if the following condition is satisfied:

$$\bar{l} \ll L_B \ll L_\epsilon\,, \quad \text{where} \quad L_B = \sqrt{\hbar/4eB} \quad \text{and} \quad L_\epsilon = \sqrt{\bar{l}\;\bar{l}_\epsilon}\,. \qquad (6)$$

At high temperatures the above condition does not hold and instead of Eq. (6) the relation of $\bar{l} \ll \overline{L_\epsilon} \ll L_B$ is realized and the negative magnetoresistance effect becomes small. In strong field region (B > 1 T) the positive magnetoresistance term in the Boltzmann equation cancels the negative contribution. Finally, it is noted that the majority carriers (E_{1}-band) play a dominant role in Eqs. (3) and (5).

SUMMARY

(i) Boronated graphite with B_4C contents of few wt% becomes metal with two hole Fermi surface E_1. (maj. band) and E_2. (min. band) and the electron Fermi surface disappears.

(ii) At low temperatures and in weak magnetic field the resistivity $\rho(T)$ and magnetoresistance $\Delta\rho(B)/\rho_0$ exhibit the anomalous characteristic ascribed to the 3D-weak localization effect.

(iii) In terms of the Kawabata theory (1980) extended to the SWMcC-band the observed anomalies are fairly well explained.

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