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Thickness-Dependent Electrical Resistivity of Thin Rough Metal Films

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Introduction In the treatment of the electrical conductivity of a metal thin film the percolating conduction mechanism /1/ and the possible surface roughness /2/ play an important role. The influence of the surface roughness on the electrical properties of pure metal films is well known /2 to 8/. The thickness dependence of the electrical resistivity of rough metal films was investigated thoroughly by Finzel et al. /2, 3/.

In accordance to the theory of Finzel and Wissmann /2/ the total resistivity of rough metal films consists of the contributions of the normal bulk resistivity, the well-known term of conduction electron scattering on the grain boundaries and surfaces, and an additional term due to roughness, which varies proportionally to d^{-3} /2/ if the deviations of the thickness from the mean value d are symmetrical. Finzel and Wissmann /2/ calculated the total resistivity of rough metal films with the assumption that $\lambda \ll B \ll d$, where λ and B are the mean free path of the conduction electrons and the maximum thickness deviation from the mean value d, respectively.

Crittenden and Hoffmann /4/ introduced a thickness correction term into the total resistivity expression to describe the influence of the surface roughness. Namba /5/ extended this theory assuming that the film surface can be characterized by a sinusoidal profile. Hoffmann and Vancea /6/ gave a quantitative analysis of the roughness effect. These theories can be quite correct for a "microscopic" roughness, when $B \ll \lambda \ll d$ /7, 8/.

The total resistivity of very thin films ($d \ll \lambda$) with "microscopic" surface roughness ($B \ll d$) is not investigated yet. In the case of $B \ll d \ll \lambda$ the size effect has an important role /9 to 12/. In this note we give a quantitative analysis for the thickness dependence of the electrical resistivity of very thin ($d \ll \lambda$), rough ($B \ll d$) films considering the size and roughness effect.

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For the size effect we use the Fuchs-Sondheimer-Lucas theory /11 to 14/. For the surface roughness we use the model of Finzel and Wissmann /2/, assuming that the investigated very thin film consists of a monolayer of crystallites, and the boundaries are mainly aligned perpendicular to the film surface.

The average crystallite size is d, so the average film thickness is d, too. The deviations of the thickness from this average value have a distribution function f(y). This distribution has a cut-off because $-B \leqq y \leqq B$, where B is the maximum value of these deviations. We assume a symmetrical distribution of the film thickness around the mean value d. Such a distribution has been experimentally established by several authors /2, 15, 16/.

Analysis The resistivity of a crystallite with size d-y is /2/

$$\varrho_c(y) = \varrho_o\left(1 + \frac{k}{d-y}\right), \quad k = z\sigma\lambda = \text{const}, \tag{1}$$

where z, σ, λ, d, y, ϱ_o are the number of scattering centres per unit surface, the scattering cross section, the bulk mean free path of the conduction electrons, the mean crystallite size, the deviation of the thickness from its mean value d, and the resistivity of very thin crystallites, respectively. By the model of Finzel and Wissmann /2/ the total resistivity of the film is the average of the resistivity contributions of crystallites of different size:

$$\varrho_f = \frac{\int_{-B}^{B} \varrho_c(y) f(y)\,dy}{\int_{-B}^{B} f(y)\,dy}, \tag{2}$$

where f(y) is the distribution function of the grain size. In very thin films the resistivity ϱ_o increases because of the size effect. On the basis of the Fuchs-Sondheimer-Lucas theory /11 to 13/ in the case $d \ll \lambda$ the resistivity ϱ_o is

$$\varrho_o = \varrho_b\left[1 + \frac{A\,\lambda}{(d-y)\ln\left(\frac{\lambda}{d-y}\right)}\right], \quad A = \frac{4(1-pq)}{3(1+p)(1+q)}, \tag{3}$$

where ϱ_b is the resistivity of the bulk material with the same densities of lattice defects as in the film. The parameters p and q give the fractions of conduction electrons scattered elastically on the two boundary surfaces of the grains. We introduce the notation

$$x = y/B \tag{4}$$

and from (1) to (4) we obtain

$$\varrho_f = \varrho_b \frac{\int_{-1}^{1} \left(1 + \frac{k/d}{1 - Bx/d}\right)\left[1 + \frac{A\lambda/d}{(1 - Bx/d)\ln\left(\frac{\lambda/d}{1 - Bx/d}\right)}\right] f(x)\,dx}{\int_{-1}^{1} f(x)\,dx} . \tag{5}$$

The nominators in (5)

$$(1 - Bx/d)^{-1} , \quad \left[(1 - Bx/d)\ln\left(\frac{\lambda/d}{1 - Bx/d}\right)\right]^{-1} \tag{6}$$

can be expanded in a power series of Bx/d because of $Bx/d \ll 1$ in the case $-1 \leqq x \leqq 1$ and $B/d \ll 1$. When the distribution function $f(y)$ is symmetrical, all the odd terms of the expansion vanish by the integration, so we can write

$$\varrho_f = \varrho_b + \varrho_b \frac{k}{d} + \varrho_b \frac{B^2 G_2 k}{d^3} + \varrho_b \frac{A\lambda}{d \ln(\lambda/d)} + \varrho_b \frac{Ak\lambda}{d^2 \ln(\lambda/d)} +$$

$$+ \varrho_b \frac{B^2 G_2 A\lambda}{2d^3 \ln(\lambda/d)} \left[2 - \frac{3}{\ln(\lambda/d)} + \frac{2}{\ln^2(\lambda/d)}\right] + \dots$$

$$= \varrho_b + \varrho_{sc} + \varrho_r^{(sc)} + \varrho_{si} + \varrho_{si}^{(sc)} + \varrho_{si}^{(r)} + \dots , \tag{7}$$

where

$$G_n = \frac{\int_{-1}^{1} x^n f(x)\,dx}{\int_{-1}^{1} f(x)\,dx} , \quad n = 2, 4, \dots . \tag{8}$$

In the case $d \gg k$ the terms of higher order can be neglected compared with the first six terms in (7).

If the distribution function $f(y)$ is not symmetrical, then in the cases $B \ll d \ll \lambda$ and $d \gg k$ further resistivity terms appear in the total resistivity, which can be calculated from (5):

$$\varrho_1 = \varrho_b \frac{BkG_1}{d^2}, \quad \varrho_2 = \varrho_b \frac{ABk\lambda G_1}{d^3 \ln(\lambda/d)} \left[2 - \frac{1}{\ln(\lambda/d)} \right],$$

$$\varrho_3 = \varrho_b \frac{AB\lambda G_1}{d^2 \ln(\lambda/d)} \left[1 - \frac{1}{\ln(\lambda/d)} \right]. \tag{9}$$

Conclusions The assumptions of our calculations are that the thickness deviations from a mean value are symmetrical, the maximum deviation is much smaller than the mean thickness, and the mean thickness is much smaller than the bulk mean free path of the conduction electrons ($B \ll d \ll \lambda$).

The total resistivity is given by six resistivity terms under these conditions. The first three terms are the well known normal bulk resistivity (ϱ_b), the contribution of the scattering of the conduction electrons on grain boundaries and surfaces (ϱ_{sc}), and the roughness term ($\varrho_r^{(sc)}$).

The new additional three resistivity terms belong to the size effect ($d \ll \lambda$). The first additional term ϱ_{si} is due to the size effect only, and varies as $(d \ln(\lambda/d))^{-1}$. The second one $\varrho_{si}^{(sc)}$ describes the combination the size effect and the scattering of the electrons on the grain boundaries and surfaces, which varies as $(d^2 \ln(\lambda/d))^{-1}$. The third additional resistivity term $\varrho_{si}^{(r)}$ depending on the thickness is most complicated, it varies as $F(\ln(\lambda/d))d^{-3}$ and it is due to the combination of the size and roughness effect.

In very thin films ($d \ll \lambda$) the additional three resistivity terms have primary relevance in the total resistivity. The parameters ϱ_b, k, B, G_2, A, and λ can be evaluated from experimental data measuring the thickness dependence of the resistivity.

When the thickness deviations from the mean value d are not symmetrical, then some further terms appear in the total resistivity. These terms are due to the combination of the roughness effect and the scattering (on the grain boundaries and the surfaces) (ϱ_1); the size and the roughness effect plus scattering (ϱ_2), the size and the roughness effect (ϱ_3).

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