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Consequence of electron scattering mechanisms on the conductivity of semi-metal films

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A general expression for the resistivity of an infinitely thick polycrystalline semi-metal films is calculated starting from the Mayadas–Shatzkes conduction model. Good agreement with the experimental data related to antimony films is observed. Variations of the thermaly dependent term in conductivity with conductivity at low temperature cannot be neglected.

1. Introduction

Previously published data [1], related to antimony films, gave evidence for the validity of the extension of the Mayadas–Shatzkes equations [2] for describing the electrical conduction in semi-metal films which exhibit an energy-dependent relaxation time, τ, in the form:

$$\tau \sim E_F^{-1/2},$$

where E_F is the Fermi energy.

The purpose of this paper is to give the general expression for the resistivity of an infinitely thick polycrystalline semi-metal films, starting from the Mayadas–Shatzkes conduction model [2], and then to examine some consequences.

2. Theory

Starting from a general theoretical treatment of the electronic transport properties of metals, Ziman [3] has shown that the electrical conduction, i_{EE}, in a metal sample is given by the following equation:

$$i_{EE} = \sigma(E) + \frac{\pi^2 B^2 T^2}{6} \frac{\partial^2}{\partial E^2} \sigma(E) \bigg|_{E=E_F} \quad (1)$$

where $\sigma(E)$ is the electrical conductivity of the metal sample at low temperature, E is the electron energy, B is the Boltzmann constant, and T the absolute temperature in K.

If the Mayadas–Shatzkes conduction model [2] is used for expressing the electrical conductivity of an infinitely thick film, Equation 1 takes the following form:

$$\sigma_g = \sigma_0 \left[f(\alpha) + \frac{1}{6}\left(\frac{\pi B T}{E_F}\right)^2 h(\alpha) \right] \quad (2)$$

where σ_0 is the electrical conductivity of the bulk material, and $f(\alpha)$ is the usual M.S. function given by [2]:

$$f(\alpha) = 1 - \frac{3}{2}\alpha + 3\alpha^2 - 3\alpha^3 \ln\left(1 + \frac{1}{\alpha}\right) \quad (3)$$

with

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$$\alpha = \frac{(2m)^{1/2}}{\hbar^2} \frac{S^2 \tau}{E_F^{1/2}} \frac{1}{D}, \quad (4)$$

where m is the electron effective mass, $\hbar$ is the modified Planck constant, S the so-called [2] strength of the grain boundary, τ the electronic relaxation time in the bulk material, and D the average grain diameter. The procedure for calculating $h(\alpha)$ is presented in the next paragraph.

For an adequate description of transport properties in semi-metals it has been shown by several authors [1, 4–8] that the energy dependence of τ could be described by the following relations:

$$\tau_e = (\tau_0)_e E_{F_e}^s \quad (5)$$

$$\tau_h = (\tau_0)_h E_{F_h}^s \quad (6)$$

where subscripts e and h denote electrons and holes, respectively. By using a two-band multivalley model for the Fermi pockets of electrons and holes, we obtain:

$$\sigma_g = \sigma_{g_{e,h}} = \sigma_{g_e} + \sigma_{g_h} \quad (7)$$

with:

$$\sigma_{g_{e,h}} = \sigma_0 \sum_{e,h} \left[f(\alpha_{e,h}) + \frac{1}{60} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 h(\alpha_{e,h}) \right] \quad (8)$$

and

$$\alpha_{e,h} = \frac{(2m_{e,h})^{1/2}}{h^2} \frac{S^2 \tau_{e,h}}{E_{F_{e,h}}^{1/2}} \cdot \frac{1}{D}. \quad (9)$$

Partial derivatives of $\sigma_0 \cdot f(\alpha_{e,h})$ are performed in the way given by Equations 1, 3, 4 and 5. It gives:

$$h(\alpha_{e,h}) = 4s(s-1)f(\alpha_{e,h}) - 3(s-\tfrac{1}{2})(5s+\tfrac{1}{2}) (1+\alpha_{e,h})^{-1} + 3(s-\tfrac{1}{2})^2 \alpha_{e,h}(1+\alpha_{e,h})^{-2}. \quad (10)$$

Introducing Equation 10 into Equation 2, and reordering gives:

$$\sigma_g = \sigma_0 \sum_{e,h} \left\{ \left[1 + \frac{2}{3} s(4s-1) \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 \right] f(\alpha_{e,h}) + \frac{1}{2} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 (s-\tfrac{1}{2}) \left[(-5s-\tfrac{1}{2}) (1+\alpha_{e,h})^{-1} + (s-\tfrac{1}{2}) \alpha_{e,h} (1+\alpha_{e,h})^{-2} \right] \right\} \quad (11)$$

In the limiting cases of low and high values for α, $f(\alpha)$ takes the following approximate expressions [2]:

$$f(\alpha) \approx \frac{3}{4\alpha} - \frac{3}{5\alpha^2}, \quad \alpha \gg 1 \quad (12)$$

$$f(\alpha) \approx 1 - \frac{3}{2}\alpha, \quad \alpha \ll 1. \quad (13)$$

The approximate expressions for σ_g are then:

$$\frac{\sigma_g}{\sigma_0} \approx \sum_{e,h} \left\{ \frac{3}{4\alpha_{e,h}} \left[1 + \frac{1}{3} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 \right] - \frac{3}{5\alpha_{e,h}^2} \left[1 + \frac{1}{6} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 (s^2 - 4s + \tfrac{15}{4}) \right] \right\} \quad \alpha \gg 1 \quad (14)$$

$$\frac{\sigma_g}{\sigma_0} \approx \sum_{e,h} \left\{ 1 + \frac{1}{6} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 (s+\tfrac{1}{2})(s+\tfrac{3}{2}) - \frac{3\alpha_{e,h}}{2} \left[1 + \frac{2}{3} \left(\frac{\pi BT}{E_{F_{e,h}}}\right)^2 s(s+\tfrac{1}{2}) \right] \right\} \quad \alpha \gg 1. \quad (15)$$

3. Comparison with experiment

3.1. Experimental determination of the strength S

Extended data about grain-boundary conductivity in antimony semi-metal films have been published previously [1] and it was established that Equation 4 even holds assuming that S takes the same values for electrons and holes and that $(2m)^{1/2} \cdot \tau$ is an average value [1].

Introducing the term $(\pi BT/E_F)^2$, the values of B and E_F, for antimony, available in the literature [4], show that $(\pi BT/E_F)^2$ takes negligible values for $T \ll 80$ K and $D < 20 \times 10^3$ nm. Hence Equation 14 becomes

$$\frac{\sigma_g}{\sigma_0} \approx \frac{3}{4\alpha}, \quad \alpha \gg 1 \quad (16)$$

which is the usual asymptotic equation for metal films [2].

From Equation 16 it can be predicted that a linear law is obtained for the variations in σ_g/σ_0 against D. This feature agrees with experimental data related to antimony films (Fig. 1).

Moreover if it is assumed, as usually [1, 4], that $s = -\frac{1}{2}$, in the case of antimony, the slope of the linear plot allow the calculation of the strength S, from Equations 16 and 4.

The calculated value is $S = 5.28 \times 10^{-29}$ Jsec in good agreement with the value $S = 5.2 \times 10^{-29}$ Jsec which gave the best fit [1] to experimental variations in conductivity with grain diameter (for $D < 10^4$ mn) at 300 K.

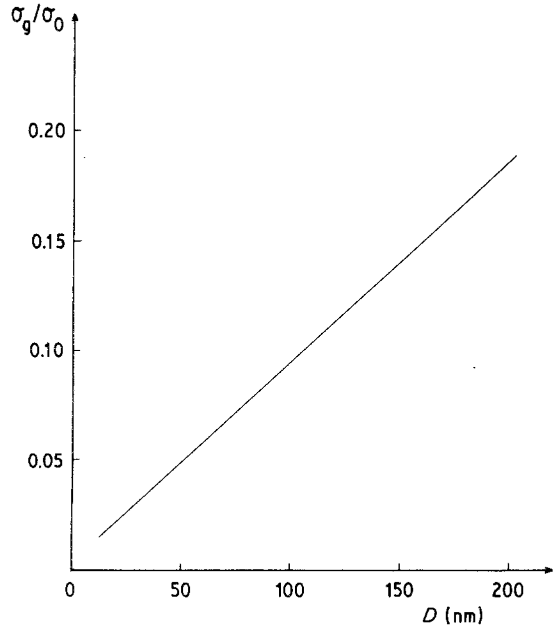

Figure 1 Plot of σ_g/σ_0 against D.

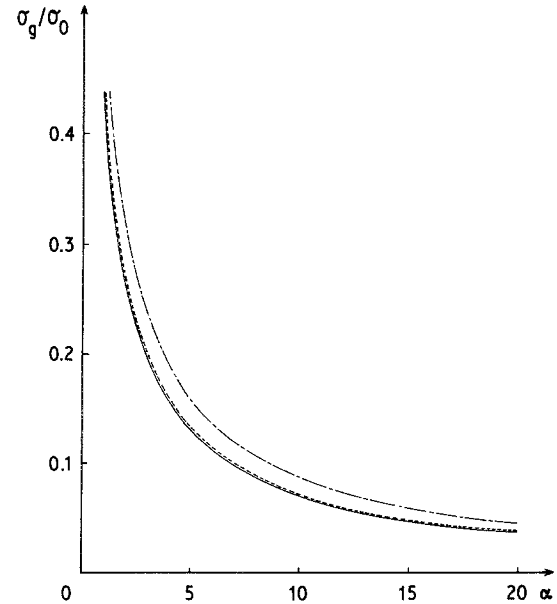

Figure 3 Plot of σ_g/σ_0 against α: ---, σ_g/σ_0 at $T = 350$ K; -----, σ_g/σ_0 at $T = 77$ K; ——, $f(\alpha)$.

3.2. Magnitude of the temperature-dependent extra term in conductivity

From theoretical Equations 2, 3 and 10 are drawn the variations in σ_g/σ_0 with α at 77 K and 350 K, in the case of antimony, i.e. for $s = -\frac{1}{2}$ (Figs 2 and 3). It is seen that, at 350 K, the theoretical grain-boundary conductivity of antimony films deviates from the Mayadas–Shatzkes function; the variations in the ratio:

$$\frac{1}{6}\left(\frac{\pi BT}{E_F}\right)^2 \cdot \frac{h(\alpha)}{f(\alpha)},$$

of the thermally-dependent term in conductivity to the conductivity at low temperature are plotted against α, s acting as a parameter (Fig. 4).

It may be noted that this extra term becomes negligible at 350 K (ratio $< 5\%$) for $\alpha < 0.5$, which corresponds to $D > 15 \times 10^3$ nm.

These theoretical predictions agree with experimental data [1] as shown by experimental points drawn in Fig. 2.

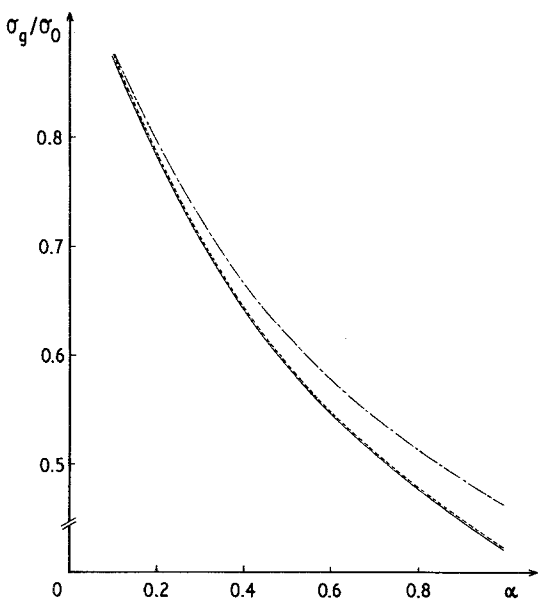

Figure 2 Plot of σ_g/σ_0 against α: ---, σ_g/σ_0 at $T = 350$ K; -----, σ_g/σ_0 at $T = 77$ K, ——, $f(\alpha)$.

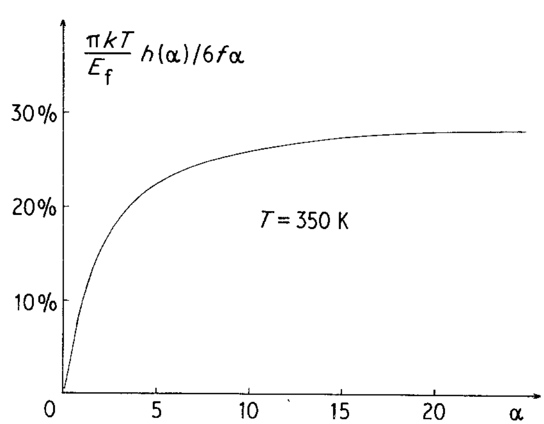

Figure 4 Variation in the ratio $\frac{1}{6}(\pi kT/E_F)^2 \cdot (h(\alpha)/f(\alpha))$ against α at $T = 350$ K.

4. Special features

Some unexpected consequences can be deduced from Equations 14 and 15.

First, in fine grained films ($\alpha \gg 1$), the reduced conductivity may be written, to a first approximation, in the form:

$$\frac{\sigma_g}{\sigma_0} \approx \frac{3}{4\alpha} \left[1 + \frac{1}{3}\left(\frac{\pi BT}{E_F}\right)^2\right], \quad \alpha \gg 1.$$

It clearly shows that the temperature-dependent term in the conductivity has the same expression, whatever the scattering kinetics may be, i.e. for any value of s. No physical explanation can be proposed for this feature.

Moreover, for large grain diameter ($\alpha \ll 1$), the temperature-dependent terms in the conductivity equation (Equation 15) vanish for $s = -\frac{1}{2}$ and Equation 15 reduces to Equation 13, which is valid for metal films.

In the case of antimony films, it is observed that Equation 13 gives a good fit for variations in conductivity at 500 K for $D > 10^4$ nm.

Equation 15 also satisfies an essential physical requirement: for $\alpha = 0$, which corresponds to a Fuchs–Sondheimer conduction model for a bulk material, Equation 11 reduces to:

$$\frac{\sigma_g}{\sigma_0} \approx 1 + \frac{1}{6}\left(\frac{\pi BT}{E_F}\right)^2 (s + \tfrac{1}{2})(s + \tfrac{3}{2}),$$

in good agreement with the general expression that can be obtained by an extension of the expression proposed by Jain and Verma [7] in the limiting case of diffuse electron scattering at the film surface, whereas perfectly specular scattering is an alternative description of an infinitely thick film.

Equation 7 shows that $s = \frac{1}{2}$ is the only case where the size effect function, at a given temperature, is proportional to the Mayadas–Shatzkes function $f(\alpha)$, for any α. Equation 11 thus becomes:

$$\frac{\sigma_g}{\sigma_0} = \left[1 + \frac{1}{3}\left(\frac{\pi BT}{E_F}\right)^2\right] f(\alpha), \quad s = \tfrac{1}{2}.$$

The above discussion shows that no simple procedure is available for calculating the exponent s (Equations 5 and 6); however, a rough indication can be derived from the thermal variations in σ_g/σ_0 with temperature (Equation 15) for large grains.

5. Conclusions

A theoretical expression for the electrical conductivity in infinitely thick polycrystalline semi-metal films can be derived from the Mayadas–Shatzkes theory; a good agreement with experimental data related to antimony films is observed.

Predictions are given for the deviations in the linear dependence of electrical conductivity of a semi-metal film with temperature.

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