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Three-dimensional analytical expressions of strain gauge coefficients of infinitely thick polycrystalline metal films

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Theoretical equations for the longitudinal and transverse strain coefficients of resistivity in infinitely-thick polycrystalline films are derived from a three-dimensional conduction model; the changes in the grain sizes in the directions parallel and perpendicular to the applied electric field are considered. Numerical calculations are performed in the typical case of silver, the strain coefficients are found to depend mainly on the grain parameter ν.

1. Introduction

In the past few years the electrical resistivity, ρ_g, of infinitely thick polycrystalline films was found [1–12] to depend on grain-boundary scattering effects. These effects have been recently studied [13] by taking into account the scattering effects due to three arrays of grain-boundaries respectively perpendicular to the x-, y- and z-axes (see Fig. 1) and by introducing [13, 14] a transmission coefficient, t, to describe the average property of the boundaries.

Hence it is reasonable to expect that the scatterings from the grain-boundary will affect all the transport properties and therefore the strain coefficient of resistivity. The purpose of the present paper is to derive a general expression for the strain coefficient of resistivity, γ_g, in infinitely-thick polycrystalline metal films.

2. Theoretical work

When the substrate is bent to produce a longitudinal (or a transverse) strain it is reasonable to expect variations in length L, width w, and also in the average grain-boundary spacings a_x, a_y and a_z (Fig. 1) which lie in the x-, y- and z-directions, respectively, and which are commonly identified with the grain size [13]. At the same time the strain introduces a change in the background mean free path l_0 and in the background resistivity ρ_0.

In terms of a three-dimensional model [13] the total film resistivity is represented by the function

$$\rho_g = \rho_g(\rho_0, l_0, a_x, a_y, a_z), \quad (1)$$

but it is not easy to determine the strain coefficient by using the general expression of the polycrystalline film resistivity commonly derived from the three-dimensional model [13].

The difficulty may be overcome by separately considering the contributions to the total resistivity ρ_g of the three distributions of grain-boundaries.

2.1. The film resistivity

It has recently been shown [15] that such an approximate analysis leads to small deviations in the total film resistivity ρ_g provided that the grain boundary parameter ν_i, defined [13] as

$$\nu_i = a_i l_0^{-1} \left(\ln \frac{1}{t}\right)^{-1} \quad \text{for } i = x, y, z, \quad (2)$$

keeps values greater than 0.4.

Let us recall that in terms of the above approximate model the contribution to the resistivity, $\rho_\perp$, of the boundaries perpendicular to the applied electric field $\mathbf{E}_x$ is given by [15]

$$\rho_\perp/\rho_0 = [F(\nu_x)]^{-1} - 1, \quad (3)$$

where [14]

$$F(\nu_x) = 3\nu_x \{\tfrac{1}{2} - \nu_x + \nu_x^2 \ln(1 + \nu_x^{-1})\}. \quad (4)$$

The contribution to the resistivity, $\rho_\parallel$, of the grain-boundaries parallel to the electric field $\mathbf{E}_x$ is

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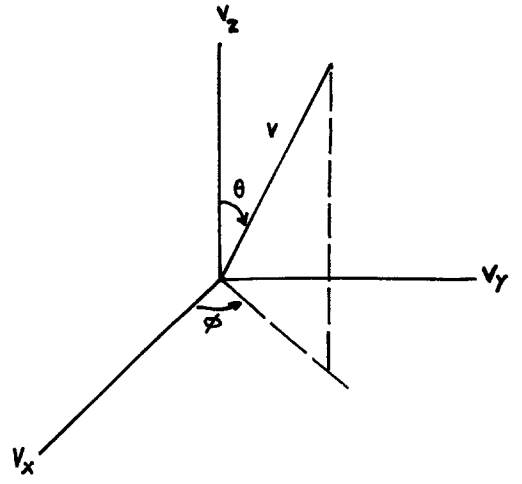

Figure 1 The geometry of the model.

expressed [15] as

$$\frac{\rho_{\parallel}}{\rho_0} = [G(\nu_i)]^{-1} - 1 \quad \text{for } i = y, z, \tag{5}$$

where

$$G(\nu_i) = \tfrac{3}{2}\nu_i\{\nu_i - \tfrac{1}{2} + (1 - \nu_i^2)\ln(1 + \nu_i^{-1}). \tag{6}$$

Hence, the approximate form of the polycrystalline film resistivity becomes

$$\rho_g/\rho_0 = M(\nu_x, \nu_y, \nu_z) = [F(\nu_x)]^{-1} + [G(\nu_y)]^{-1} + [G(\nu_z)]^{-1} - 2. \tag{7}$$

2.2. The strain coefficient

According to the preceding discussion, when a longitudinal strain dL/L is applied to the substrate, the elasticity formulae [16–19] yield the following equations

$$\frac{da_x}{a_x} \approx \frac{dL}{L}, \tag{8}$$

$$\frac{da_y}{a_y} \approx \frac{dW}{W} = -\mu_s\left(\frac{dL}{L}\right), \tag{9}$$

$$\frac{da_z}{a_z} \approx \frac{da}{a} = -\mu\frac{1-\mu_s}{1-\mu}\left(\frac{dL}{L}\right) = -\mu'\left(\frac{dL}{L}\right), \tag{10}$$

where a is the film thickness, dW/W is the transverse strain and μ and μ_s are the Poisson's ratio of the film and substrate materials, respectively.

In a similar way, when a transverse strain dW/W is applied to the substrate, the strain equations can be written

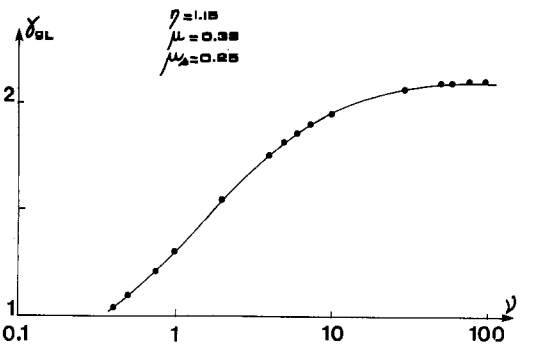

Figure 2 The grain-boundary longitudinal gauge factor, γ_{gL}, as a function of the grain-parameter, ν, for $\eta = 1.15$, $\mu = 0.38$ and $\mu_s = 0.25$.

$$\frac{da_x}{a_x} \approx -\mu_s\left(\frac{dW}{W}\right) \tag{11}$$

$$\frac{da_y}{a_y} \approx \frac{dW}{W} \tag{12}$$

$$\frac{da_z}{a_z} \approx -\mu'\left(\frac{dW}{W}\right) \tag{13}$$

With the assumptions that the film material is isotropic and that the variations in l_0 with deformation may be entirely attributed to the change in the amplitude of the thermal vibrations of atoms [20], the strain coefficients of ρ_0 and l_0 are given by [20]

$$d\ln \rho_0/d\epsilon = \eta + 1, \tag{14}$$

$$d\ln l_0/d\epsilon = -\eta, \tag{15}$$

where $d\epsilon$ is the change in general strain ϵ and $\eta = 2g(1 - 2\mu)$, where g is Grüneisen's constant.

Logarithmic differentiation of Equation 7 gives

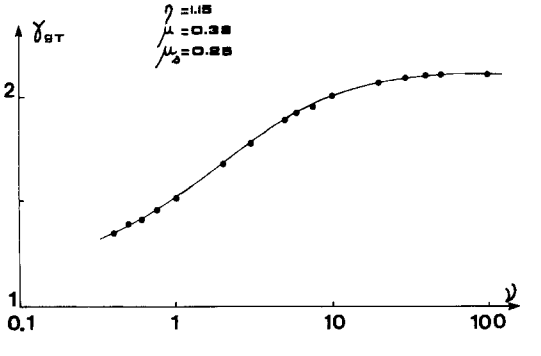

Figure 3 The grain-boundary transverse gauge factor, γ_{gT}, as a function of the grain-parameter, ν, for $\eta = 1.15$, $\mu = 0.38$ and $\mu_s = 0.25$.

$$\frac{d\rho_g}{\rho_g} - \frac{d\rho_0}{\rho_0} = -\frac{1}{M(\nu_x, \nu_y, \nu_z)}\left\{\frac{1}{F^2(\nu_x)}\frac{dF(\nu_x)}{d\nu_x}\,d\nu_x + \frac{1}{G^2(\nu_y)}\frac{dG(\nu_y)}{d\nu_y}\,d\nu_y + \frac{1}{G^2(\nu_z)}\frac{dG(\nu_z)}{d\nu_z}\,d\nu_z\right\} \quad (16)$$

Taking into account Equation 2 and noting that

$$\frac{d\nu_i}{\nu_i} = \frac{da_i}{a_i} - \frac{dl_0}{l_0}; i = x, y, z, \quad (17)$$

and further introducing, for convenience, the functions

$$\nu_x \frac{dF(\nu_x)}{d\nu_x}[F(\nu_x)]^{-2} = F^*(\nu_x) \quad (18)$$

$$\nu_i \frac{dG(\nu_i)}{d\nu_i}[G(\nu_i)]^{-2} = G^*(\nu_i); i = y, z, \quad (19)$$

where

$$\frac{dF(\nu_x)}{d\nu_x} = \frac{3}{2} - 6\nu_x + 9\nu_x^2 \ln(1 + \nu_x^{-1}) - 3\nu_x^2(1 + \nu_x)^{-1} \quad (20)$$

and

$$\frac{dG(\nu_i)}{d\nu_i} = \frac{3}{2}\left\{3\nu_i - \frac{3}{2} + (1 - 3\nu_i^2)\ln(1 + \nu_i^{-1})\right\}, \quad (21)$$

finally, after some rearrangements, the relation is obtained that

$$\frac{d\rho_g}{\rho_g} - \frac{d\rho_0}{\rho_0} = \frac{1}{M(\nu_x, \nu_y, \nu_z)}\left\{\frac{dl_0}{l_0}[F^*(\nu_x) + G^*(\nu_y) + G^*(\nu_z)] - F^*(\nu_x)\frac{da_x}{a_x} - G^*(\nu_y) \times \frac{da_y}{a_y} - G^*(\nu_z)\frac{da_z}{a_z}\right\}. \quad (22)$$

Inserting Equations 8 to 10 and 14 and 15 into Equation 22, the longitudinal strain coefficient of grain boundary resistivity, $\gamma_{gL} = d \ln \rho_g (dL/L)^{-1}$ is found to be

$$\gamma_{gL} = (\eta + 1) - \eta\frac{F^*(\nu_x) + G^*(\nu_y) + G^*(\nu_z)}{M(\nu_x, \nu_y, \nu_z)} - \frac{F^*(\nu_x)}{M(\nu_x, \nu_y, \nu_z)} + \mu_s\frac{G^*(\nu_y)}{M(\nu_x, \nu_y, \nu_z)} + \mu'\frac{G^*(\nu_z)}{M(\nu_x, \nu_y, \nu_z)}. \quad (23)$$

In a similar way the transverse strain coefficient of grain boundary resistivity, γ_{gT}, takes the form

$$\gamma_{gT} = (\eta + 1) - \eta\frac{F^*(\nu_x) + G^*(\nu_y) + G^*(\nu_z)}{M(\nu_x, \nu_y, \nu_z)} - \frac{G^*(\nu_y)}{M(\nu_x, \nu_y, \nu_z)} + \mu_s\frac{F^*(\nu_x)}{M(\nu_x, \nu_y, \nu_z)} + \mu'\frac{G^*(\nu_z)}{M(\nu_x, \nu_y, \nu_z)}. \quad (24)$$

Simple analytical expressions for the film strain coefficients can then be expressed from the grain-boundary strain coefficients by introducing an approximate linear effective size-effect function [21].

Equations 23 and 24 can then be helpful for analysing the strain effects in polycrystalline films.

In the three-dimensional conduction model proposed by Pichard *et al.* [13] it is assumed that the grain sizes measured in the x-, y- and z-directions take equal values (i.e. $\nu_x = \nu_y = \nu_z = \nu$). Figs 2 and 3 show the variations of the longitudinal and transverse gauge factor with the grain parameter, ν, taking the values of μ and η typical for silver ($\eta = 1.15$, $\mu = 0.38$, [20]) and the value of μ_s typical for glass ($\mu_s = 0.25$, [17]). It is seen that the values of gauge factors γ_{gL} and γ_{gT} slightly decrease with decreasing values of ν, that is, when the grain-boundaries act as more efficient scatterers.

The gauge factors γ_{gL} and γ_{gT} appear to reach the bulk values γ_{L_0} and γ_{T_0} when the grain parameter ν takes values greater than 50. This result is not surprising and could be deduced from the limiting forms of $F(\nu)$, $G(\nu)$ and their respective derivatives (with respect to ν). Effectively in the limit of very large ν, Equations 4, 6, 20 and 21 reduce to the simple forms

$$F(\nu)|_{\nu \to \infty} \approx 1 - \frac{3}{4\nu}, \quad (25)$$

$$G(\nu)|_{\nu \to \infty} \approx 1 - \frac{3}{8\nu}, \quad (26)$$

$$\left.\frac{dF(\nu)}{d\nu}\right|_{\nu \to \infty} \approx \frac{3}{4\nu^2}, \quad (27)$$

$$\left.\frac{dG(\nu)}{d\nu}\right|_{\nu \to \infty} \approx \frac{3}{8\nu^2}. \quad (28)$$

3. Conclusions

An approximate form of the electrical resistivity of polycrystalline film previously derived in the light of the three-dimensional model of grain-boundaries gives analytical expressions for the strain coefficients of resistivity which mainly depend on the average grain parameter, ν, and tend to bulk values when the efficiency of the grain-boundary scattering processes is low.

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