

# THE ELECTRICAL RESISTIVITY OF MONOCRYSTALLINE FILMS DEDUCED FROM DERIVATION OF THE MAYADAS-SHATZKES EQUATIONS

C. R. TELLIER and A. J. TOSSER

Université de Nancy-I Laboratoire d'Electronique. Case Officielle 140 – 54037 NANCY Cedex – FRANCE

(Received March 23, 1976; in final form August 29, 1976)

The theoretical expression deduced by Mola and Heras from the Mayadas–Shatzkes model of monocrystalline thin film resistivity is approximated assuming that the Sommerfeld relation is valid and introducing corrections to the Matthiessen's rule.

The approximate expression of  $k\rho_f/\rho_0$  deviates from less than 6% in the 0.01–2 k-range, 0–0.5 p-range and 0.1–0.62 r-range.

## 1 INTRODUCTION

Mayadas and Shatzkes<sup>1</sup> have proposed a theoretical calculation of the electrical resistivity of thin metallic films; they have considered the simultaneous action of isotropic electron scattering, surface scattering and grain boundary scattering. Mola and Heras<sup>2</sup> have tabulated the exact values of the electrical resistivity of monocrystalline and polycrystalline metal films and given linearized expressions<sup>3</sup> which are valid in some special cases ( $p = 0$ ,  $0.1 \leq k \leq 5$ ,  $0.1 \leq r \leq 0.52$ ). In this paper we propose an approximate expression of the resistivity of monocrystalline films which is valid in larger ranges.

## 2 APPROXIMATE EXPRESSION OF MONOCRYSTALLINE FILM RESISTIVITY

The resistivity  $\rho_f$  of a monocrystalline film is<sup>3</sup> given by

$$\rho_f/\rho_0 = [f(\alpha) - A]^{-1} \quad (1)$$

in which  $\rho_0$  is the resistivity of an infinitely thick monocrystalline film, i.e. without Fuchs–Sondheimer<sup>4</sup> size effects, where

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

and where

$$f(\alpha) = 1 - \frac{3\alpha}{2} + 3\alpha^2 - 3\alpha^3 \text{Log}_e \left( 1 + \frac{1}{\alpha} \right) \quad (3)$$

The variable  $p$  is the fraction of electrons specularly scattered at the external surfaces and  $k$  is the ratio of film thickness,  $d$ , to electron mean free path,  $l_0$ .

$$k = d/l_0 \quad (4)$$

$$\alpha = (1/k) \cdot r \cdot (1-r)^{-1} \quad (5)$$

where  $r$  is the electron reflection coefficient defined by the relation<sup>1</sup>

$$r(1-r)^{-1} = \frac{1}{2}(V \cdot a)^2 \cdot (\hbar^2 k_f / 2m)^{-2} \quad (6)$$

in which  $V$  is the height of the potential well at grain-boundary and  $a$  is the potential well width,  $\hbar$  is the modified Planck's constant,  $k_f$  the magnitude of the Fermi wave vector and  $m$  the electron effective mass.

$$H(t, \phi) = 1 + \alpha(\cos \phi)^{-1} \cdot (1 - 1/t^2)^{-1/2} \quad (7)$$

After logarithmic differentiation Eq. (1) becomes

$$\frac{d\rho_f}{\rho_f} - \frac{d\rho_0}{\rho_0} = -\frac{df - dA}{f(\alpha) - A} \quad (8)$$

For  $p = p_0$  and  $r = r_0$  we deduce from Eq. (3) to (7):

$$-(df - dA) = \left[ -\frac{\partial f}{\partial \alpha} \frac{\partial \alpha}{\partial k} + \frac{\partial A}{\partial k} + \frac{\partial A}{\partial H} \frac{\partial H}{\partial \alpha} \frac{\partial \alpha}{\partial k} \right] dk$$

or

$$-(df - dA) = U(k, p) \cdot dk \quad (9)$$

If the variation in  $k$  is due only to variation in  $l_0$ , equation (4) gives:

$$\frac{dk}{k} = - \frac{dl_0}{l_0} \tag{10}$$

Assuming<sup>3</sup> the Sommerfeld relation to be valid and the number of conduction electrons per unit volume to be temperature independent and assuming that the T.C.R. of bulk metallic layers is

$$- \frac{dl_0}{l_0 dT} = \beta_0 \tag{11}$$

where  $T$  is temperature Eq. (8) becomes:

$$\beta_f - \beta_0 = \frac{k \cdot U(k, p)}{f(\alpha) - A} \cdot \beta_0 \tag{12}$$

or

$$\beta_f/\beta_0 = \frac{1 + k \cdot U(k, p)}{f(\alpha) - A} \tag{13}$$

From eq. (1) we deduce:

$$k\rho_f/\rho_0 = k[f(\alpha) - A]^{-1} \tag{14}$$

By differentiating Eq. (14) we obtain

$$\frac{dk\rho_f/\rho_0}{k\rho_f/\rho_0} = \frac{dk}{k} - \frac{df - dA}{f(\alpha) - A} \tag{15}$$

Substituting Eq. 9 in Eq. 14 we obtain

$$\frac{dk\rho_f/\rho_0}{k\rho_f/\rho_0} = \left(1 + \frac{k \cdot U(k, p)}{f(\alpha) - A}\right) \frac{dk}{k} \tag{16}$$

Eq. (13) leads to

$$dk\rho_f/\rho_0 = (\rho_f \beta_f)(\rho_0 \beta_0)^{-1} dk \tag{17}$$

Assuming the Mathiessen's rule<sup>5</sup> to be valid, we may write

$$\rho_f = \rho_0 + \rho_e \tag{18}$$

where  $\rho_e$  is an extrinsic resistivity.

If  $\rho_e$  is essentially temperature independent, then

$$(\rho_f \beta_f)(\rho_0 \beta_0)^{-1} = 1$$

Since this assumption is not completely valid, we introduce the function  $m(r)$ , measuring the deviation from the Mathiessen's rule, in the expression of  $k\rho_f/\rho_0$  related to a given value of  $p$ . Hence:

$$\Delta[k\rho_f/\rho_0] = [1 + m(r)] \Delta k \tag{19}$$

It may also be expressed as:

$$k\rho_f/\rho_0 = [k\rho_f/\rho_0]_{k=k_0} + [1 + m(r)] [k - k_0] \tag{20}$$

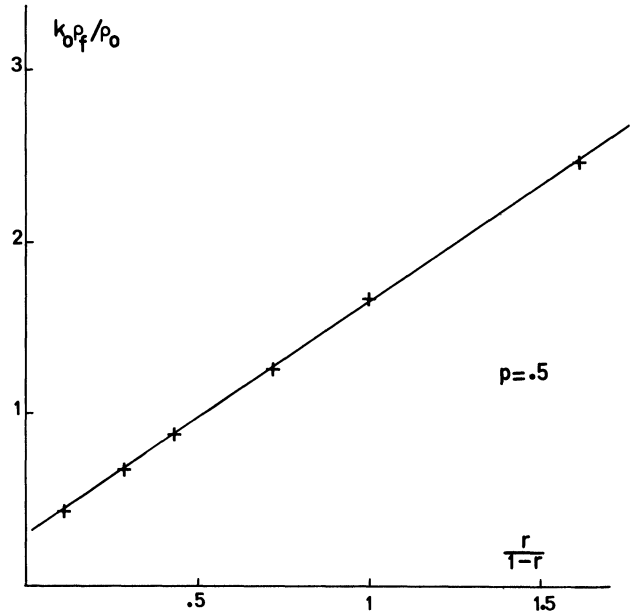


FIGURE 1 Exact values of  $k_0 \rho_f/\rho_0$  versus  $r/(1 - r)$  for an electronic specular reflection coefficient,  $p$ , of 0.5.

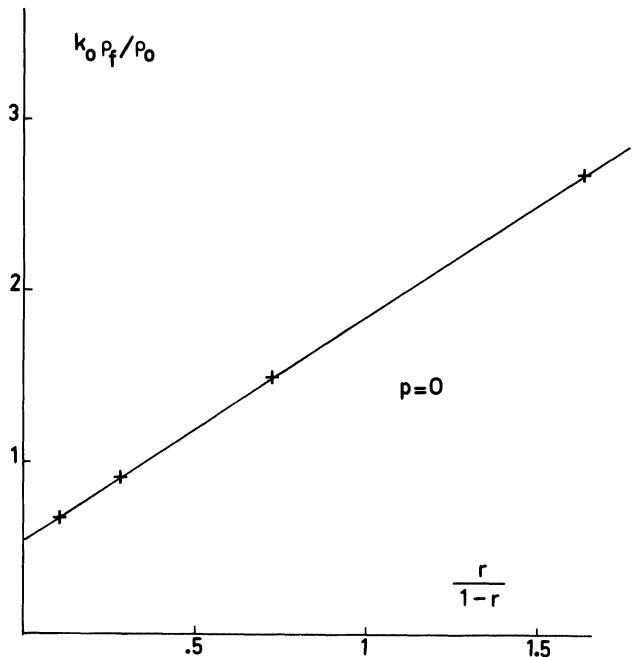


FIGURE 2 Exact values of  $k_0 \rho_f/\rho_0$  versus  $r/(1 - r)$  for an electronic specular reflection coefficient of 0.

TABLE I

$r$	$[k\rho_f/\rho_0]_{k=0.1}$ Eq. (21)		$[k\rho_f/\rho_0]_{k=0.1}$ exact values	
	$p=0$	$p=0.5$	$p=0$	$p=0.5$
0.1	0.676	0.4466	0.6687	0.4336
0.22	0.902	0.6723	0.912	0.6685
0.42	1.4858	1.2558	1.4912	1.2579
0.62	2.683	2.4536	2.687	2.4613

TABLE II

$k$	Thieme-Kirstein Eq. (24)			Approx. Eq. (25)			M-S exact values Eq. (1)		
	$p=0$ $r=0.22$	$r=0.42$	$r=0.62$	$r=0.22$	$r=0.42$	$r=0.62$	$r=0.22$	$r=0.42$	$r=0.62$
0.05	0.8480	1.5112	2.8723	0.849	1.4345	2.632	0.8559	1.4392	2.6163
0.1	0.8980	1.5612	2.9223	0.902	1.4858	2.683	0.912	1.4916	2.687
0.5	1.2980	1.9612	3.3223	1.3256	1.8958	3.087	1.335	1.9058	3.0874
1	1.7980	2.4612	3.8223	1.855	2.4083	3.592	1.8356	2.4137	3.6064
2	2.798	3.4612	4.8223	2.914	3.4333	4.602	2.8268	3.4216	4.6348
$k$	$p=0.5$ $r=0.22$	$r=0.42$	$r=0.62$	$r=0.22$	$r=0.42$	$r=0.62$	$r=0.22$	$r=0.42$	$r=0.62$
0.05	0.6605	1.3237	2.6848	0.6193	1.2045	2.4030	0.6141	1.2048	2.4084
0.1	0.7105	1.3737	2.7348	0.6723	1.2558	2.4536	0.6685	1.2579	2.4613
0.5	1.1105	1.7737	3.1348	1.0959	1.6658	2.8576	1.0879	1.6775	2.8836
1	1.6105	2.2737	3.6348	1.6254	2.1783	3.3626	1.5967	2.1928	3.406
2	2.6105	3.2737	4.6348	2.6844	3.2033	4.3726	2.6022	3.2106	4.4388

TABLE III

$k$	$k\rho_f/\rho_0$ Exact Eq. (1)				$k\rho_f/\rho_0$ Approximate Eq. (25)			
	$r=0.1$	$r=0.22$	$r=0.42$	$r=0.62$	$r=0.1$	$r=0.22$	$r=0.42$	$r=0.62$
$p=0$								
0.01	0.5487	0.8100	1.3973	2.5749	0.5779	0.8066	1.3935	2.592
0.02	0.5631	0.8216	1.4079	2.5855	0.5888	0.8172	1.4038	2.602
0.03	0.5769	0.8328	1.4178	2.5947	0.5997	0.8278	1.414	2.612
0.04	0.5908	0.8444	1.4285	2.6056	0.6106	0.8384	1.4243	2.6224
0.05	0.6043	0.8559	1.4392	2.6163	0.6215	0.8490	1.4345	2.632
0.06	0.6175	0.8671	1.4494	2.6264	0.6324	0.8596	1.4448	2.6426
0.07	0.6306	0.8785	1.4601	2.6371	0.6433	0.870	1.4550	2.6527
0.08	0.6435	0.8897	1.4707	2.6478	0.6540	0.8808	1.4653	2.6628
0.09	0.6561	0.9008	1.4810	2.6580	0.6650	0.8914	1.4755	2.6729
0.1	0.6687	0.9120	1.4916	2.6870	0.6760	0.902	1.4858	2.683
0.2	0.7873	1.0211	1.5960	2.7736	0.7850	1.0079	1.5883	2.784
0.3	0.8941	1.1271	1.6997	2.8785	0.894	1.1138	1.6908	2.885
0.4	1.0050	1.2310	1.8028	2.9831	1.003	1.2197	1.7933	2.986
0.5	1.1090	1.3350	1.9053	3.0874	1.112	1.3256	1.8958	3.087
0.6	1.2111	1.4350	1.0075	3.1916	1.221	1.4315	1.9983	3.188
0.7	1.3120	1.5358	2.1093	3.2955	1.330	1.5374	2.1008	3.289
0.8	1.4121	1.6360	2.2110	3.3993	1.439	1.6433	2.1928	3.390
0.9	1.5116	1.7359	2.3124	3.5029	1.548	1.7492	2.3058	3.491
1	1.6107	1.8356	2.4137	3.6064	1.657	1.855	2.4083	3.592
2	2.5944	2.8268	3.4216	4.6348	2.747	2.914	3.4333	4.602

We thus obtain approximate expressions of  $k\rho_f/\rho_0$  if the exact value of  $[k\rho_f/\rho_0]_{k=k_0}$  is known, slight deviations from the exact values (tabulated by Mola and al<sup>2</sup>) are obtained with  $p$  independent values of  $m(r)$ .

Furthermore, we may observe that the exact values<sup>2</sup> of  $k\rho_f/\rho_0$  for  $k = 0.1$  are linear with  $r/1 - r$  when  $p = 0$  or  $p = 0.5$  (Figure 1, 2). Hence:

$$(k\rho_f/\rho_0)_{k=0.1} \approx 0.1 + [0.37(1-p) + 0.06(1-p)^2] + 1.32 \frac{r}{1-r} \quad (21)$$

This expression is valid with a deviation less than 2% from the exact values in the 0 to 0.5  $p$ -range and in the 0.22 to 0.62  $r$ -range (Table I)

Making use of Mathiessen's rule Wissman<sup>6</sup> had obtained

$$\rho_f = \rho_0 \left[ 1 + K \cdot \frac{1}{k} + \frac{3}{8} \cdot \frac{1-p}{k} \right] \quad (22)$$

Thieme and Kirstein<sup>7</sup> use

$$K = \frac{3}{2} \cdot \frac{r}{1-r} \quad (23)$$

Hence

$$k\rho_f/\rho_0 = k + 0.375(1-p) + 1.5 \frac{r}{1-r} \quad (24)$$

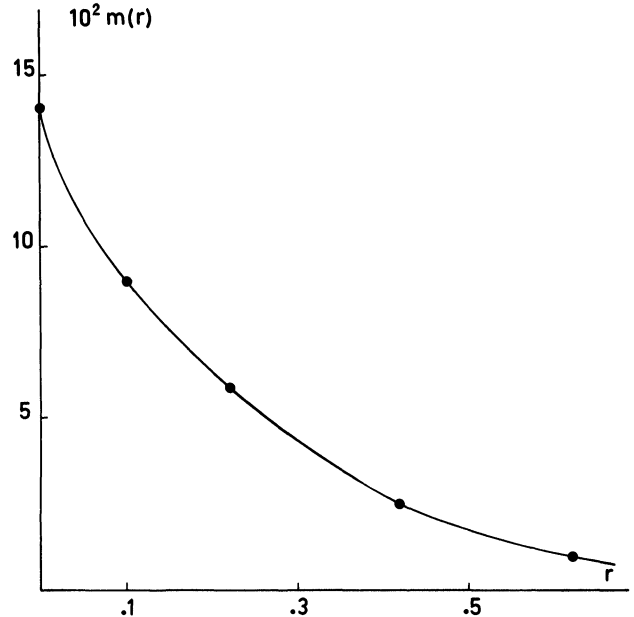


FIGURE 3 Variations in  $m(r)$  (a measure of deviation from Mathiessen's rule) with  $r$  (from Eq. 25).

In the ranges considered, this equation leads to most significant deviations (Table II).

Values of  $(k\rho_f/\rho_0)$  calculated from Eq. (21) are reported in Eq. (20). Hence

TABLE IV

$k$	$k\rho_f/\rho_0$ Exact Eq. (1)				$k\rho_f/\rho_0$ Approximate Eq. (25)			
	$r = 0.1$	$r = 0.22$	$r = 0.42$	$r = 0.62$	$r = 0.1$	$r = 0.22$	$r = 0.42$	$r = 0.62$
$p = 0.5$								
0.01	0.3280	0.5700	1.1624	2.3665	0.3485	0.5769	1.1635	2.3627
0.02	0.3403	0.5811	1.1731	2.3772	0.3594	0.5875	1.1738	2.3728
0.03	0.3522	0.5919	1.1832	2.3866	0.3703	0.5981	1.8140	2.3829
0.04	0.3642	0.6030	1.1941	2.3976	0.3812	0.6087	1.1943	2.3930
0.05	0.3761	0.6141	1.2048	2.4084	0.3921	0.6193	1.2045	2.4030
0.06	0.3877	0.6249	1.2153	2.4186	0.4030	0.6299	1.2148	2.4132
0.07	0.3993	0.6359	1.2260	2.4294	0.4139	0.6405	1.2250	2.4233
0.08	0.4109	0.6469	1.2367	2.4402	0.4248	0.6511	1.2353	2.4334
0.09	0.4222	0.6577	1.2472	2.4505	0.4357	0.6617	1.2455	2.4435
0.1	0.4336	0.6685	1.2579	2.4613	0.4466	0.6723	1.2558	2.4536
0.2	0.5435	0.7755	1.3638	2.5672	0.5556	0.7782	1.3583	2.5546
0.3	0.6497	0.8808	1.4689	2.673	0.6646	0.8841	1.4608	2.6556
0.4	0.7538	0.9847	1.5735	2.7785	0.7736	0.9900	1.5633	2.7566
0.5	0.8566	1.0879	1.6775	2.8836	0.8826	1.0959	1.6658	2.8576
0.6	0.9586	1.1904	1.7812	2.9886	0.9916	1.2018	1.7683	2.9586
0.7	1.0600	1.2924	1.8845	3.0932	1.1006	1.3077	1.8708	3.0596
0.8	1.1610	1.3941	1.9875	3.1976	1.209	1.4136	1.9733	3.1606
0.9	1.2618	1.4955	2.0903	3.3019	1.3186	1.5195	2.0758	3.2616
1	1.3622	1.5967	2.1928	3.4060	1.4276	1.6254	2.1783	3.3626
2	2.3622	2.6022	3.2106	4.4388	2.5176	2.6844	3.2033	4.3726

$$k\rho_f/\rho_0 \approx 0.1 + [0.37(1-p) + 0.06(1-p)^2] + 1.32 \cdot \frac{r}{1-r} + [1 + m(r)] [k - 0.1] \quad (25)$$

Variation of  $m(r)$  with  $r$  is given in Fig. 3.

Deviation of less than 6% is obtained in the 0.01 to 2  $k$ -range, 0 to 0.5  $p$ -range, 0.1 to 0.62  $r$ -range. (Tables III and IV).

### 3. CONCLUSION

Under the assumption that the effects due to surface scattering and to grain-boundary scattering may be treated separately, we obtain an approximate expression containing a term directly related to grain-boundary scattering and another related to surface scattering. A correction term is necessary for a

complete description of surface scattering. We also must introduce a term describing the combined action of isotropic scattering and grain scattering. We shall attempt to give further theoretical considerations to this point in a future paper.

### REFERENCES

1. A. F. Mayadas and M. Shatzkes, *Phys. Rev. B*, **1**, 1382–1389 (1970).
2. E. E. Mola and J. M. Heras, *Electrocomp. Sci. Tech.*, **1**, 77–80 (1974).
3. E. E. Mola and J. M. Heras, *Thin Solid Films*, **18**, 137–144 (1973).
4. T. J. Coutts, *Thin Solid Films*, **7**, 77–100 (1971).
5. L. I. Maissel in “*Hand book of Thin Film Technology*”, McGraw-Hill Book Co., (1970) p. 13–4.
6. P. Wissman, *Thin Solid Films*, **5**, 329–338 (1970).
7. F. Thieme and W. Kirslein, *Thin Solid Films*, **30**, 371–375 (1975).



**Hindawi**

Submit your manuscripts at  
<http://www.hindawi.com>

