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SHORT COMMUNICATION
Hyperbolic Approximate Form of the Mayadas-Shatzkes Function

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In order to take into account the effect of grain boundaries scattering on the electronic transport properties of metal films, Mayadas and Shatzkes[1] have proposed a conduction model in which the conductivity σ_g of an infinitely thick polycrystalline film is expressed by the following equation:

$$\sigma_g = \sigma_0 \, . \, f(\alpha) \tag{1}$$

where σ_0 is the bulk conductivity, f is the M–S (Mayadas–Shatzkes) function, and α is a parameter defined by:

$$\alpha = l_0 \; a_g^{-1} \; r(1-r)^{-1} \tag{2}$$

where l_0 is the electronic mean free path in the bulk material, a_g is the mean grain diameter and r the electronic reflection coefficient at the grain boundary.

The literal expression of $f(\alpha)$ is complicated and a new approximate form of the M–S function is examined in this paper.

The temperature coefficient of the resistivity β is usually defined[2] by:

$$\beta = -\mathrm{d} \ln \sigma / \mathrm{d}T$$

where T is temperature, and theoretical calculations[3,4] can be derived from Eq. (1).

The ratio of grain boundary t.c.r. β_g and bulk t.c.r. β_0 is then given by:[4]

$$\beta_g/\beta_0 = 1 + f(\alpha)^{-1} \; \alpha \, \frac{\mathrm{d}f(\alpha)}{\mathrm{d}\alpha} \tag{3}$$

Experiments on polycrystalline metal films[5,6] have shown that:

$$\beta_g/\sigma_g \approx \beta_0/\sigma_0 \tag{4}$$

Eq. (1), (3) and (4) then give:

$$\frac{\mathrm{d}f(\alpha)}{f(\alpha)\,[f(\alpha)-1]} \approx \frac{\mathrm{d}\alpha}{\alpha} \tag{5}$$

whose solution is:

$$f^*(\alpha) = (1 + C_1\alpha)^{-1} \tag{6}$$

where C_1 is a constant.

$f^*(\alpha)$ is an hyperbolic approximate form of the M–S function $f(\alpha)$.

A perfect fit could be obtained if C_1 could vary with α; but since a variation ΔC_1 in C_1 induces a variation Δf^* in $f^*(\alpha)$, whose value is derived from Eq. (6):

$$\frac{\Delta f^*}{f^*(\alpha)} = -[1 - f^*(\alpha)] \, \frac{\Delta C_1}{C_1} \tag{7}$$

the deviation from the ideal value is lowest when $f^*(\alpha)$ takes values near unity, i.e. for lowest values of α[1], the value which gives a good fit for the higher values of α is chosen. In this case, the value of C_1 is chosen in order that approximate and exact values of the M–S function coincide for $\alpha = 10$; higher values of α are rarely obtained at room temperature.[2]

For $C_1 = 1.34$, the deviation is less than 4% for the α values situated between 0.01 and 10 (Table I).

In spherical polar coordinates, the conductivity σ_g is expressed by:[7]

$$\sigma_g/\sigma_0 = \frac{3}{4\pi} \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \frac{\sin^3\theta \cos^2\phi}{1 + l_0 \, . \, l^{-1}} \, \mathrm{d}\phi$$

where l is the mean free path due to grain boundary scattering.

Assuming that l is independent of θ and ϕ, then:

$$\sigma_g/\sigma_0 = \frac{1}{1 + l_0 \, . \, l^{-1}} \tag{8}$$

Introducing Eq. (6) in Eq. (1) and comparing with Eq. (8) yields:

$$(l/l_0)^{-1} = C_1 \; \alpha \tag{9}$$

TABLE I
Comparison between the Mayadas–Shatzkes function, f, and the hyperbolic approximation, f^*.

α	$C_1 \alpha$	$1 + C_1 \alpha$	f^*	f
0.01	0.0134	1.0134	0.9868	0.985286
0.05	0.067	1.067	0.9372	0.931358
0.1	0.134	1.134	0.8818	0.872806
0.5	0.67	1.67	0.5888	0.588000
1	1.34	2.34	0.42735	0.420558
2	2.68	3.68	0.2717	0.268837
3	4.02	5.02	0.1992	0.197752
4	5.36	6.36	0.1572	0.156438
5	6.7	7.7	0.1299	0.129416
10	13.4	14.4	0.0694	0.069461

In the M–S model the exact expression is [Mayadas and Shatzkes[1], Eq. (9)]:

$$(1/l_0)_{ex}^{-1} = \frac{\alpha}{\tau} \frac{k_F}{|k_x|} \quad (10)$$

where τ is the electronic relaxation time in the bulk material, k the wave vector, the index F and x being, respectively, related to the Fermi surface and the x-direction.

Comparing Eqs. (9) and (10) shows that the approximate hyperbolic form $f^*(\alpha)$ is obtained when assuming that the scattering is an isotropic process.

Approximate hyperbolic forms of the M–S function can be obtained under the assumption of an isotropic scattering at the grain boundary; slight deviations from the exact M–S values are obtained.

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