SHORT COMMUNICATION

Adequate Use of the Cottey Model for the Description of Conduction in Polycrystalline Films

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An attempt has been recently made¹ to give a new model of electrical conduction in polycrystalline metal films. Some points are discussed in this paper. In the theoretical calculations related to a new grain boundary scattering model for conduction in metals [1], the current density J is written as

$$J = e \int v_x \cdot f_1(\theta, \phi) d^3p \quad (1)$$

where e is the electron charge, v_x the component of electron velocity v in the direction of the applied electric field and f_1 stands for the deviation from the equilibrium function of Fermi distribution.

Eq. (1) has been given by COTTEY² (p. 301) and is valid in spherical polar coordinates (r, θ, ϕ) with:

$$z = r \cos \theta$$

$$x = r \sin \theta \cos \phi$$

as shown in Figure 1.

Let us remember that in the Mayadas-Shatzkes conduction model³ the grain boundaries are represented by two types of randomly spaced planes,

FIGURE 1 Definition of spherical polar coordinates.

those parallel to the electric field, which produce only specular reflection, and those perpendicular whose effects are represented by a grain-boundary relaxation time $[2F(|k_x|)]^{-1}$ (Refer to Mayadas and Shatzkes³, Eqs. 6b and 7b) introduced in the Boltzmann equation.

The positions of the planes are defined by a Gaussian law [Mayadas and Shatzkes³ Eq. 3] whose standard deviation is s . In the limit $s \rightarrow 0$ no grain boundary resistivity is observed. This means that a periodic array of planes provides no resistance. However the average separation of the planes (which is identified with the average grain diameter D) could be used if the travelling distance of electrons l satisfies the condition

$$l \gg D \quad (2)$$

The transmission of electrons across grain boundaries can be conveniently¹ described with the COTTEY model, using the same assumptions as COTTEY², specially if the effect of boundaries on electrons can be described by an exponential function P of the travelling distance. This feature requires that the effect of any boundary could be expressed by a given differential variation of P and that the electron path between two boundaries could be considered as a differential variation of l . In the new proposed model the first condition must be written in the form:

$$r \approx 1 \quad (3)$$

Furthermore, under this assumption, the term $\vec{v} \cdot \text{grad}_r f$ can be neglected in the Boltzmann equation [Sondheimer⁴, Eq. 5].

The second condition must be expressed as:

$$l \gg D' \quad \text{for } \theta \approx \frac{\pi}{2} \quad (4)$$

where D' is the boundary spacing measured in the vertical plane ($z = 0 = \rho$) containing $\vec{v}$ (Figure 2).

If Eq. 4 is satisfied, the probability of electrons

FIGURE 2 The geometry of the grain-boundary model.

travelling through n grain boundaries P is defined by^{1,2}

$$P = r^n \quad (5)$$

$$dP = -\frac{P}{\lambda_D} dl \quad \text{which gives}$$

$$P = \exp(-l/\lambda_D) \quad (6)$$

where λ_D is the mean free path associated with the influence of grain boundaries on the conduction electrons.

The travelling distance l is calculated in the $(z - O - \rho)$ plane (Figure 3).

$$l = \frac{nD'}{|\sin \theta|} \quad (7)$$

FIGURE 3 The geometry of the Warkusz model¹.

where (Figure 2)

$$D' = D/|\cos \phi|. \quad (8)$$

Hence the theoretical expression of λ_D

$$\lambda_D = \frac{D}{|\sin \theta| |\cos \phi| \ln \frac{1}{r}} \quad (9)$$

This expression does not agree with the expression previously proposed [Warkusz¹, Eq. 4], since the author did calculate the travelling distance from the relation:

$$l = \frac{nD}{|\sin \theta|} \quad (10)$$

which is only valid for cylindrical grain boundaries. Hence, all equations derived are questionable [Warkusz¹, Eq. 8, 9, 10, 11, 12].

Assuming that grain boundary and background scattering are independent, the mean free path $\lambda(\theta, \phi, r)$ for both scatterings is^{4,1}.

$$\frac{1}{\lambda(\theta, \phi, r)} = \frac{1}{\lambda_0} + \frac{1}{\lambda_D} \quad (11)$$

where λ_0 is the bulk mean free path.

Solving the Boltzmann equation gives:

$$\sigma_g/\sigma_0 = \frac{3}{4\pi} \int_0^\pi \int_0^{2\pi} \frac{\sin^3 \theta \cos^2 \phi}{1 + \frac{\lambda_0}{D} |\cos \phi| |\sin \theta| \ln \frac{1}{r}} d\theta d\phi \quad (12)$$

where σ_g is the grain boundary conductivity, i.e. the conductivity of an infinitely thick polycrystalline film, and σ_0 the bulk conductivity.

Eq. 12 is not easily integrated in these coordinates but more convenient coordinates could be used.

As it has been shown above Eq. 12 is valid if r takes values near 1.

Finally it appears that the new model recently proposed¹ is of slight physical interest and somewhat questionable whereas the alternative expression for Mayadas-Shatzkes equation is somewhat complicated. Further studies would be necessary.

REFERENCES

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