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ELECTRICAL PROPERTIES OF EPITAXIAL ALUMINIUM FILMS

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The resistivity of monocrystalline Al films was measured and compared with the resistivity calculated in terms of the function which takes into account both the external and the internal size effects. A comparison of the theoretical and experimental curves shows that the specular reflection coefficient (p) is small, while the coefficient of electron transmission through the grain boundary (r) increases with increasing film thickness.

1. INTRODUCTION

The resistivity of metal films is known to be thickness and grain-size dependent.[1–3] Based on Fuchs's model of electron scattering,[4] Mayadas and Shatzkes[2] have developed a function which takes into account the influence of both external and internal size effects on the resistivity of the film. Using the layer model proposed by Cottey[5] the scattering function $W(\mu,\nu)$[3] was derived, which describes the dependence of the film resistivity on film thickness and grain diameter. The comparison of experimental resistivities and the resistivities calculated in terms of the Mayadas-Shatzkes grain-boundary scattering function and Cottey's surface scattering function is presented elsewhere by the authors.[6] In this paper the function $W(\mu,\nu)$ is used to calculate the resistivity vs. grain diameter (b) for two series of Al films exhibiting various thicknesses (a). The accepted values of a and b were obtained from measurements. Theoretical and experimental curves are compared.

2. THEORY

Considering the electron scattering on the external surfaces and on the grain boundaries the resistivity of the film (ρ_f) can be represented as follows

$$\rho_f = \frac{\rho_B}{W(\mu,\nu)} \tag{1}$$

where ρ_B denotes the resistivity of the bulk material, and $W(\mu,\nu)$ refers to the function derived by Warkusz[3] which depends on the film thickness (a), on the fraction of electrons specularly scattered at the film surface (p), on the grain diameter (b), on the coefficient of electron transmission through the grain boundary (r) and finally on the electron mean free path λ, whereas

$$\mu = \frac{a}{\lambda \ln 1/p} \tag{2}$$

and

$$\nu = \frac{b}{\lambda \ln 1/r} \tag{3}$$

Depending on the parameters μ and ν, the function $W(\mu,\nu)$ takes the following form:

$$\begin{aligned} &W_1(\mu,\nu) \text{ if } \mu \neq 1, \frac{1}{\mu^2}+\frac{1}{\nu^2} > 1 \\ &W_2(1,\nu) \text{ if } \mu = 1, \frac{1}{\mu^2}+\frac{1}{\nu^2} > 1 \\ &W_3(\mu,\nu) \text{ if } \frac{1}{\mu^2}+\frac{1}{\nu^2} = 1 \\ &W_4(\mu,\nu) \text{ if } \frac{1}{\mu^2}+\frac{1}{\nu^2} < 1 \end{aligned} \tag{4}$$

W_1, W_2, W_3 and W_4 are given by Warkusz.[3]
The extreme terms of these functions required in our calculations are presented below. If the film thickness is sufficiently high ($a/\lambda \to \infty$) or if $p \to 1$, then in

terms of Eq. (2) $\mu \to \infty$ and $W_1(\mu,\nu) = F_1(\nu)$ or $W_4(\mu,\nu) = F_2(\nu)$ where

$$F_1(\nu) = \frac{3}{2}\nu\left(\frac{\pi}{4} - \nu + \frac{\pi}{2}\nu^2 + \frac{\nu^3}{\sqrt{1-\nu^2}} \ln \frac{\nu}{1+\sqrt{1-\nu^2}}\right) \text{for } \nu < 1 \quad (5)$$

$$F_2(\nu) = \frac{3}{2}\nu\left(\frac{\pi}{4} - \nu + \frac{\pi}{2}\nu^2 - \frac{\nu^3}{\sqrt{\nu^2-1}} \arcsin\sqrt{1-1/\nu^2}\right) \text{for } \nu > 1 \quad (6)$$

If the films of interest exhibit a large grain size ($b/\lambda \to \infty$) or if $r \to 1$, then $W_1(\mu,\nu) = W_4(\mu,\nu) = F(\mu)$ where

$$F(\mu) = \frac{3}{2}\mu\left\{\mu - \frac{1}{2} + (1-\mu^2)\ln\left(1+\frac{1}{\mu}\right)\right\} \quad (7)$$

For a sufficiently thick film with large grain size

$$\lim_{\substack{\mu\to\infty \\ \nu\to\infty}} W(\mu,\nu) = 1.$$

The product $F(\mu)\cdot F_2(\nu)$ also tends to unity,

$$\lim_{\substack{\mu\to\infty \\ \nu\to\infty}} F(\mu)F_2(\nu) = 1.$$

Hence, $W(\mu,\nu)$ can be replaced by $F(\mu)\cdot F_2(\nu)$ and Eq. (1) becomes

$$\rho_f = \frac{\rho_B}{F(\mu)F_2(\nu)} \quad (8)$$

Considering Eq. (1) and Eq. (8) the ρ_f/ρ_B ratio is calculated as a function of a/λ and b/λ for the given parameters p and r. The results are listed in Tables I and II. It is seen that ρ_f/ρ_B tends to unity, if the values of a/λ and b/λ are high and if p or r approaches unity. Then, the values of ρ_f/ρ_B calculated in terms of Eq. (1) and Eq. (8) are insignificantly different.

3. EXPERIMENTAL

Monocrystalline and textured Al films were obtained by using the method reported elsewhere by the authors,[7,8] and by applying a parallel or perpendicular electric field during evaporation.[9] Resistivity measurements were carried out for films of the following thicknesses: a = 600 Å ± 150 Å and 2000 Å $\leqslant a \leqslant$ 3800 Å; the measuring accuracy being of the order of 10%. To determine the average grain diameter, the size of about 300 grains on given fragments of the sample was established from electron micrographs. The grain diameters of the series of thin films ($0.7 \leqslant a/\lambda \leqslant 1.25$) were between 1300 Å and 4000 Å, and the grain diameters of the series of thicker films ($3.0 \leqslant a/\lambda \leqslant 6.5$) fell between

TABLE I

ρ_f/ρ_B calculated from Eq. (1) and Eq. (8) (with asterisk) for p = 0.2 and r = 0.5; δ is the percent relative error.

b/λ	a/λ											
	0.1	δ [%]	0.5	δ [%]	1	δ [%]	2	δ [%]	5	δ [%]	10	δ [%]
0.1	12.450 31.244*	150.9	8.321 13.415*	61.2	7.675 10.503*	36.8	7.325 8.848*	20.8	7.104 7.750*	9.1	7.028 7.361*	4.7
0.5	6.454 9.911*	53.5	3.321 4.255*	28.1	2.811 3.332*	18.5	2.525 2.807*	11.2	2.338 2.458*	5.1	2.273 2.335*	2.7
1	5.539 7.214*	30.2	2.646 3.097*	17.0	2.174 2.425*	11.5	1.907 2.043*	7.1	1.732 1.789*	3.3	1.670 1.699*	1.7
2	5.040 5.861*	16.3	2.296 2.517*	9.6	1.847 1.970*	6.7	1.593 1.660*	4.2	1.426 1.454*	1.9	1.366 1.381*	1.1
5	4.720 5.043*	6.8	2.079 2.165*	4.1	1.647 1.695*	2.9	1.402 1.428*	1.9	1.240 1.251*	0.89	1.182 1.188*	0.50
10	4.609 4.769*	3.5	2.005 2.048*	2.1	1.579 1.603*	1.5	1.338 1.351*	0.97	1.178 1.183*	0.42	1.121 1.123*	0.23

TABLE II
ρ_f/ρ_B calculated from Eq. (1) and Eq. (8) (with asterisk) for $p = 0.5$ and $r = 0.5$; δ is the percent relative error.

b/λ	a/λ											
	0.1	δ [%]	0.5	δ [%]	1	δ [%]	2	δ [%]	5	δ [%]	10	δ [%]
0.1	9.657 19.226*	99.1	7.580 10.058*	32.7	7.275 8.598*	18.2	7.116 7.813*	9.8	7.018 7.305*	4.1	6.984 7.132*	2.1
0.5	4.346 6.099*	40.3	2.734 3.191*	16.7	2.483 2.727*	9.8	2.348 2.478*	5.5	2.264 2.317*	2.3	2.235 2.262*	1.2
1	3.592 4.439*	23.6	2.102 2.222*	10.5	1.868 1.985*	6.3	1.741 1.804*	3.6	1.661 1.687*	1.5	1.634 1.646*	0.78
2	3.192 3.607*	13.0	1.779 1.887*	6.1	1.556 1.613*	3.6	1.435 1.466*	2.1	1.358 1.370*	0.92	1.331 1.338*	0.50
5	2.941 3.103*	5.5	1.582 1.623*	2.6	1.366 1.388*	1.6	1.249 1.261*	0.97	1.174 1.179*	0.44	1.148 1.151*	0.28
10	2.854 2.935*	2.8	1.515 1.535*	1.3	1.302 1.312*	0.81	1.186 1.193*	0.56	1.113 1.115*	0.19	1.087 1.089*	0.15

2000 Å and 18000 Å. Resistivity measurements for films drawn from the vacuum chamber were performed at room temperature with the use of the four-point microprobe method.

4. DISCUSSION OF RESULTS AND CONCLUSIONS

Figure 1 represents the experimental curves (full lines) illustrating the dependence of ρ_f/ρ_B on b/λ for two groups of the parameters a/λ. Using Eq. (1) the theoretical curves (dotted lines) are calculated with the assumption that $\lambda = 600$ Å and $\rho_B = 2.5 \times 10^{-6}\ \Omega$ cm. A qualitative agreement between the theoretical and experimental results if found. The resistivity of Al films is grain size dependent. This dependence, however, is more pronounced in thinner films. The values of resistivity which correspond to the same grain diameter but various film thicknesses show considerable differences. For thin Al films good

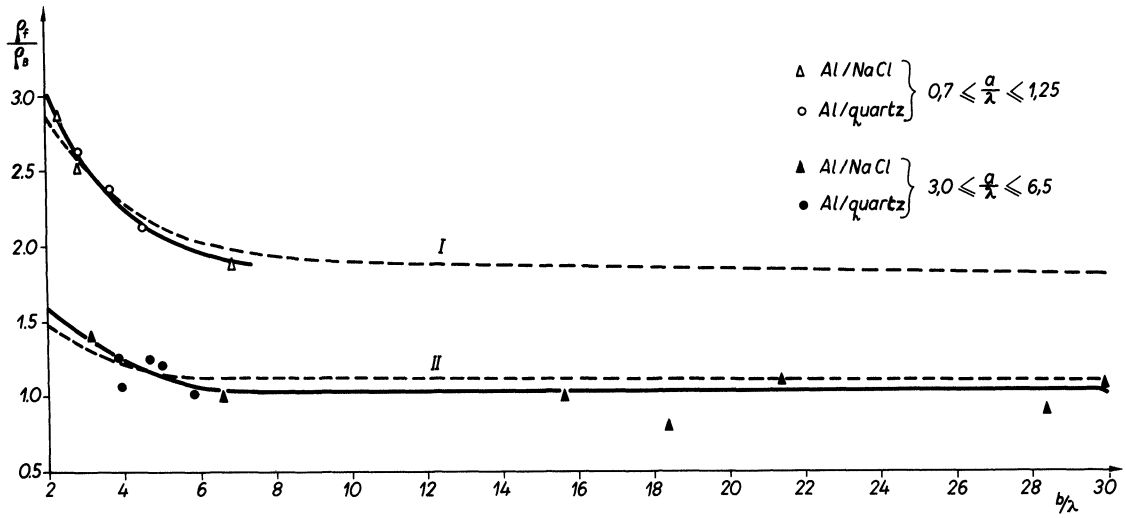

FIGURE 1 ρ_f/ρ_B versus b/λ curves. Theoretical curves (dotted lines) are calculated from Eq. (1) with $p = 0.1$, $r = 0.1$ ($R^* = 0.58$) and $a/\lambda = 1$ for curve I, and $p = 0.1$, $r = 0.5$ ($R^* = 0.30$) and $a/\lambda = 5$ for curve II.

agreement between the theoretical and experimental curves is obtained when both p and r are assumed to be equal to 0.1. For thick films the accepted p and r values are 0.1 and 0.5, respectively. It follows from Figure 1 that the specular reflection coefficient p remains small ($p = 0.1$) both for thin and thick films. The coefficient of electron transmission through the grain boundary r shows lower values ($r = 0.1$) for thin films and higher values ($r = 0.5$) for thick films.

A relationship is found between the parameter r and the grain boundary scattering coefficient R^*[3], where R^* is defined as the ratio of the number of electrons scattered by the boundary, compared with the total number of electrons impinging on the boundary.

$$\frac{R^*}{1 - R^*} = 0.62 \ln \frac{1}{r} \tag{9}$$

Thus, in the case of thin films $R^* \approx 0.58$, and in the case of thick films $R^* \approx 0.30$. Similar results for Al films are reported by Tellier and Tosser[10] and by Mayadas and Shatzkes.[2] For 110 Å $\leqslant a \leqslant$ 900 Å thicknesses, $R^* = 0.519$[10] and for significantly thicker films $R^* = 0.17$.[2]

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