

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 Shatzkes¹ have proposed a conduction model in which the conductivity σ_g of an infinitely thick polycrystalline film is expressed by the following equation:

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

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 defined² by:

$$\beta = -d \ln \sigma / dT$$

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

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

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:

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

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 , 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

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

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

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

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

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 Shatzkes¹, 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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