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Linearization of polycrystalline film gauge factors

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Résumé. — Une équation linéaire est proposée pour décrire la dépendance, en fonction de l'épaisseur, du facteur de jauge γ_F , d'un film polycristallin. Finalement la variation théorique de γ_F est représentée par une équation générale dont la forme est similaire à celle correspondant aux équations linéarisées, préalablement obtenues pour l'étude de la résistivité de films polycristallins et de leur T.C.R. Des comparaisons des valeurs exactes et approchées montrent une déviation inférieure à 10 % sur des domaines étendus du coefficient de diffusion spéculaire p , de la distance moyenne entre les joints de grains a_g , et du rapport k de l'épaisseur du film au libre parcours moyen.

Abstract. — A linearized equation is proposed to describe the thickness dependence of the polycrystalline film gauge factor γ_F . Finally the theoretical variation of γ_F is represented by a general equation whose form is similar to those related to linearized equations previously derived for analyzing polycrystalline film resistivity and T.C.R. Comparisons of exact and approximate values indicate a deviation less than 10 % over large ranges of the surface scattering specularity parameter, p , the average random distance between grain boundaries, a_g , and the ratio, k , of the film thickness to background mean free path.

1. Introduction. — In the recent years it has been observed that evaporated [1-4] and sputtered [5-9] thin metal films exhibit a fine grained structure and thus grain-boundary scattering can significantly dominates the electromechanical properties of these films [10-13]. Mayadas and Shatzkes [14] have taken into account the grain boundary scattering and have proposed a conduction model [14] which describes the combined effects of grain-boundary, external surfaces and background scatterings. The electrical resistivity ρ_F of polycrystalline films is related to the resistivity ρ_g of an infinitely thick polycrystalline film by :

$$\rho_F/\rho_g = \left[1 - \frac{A}{f(\alpha)} \right]^{-1} \quad (1)$$

with :

$$A = \frac{6}{\pi k} (1 - p) \int_0^{\pi/2} d\varphi \int_1^\infty \frac{\cos^2 \varphi}{H^2(t, \varphi)} \left(\frac{1}{t^3} - \frac{1}{t^5} \right) \times \\ \times \frac{1 - \exp\{-ktH(t, \varphi)\}}{1 - p \exp\{-ktH(t, \varphi)\}} dt \quad (2)$$

$$H(t, \varphi) = 1 + \alpha \cdot (\cos \varphi)^{-1} \cdot (1 - 1/t^2)^{-1/2} \quad (3)$$

$$\rho_0/\rho_g = f(\alpha) = 1 - \frac{3}{2}\alpha + 3\alpha^2 - 3\alpha^3 \ln \left(1 + \frac{1}{\alpha} \right) \quad (4)$$

where ρ_0 is the bulk resistivity, k is the reduced thickness a/l_0 and p the specularity parameter. α is related to the bulk mean free path (mfp) l_0 , the average random distance between scattering planes which is assumed equal to the average grain diameter, a_g in the M-S model and the grain-boundary reflection coefficient r by :

$$\alpha = \frac{l_0}{a_g} \frac{r}{1 - r} \quad (5)$$

Tellier and Tosser [10] have developed a mathematical model for the longitudinal and transverse strain coefficient of resistance in thin metallic polycrystalline films.

The longitudinal and transverse strain coefficient of resistivity, γ_{FL} and γ_{FT} , can be defined by the equations :

$$\gamma_{FL} = \frac{d \ln \rho_F}{\left(\frac{dL}{L} \right)}$$

$$\gamma_{FT} = \frac{d \ln \rho_F}{\left(\frac{dw}{w} \right)}$$

and their expressions in the M-S model can be deduced from the previously published results [10].

It yields :

$$\gamma_{FL} = (\eta + 1) + [f(\alpha) - A]^{-1} \cdot \left\{ X(\eta + 1) + Y \left(-1 - \mu \frac{(1 - \mu_s)}{1 - \mu} \right) \right\} \quad (6)$$

$$\gamma_{FT} = (\eta + 1) + [f(\alpha) - A]^{-1} \cdot \left\{ X(\eta - \mu_s) + Y \left(\mu_s - \mu \frac{(1 - \mu_s)}{1 - \mu} \right) \right\} \quad (7)$$

where :

$$X = g(\alpha) - A + B + C \quad (8)$$

$$Y = D - A \quad (9)$$

$$g(\alpha) = \alpha \frac{df(\alpha)}{d\alpha}.$$

A is defined by eq. (2)

$$B = \frac{6}{\pi} (1 - p)^2 \int_0^{\pi/2} d\varphi \int_1^\infty \frac{\cos^2 \varphi}{H^2(t, \varphi)} \left(\frac{1}{t^2} - \frac{1}{t^4} \right) \frac{\exp\{-ktH(t, \varphi)\}}{[1 - p \exp\{-ktH(t, \varphi)\}]^2} dt \quad (10)$$

$$C = \frac{12\alpha}{\pi k} (1 - p) \int_0^{\pi/2} d\varphi \int_1^\infty \frac{\cos \varphi}{H^3(t, \varphi)} \left(\frac{1}{t^2} - \frac{1}{t^4} \right) \frac{1}{(t^2 - 1)^{1/2}} \frac{1 - \exp\{-ktH(t, \varphi)\}}{1 - p \exp\{-ktH(t, \varphi)\}} dt \quad (11)$$

$$D = \frac{6}{\pi} (1 - p)^2 \int_0^{\pi/2} d\varphi \int_1^\infty \frac{\cos^2 \varphi}{H(t, \varphi)} \left(\frac{1}{t^2} - \frac{1}{t^4} \right) \frac{\exp\{-ktH(t, \varphi)\}}{[1 - p \exp\{-ktH(t, \varphi)\}]^2} dt. \quad (12)$$

Unfortunately the strain coefficient γ_{FL} and γ_{FT} cannot be evaluated analytically and theoretical results related to polycrystalline films have been computed [15]. However this method is complicated and we have studied analytical expressions of the gauge factors which allow a convenient description of the α , p and k dependence of strain coefficients.

2. Approximate expressions for the gauge factors of polycrystalline films. — 2.1 THE $X \cdot [f(\alpha) - A]^{-1}$ FUNCTION. — We have previously shown that the exact expression of the temperature coefficient of resistance (T.C.R.) of polycrystalline films is given by [16] :

$$\beta_F/\beta_g = \left[1 + \frac{g(\alpha)}{f(\alpha)} \right]^{-1} \cdot \left[1 + \frac{X}{f(\alpha) - A} \right] \quad (13)$$

where β_g is the T.C.R. of an infinitely thick polycrystalline film. It can be approximate with good agreement by a relation in the form [17] :

$$k \cdot \beta_F/\beta_g \simeq k - (1 - p) \cdot H(\alpha). \quad (14)$$

Values of the function $H(\alpha)$ have been previously given [18].

Then by defining for convenience :

$$m(\alpha) = 1 + g(\alpha)/f(\alpha) \quad (15)$$

we may deduce from equation (13) :

$$k \cdot \frac{X}{f(\alpha) - A} \approx k[m(\alpha) - 1] - (1 - p) \cdot H(\alpha) \cdot m(\alpha). \quad (16)$$

2.2 THE $Y \cdot [f(\alpha) - A]^{-1}$ FUNCTION. — Figure 1 shows that the following relation :

$$\ln(-Y^*) \sim \ln k^{-1} \quad (17)$$

with :

$$Y^* = Y \cdot [f(\alpha) - A]^{-1}$$

is satisfied in large α , p and k ranges. Hence for given values α_0 and p_0 of the physical parameters α and p :

$$Y^*(k, \alpha_0, p_0) \approx -k^{-1} \cdot V(\alpha_0, p_0) \quad (18)$$

where $V(\alpha_0, p_0)$ is the slope of linear part of $\ln Y^*$, $\ln k^{-1}$ curves.

Further since we may verify (Fig. 1) that :

$$Y^*(k, \alpha_0, 0) = 2 Y^*(k, \alpha_0, 0.5) = 1.333 Y^*(k, \alpha_0, 0.25),$$

equation (18) leads to :

$$Y^*(k, \alpha_0, p_0) \approx - (1 - p_0) k^{-1} \cdot U(\alpha_0). \quad (19)$$

Finally we obtain :

$$k \cdot Y \cdot [f(\alpha) - A]^{-1} = - (1 - p) \cdot U(\alpha). \quad (20)$$

The values of the $U(\alpha)$ function are given in table I.

 Fig. 1. — $-Y.[f(\alpha) - A]^{-1}$ versus k^{-1} in log scales

- 1 : $\alpha = 0.5$ $p = 0$
- 2 : $\alpha = 1$ $p = 0$
- 3 : $\alpha = 1$ $p = 0.25$
- 4 : $\alpha = 0.5$ $p = 0.5$
- 5 : $\alpha = 2$ $p = 0$
- 6 : $\alpha = 1$ $p = 0.5$
- 7 : $\alpha = 2$ $p = 0.5$

Table I.

α	0	0.25	0.5	0.75	1	2	5
$U(\alpha)$	0.400	0.260	0.200	0.170	0.145	0.095	0.045

It would be noted that the corresponding linear plot of $U^{-1}(\alpha)$ against α (Fig. 2) allows us to determine $U^{-1}(\alpha)$ graphically with a sufficient accuracy (2 %).

The difference between the exact values and those deduced from equation (20) is less than 10 % for k between 0.6 and 10 with $0.25 \leq \alpha \leq 5$ and $0 \leq p \leq 0.5$.

 Fig. 2. — $[U(\alpha)]^{-1}$ plotted against α .

 Table II. — Comparison of the exact and approximate values of the function $-Y.[f(\alpha) - A]^{-1}$.

k	Exact values (eqs. (1) and (9))				Approximate values (eq. (20))			
	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 1$	$\alpha = 2$	$\alpha = 0.25$	$\alpha = 0.5$	$\alpha = 1$	$\alpha = 2$
$p = 0$								
0.06	1.664 2	1.880 4	1.831 1	1.486 6	4.333 3	3.333	2.416 7	1.583 3
0.1	1.226 1	1.325 8	1.243 2	0.971 6	2.60	2.00	1.45	0.950
0.2	0.822 3	0.827 8	0.724 5	0.526 4	1.30	1.00	0.725	0.475
0.4	0.543 3	0.503 4	0.403 2	0.267 4	0.65	0.500	0.362 5	0.237 5
0.6	0.414 6	0.364 7	0.275 9	0.174 4	0.433 3	0.333 3	0.241 7	0.158 3
1	0.279 8	0.230 8	0.164 1	0.100 3	0.260	0.200	0.158 3	0.095
2	0.146 2	0.113 7	0.078 0	0.047 9	0.130	0.100	0.072 5	0.047 5
4	0.070 4	0.054 3	0.037 6	0.023 4	0.065	0.050	0.036 25	0.023 8
6	0.045 9	0.035 6	0.024 7	0.015 5	0.043 3	0.033 3	0.024 2	0.015 8
10	0.027 0	0.021 0	0.014 7	0.009 2	0.26	0.020 0	0.014 5	0.009 5
$p = 0.5$								
0.06	0.918 8	0.961 9	0.883 8	0.686 7	2.166 7	1.666 7	1.208	0.791 7
0.1	0.687 7	0.685 5	0.601 6	0.462 7	1.30	1.00	0.725	0.475
0.2	0.454 3	0.422 5	0.345 8	0.240	0.650	0.50	0.362 5	0.237 5
0.4	0.283 9	0.246 8	0.188 3	0.120	0.325	0.250	0.181 3	0.118 8
0.6	0.208 0	0.174 4	0.128 1	0.081 3	0.216 7	0.166 7	0.120 8	0.079 2
1	0.134 5	0.108 5	0.076 9	0.047 8	0.130	0.100	0.072 5	0.047 5
2	0.069 2	0.054 0	0.037 5	0.023 4	0.065	0.050	0.036 3	0.023 8
4	0.034 0	0.026 4	0.018 4	0.011 6	0.032 5	0.025 0	0.018 1	0.011 9
6	0.022 5	0.017 5	0.012 2	0.007 7	0.021 7	0.016 7	0.012 1	0.007 9
10	0.013 3	0.010 4	0.007 3	0.004 6	0.013 0	0.010 0	0.007 3	0.004 8

(table II). It may be noted that when the electronic scattering on external surfaces on the film is completely specular, i.e. when $p = 1$, the conduction equations are those related to infinitely thick film; hence, there is no deviation between exact and approximate equations. It can be seen that the greater the values of α the larger the range of applicability of the approximate form becomes. In the case of diffuse scattering a deviation of less than 10 % is obtained for k between 0.6 and 10 with α equal to 0.25 and for k between 0.02 and 10 with $\alpha = 5$.

2.3 ANALYTICAL EXPRESSIONS FOR THE THIN POLYCRYSTALLINE GAUGE FACTORS. — Introducing equations (20) and (16) into equations (6) and (7) the gauge factors may be written, using equation (15) :

$$k \cdot \gamma_{FL} \approx m(\alpha) \cdot [\eta + 1] \cdot k - (1 - p) \times \{ (\eta + 1) \cdot H(\alpha) \cdot m(\alpha) - (1 + \mu') U(\alpha) \} \quad (21)$$

$$k \cdot \gamma_{FT} \approx k \left\{ (\eta + 1) + \frac{g(\alpha)}{f(\alpha)} (\eta - \mu_s) \right\} - (1 - p) \{ (\eta - \mu_s) \cdot H(\alpha) \cdot m(\alpha) + (\mu_s - \mu') U(\alpha) \} \quad (22)$$

with :

$$\mu' = \mu \frac{(1 - \mu_s)}{1 - \mu}.$$

Exact and approximate values of the strain coefficients are given in table III; it shows that a fair agreement is obtained when k takes values above 0.6.

Accordingly, a plot of $k\gamma_{FL}$ versus k (for example) should yield a straight line with the intercept as :

$$(1 - p) \{ (\eta + 1) \cdot H(\alpha) \cdot m(\alpha) - (1 + \mu') U(\alpha) \} \quad (23)$$

and the slope as :

$$m(\alpha) \cdot \{ \eta + 1 \}. \quad (24)$$

In the one hand we observe (equations (21), (22) and (23)) that, as expected, values of the slope are equal to the values γ_{gL} and γ_{gT} of gauge factors related to infinitely thick polycrystalline films [10]. Consequently it follows that the thin polycrystalline film gauge factors γ_F are given by the general formula :

$$k\gamma_F/\gamma_g \approx k - (1 - p) \cdot F(\alpha, \eta, \mu_s, \mu). \quad (25)$$

It must be pointed out that the polycrystalline film resistivity ρ_F and T.C.R. β_F are given by :

$$k \cdot \rho_F/\rho_g \approx k + (1 - p) \cdot h(\alpha) \quad (26)$$

$$k \cdot \beta_F/\beta_g \approx k - (1 - p) \cdot H(\alpha) \quad (27)$$

according to previously published works [17, 19].

Comparison of equations ((25), (26) and (27)) suggest that all the transport properties of polycrystalline films may be described with fair agreement by approximate expressions deduced by considering α and p as separated variables.

On the other hand, suppose that simultaneous

Table III. — Comparison of the exact and approximate values of γ_{FL} and γ_{FT} .

		γ_{FL}					
		Exact values [20]			Approximate values (eq. (21))		
k	α	$\alpha = 1$	$\alpha = 2$		$\alpha = 0.5$	$\alpha = 1$	$\alpha = 2$
$p = 0$							
0.1	0.5	2.231 6	1.729 3		1.632 7	1.744 4	1.453 3
0.6		1.113 1	0.761 6		1.344 9	1.067 1	0.744 4
1		1.030 0	0.692 3		1.321 9	1.012 9	0.687 7
6		0.945 9	0.616 4		1.293 1	0.945 2	0.616 8
10		0.940 1	0.610 9		1.290 8	0.939 8	0.611 1
$p = 0.5$							
0.1		1.462 2	1.076 3		1.460 0	1.338 0	1.027 9
0.6		1.010 9	0.675 9		1.316 1	0.999 4	0.673 5
1		0.976 9	0.645 4		1.304 6	0.972 3	0.645 1
6		0.938 7	0.609 5		1.290 2	0.938 4	0.609 7
10		0.935 9	0.606 8		1.289 1	0.935 7	0.606 9
		γ_{FT}					
		Exact values [20]			Approximate values (eq. (22))		
k	α	$\alpha = 1$	$\alpha = 2$		$\alpha = 0.5$	$\alpha = 1$	$\alpha = 2$
$p = 0.25$							
0.1	0.5	1.645 4	1.547 4		1.295 6	1.458 9	1.490 4
0.6		1.613 3	1.499 5		1.706 7	1.609 8	1.499 1
1		1.621 8	1.500 3		1.739 5	1.621 9	1.500 4
6		1.637 1	1.501 9		1.780 7	1.637 0	1.501 9
10		1.638 2	1.502 1		1.783 9	1.638 2	1.502 1

experimental study of the grain-boundary and size effects in electrical resistivity ρ_F and gauge factor γ_F has been undertaken ; values of the physical parameter α and specularly coefficient p are easily deduced [10, 18, 19] from resistivity data and the corresponding values of $m(\alpha)$ and $U(\alpha)$ functions may thus be obtained. For a given value of μ_s , data on the gauge factor allow us to calculate experimental values of the strain coefficient η and Poisson ratio μ of bulk material by using equation (21) or (22). Comparison of these values with theoretical values of μ and η (as given in literature) will then furnish further information on the conduction mechanisms occurring in the films, especially on the influence (on transport properties)

of other structural defects such as point defects or impurities frozen in the thin polycrystalline film during the nucleation and growth process.

3. Conclusion. — Variations in the gauge factor of polycrystalline films with thickness may be described with a good agreement by an approximate equation deduced from the Mayadas-Shatzkes conduction model by considering α and p as separated variables. The physical parameters η and μ can then be easily extracted with reasonable accuracy from experimental plots of $\gamma_F \cdot k$ against k for polycrystalline films by using these linearized approximate expression.

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