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SHORT COMMUNICATION
Numerical Evaluation of the Resistivity of Polycrystalline Metal Films with the Mayadas-Shatzkes Model

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Numerical Tables are given in order to allow a direct comparison of the electrical resistivity model for polycrystalline films proposed by Mayadas–Shatzkes with experimental data.
The tables have been calculated extending the Gauss method for one variable to many variables.

1 INTRODUCTION

In the past years, it has been a common practice to analyze electrical resistivity data of polycrystalline metal films[1] by means of the Fuchs-Sondheimer model[2] (F–S model) for the size effects. However, the granular structures of evaporated films impose a restriction about which the F–S model says nothing. In order to take this into account, Mayadas and Shatzkes[3] developed the model (M–S model) given briefly later on.

The purpose of this communication is to present numerical tables. Model possibilities and applications have been discussed elsewhere[4].

2 MAYADAS–SHATZKES MODEL

Basically, to the two electron scattering mechanisms of the well known F–S model, M–S add a third one due to the presence of crystallite boundaries.

For the evaluation of the overall film resistivity ρ_f, M–S assumed that crystallite boundaries can be represented by a Gaussian distribution of partially electron reflecting planes randomly spaced with an average distance a and a standard deviation s.

Based on the available experimental data, which shows that thin evaporated films have a column-like structure with crystallites towering from the substrate to the surface, they assumed that (i) only those planes perpendicular to the applied electric field cause the extra electron scattering; (ii) the average interplanar distance a is equivalent to the average crystallite diameter D as obtained by electron microscopy. In order to fit the model to experimental data, the electron reflecting power of the potential barrier between crystallites is interpreted by a phenomenological parameter r.

The model can be summarized by the two following equations, rearranged according to the heading assumptions to make the mathematical problem and numerical evaluation more tractable.

2.1 *Crystallite Diameter D is a Thickness Independent Constant.*

The ratio between film resistivity ρ_f and the resistivity of a polycrystalline film infinitely thick, ρ_g is given by:

$$\frac{\rho_f}{\rho_g} = \left[1 - \frac{A}{f_{(\alpha)}}\right]^{-1} \tag{1}$$

in which:

$$A = \frac{6}{k_0 \pi}(1-p)\int_0^{\pi/2} d\varphi \int_1^{\infty} \frac{\cos^2\varphi}{H^2(t,\varphi)}\left(\frac{1}{t^3} - \frac{1}{t^5}\right) \times \frac{1 - e^{-k_0 t H(t,\varphi)}}{1 - p e^{-k_0 t H(t,\varphi)}} \tag{1a}$$

with:

$$H(t,\varphi) = 1 + \alpha \Big/ \left(1 - \frac{1}{t^2}\right)^{1/2} \cos\varphi$$

$k_0 = d/l_0$; d = film thickness; l_0 = mean free path of the electrons; p = specularity parameter.

TABLE I

Numerical data according to Eq. (1). p = specularity parameter; $k_0 = d/l_0$; d = film thickness; l_0 = electron mean free path; $\alpha = (l_0/D)r/1 - r$; D = crystalline diameter; r = reflection coefficient.

k_0	$p = 0$				$p = 0.5$			
	$\alpha = 0$	$\alpha = 0.5$	$\alpha = 1.0$	$\alpha = 2.0$	$\alpha = 0$	$\alpha = 0.5$	$\alpha = 1.0$	$\alpha = 2.0$
0.01	28.1528	17.6710	13.3803	9.4128	11.9282	7.9603	6.2672	4.6383
0.02	15.5631	10.1334	7.8643	5.7071	7.1911	4.9550	3.9889	3.0523
0.03	11.2718	7.4992	5.8937	4.3444	5.4583	3.8384	3.1370	2.4567
0.04	9.0703	6.1178	4.8468	3.6138	4.5336	3.2394	2.6794	2.1371
0.05	7.7083	5.2498	4.1852	3.1516	3.9489	2.8599	2.3896	1.9351
0.06	6.7707	4.6465	3.7245	2.8302	3.5415	2.5954	2.1878	1.7948
0.07	6.0821	4.2010	3.3843	2.5934	3.2403	2.4000	2.0389	1.6916
0.08	5.5512	3.8567	3.1216	2.4109	3.0073	2.2489	1.9239	1.6122
0.09	5.1271	3.5814	2.9118	2.2655	2.8208	2.1282	1.8321	1.5490
0.10	4.7804	3.3565	2.7405	2.1469	2.6682	2.0295	1.7572	1.4976
0.20	3.0962	2.2682	1.9154	1.5813	1.9251	1.5528	1.3984	1.2545
0.30	2.4659	1.8649	1.6131	1.3797	1.6464	1.3775	1.2684	1.1688
0.40	2.1284	1.6515	1.4554	1.2775	1.4975	1.2855	1.2012	1.1252
0.50	1.9161	1.5192	1.3590	1.2167	1.4041	1.2288	1.1601	1.0991
0.60	1.7696	1.4292	1.2945	1.1768	1.3399	1.1903	1.1326	1.0818
0.70	1.6621	1.3643	1.2485	1.1489	1.2930	1.1626	1.1129	1.0696
0.80	1.5799	1.3154	1.2143	1.1284	1.2572	1.1417	1.0981	1.0604
0.90	1.5149	1.2773	1.1880	1.1127	1.2289	1.1254	1.0867	1.0534
1.00	1.4623	1.2470	1.1671	1.1004	1.2061	1.1123	1.0776	1.0478
2.00	1.2208	1.1146	1.0780	1.0479	1.1014	1.0542	1.0376	1.0234
3.00	1.1414	1.0737	1.0507	1.0314	1.0663	1.0356	1.0247	1.0155
4.00	1.1032	1.0543	1.0376	1.0234	1.0491	1.0264	1.0184	1.0116
5.00	1.0810	1.0430	1.0298	1.0186	1.0389	1.0210	1.0147	1.0092
6.00	1.0666	1.0356	1.0247	1.0155	1.0322	1.0175	1.0122	1.0077
7.00	1.0566	1.0303	1.0211	1.0132	1.0275	1.0149	1.0104	1.0066
8.00	1.0492	1.0264	1.0184	1.0116	1.0240	1.0130	1.0091	1.0057
9.00	1.0435	1.0234	1.0164	1.0102	1.0213	1.0116	1.0081	1.0051
10.00	1.0390	1.0210	1.0147	1.0092	1.0191	1.0104	1.0073	1.0046

$$\alpha = (l_0/D)^r/_{1-r}$$

and

$$f_{(\alpha)} = 1 - (3/2)\alpha + 3\alpha^2 - 3\alpha^3 \ln(1 + 1/\alpha) \quad (1b)$$

When $\alpha = 0$, Eq. (1) reduces to the F–S equation. Neverthelss the curve shapes are identical within the experimental error.

2.2 *Crystallite Diameter D is Equal to Film Thickness d.*

Then, the ratio between film resistivity ρ_f and the resistivity of a single crystal film infinitely thick, ρ_0, is:

$$\frac{\rho_f}{\rho_0} = [f_{(\alpha)} - A]^{-1} \quad (2)$$

in which A, $f_{(\alpha)}$ and α have the same meaning as in eq. (1). When $k_0 > 10$ or $r \to 0$, eq. (2) reduces to the F–S equation.

3 NUMERICAL TABLES

Unfortunately Eq. (1) and (2) cannot be evaluated analytically. Hence, in order to interpret quantitatively the experimental results it was necessary to

elaborate numerical tables. These have not been given in the literature yet and were obtained with a IBM–360/50 computer with a program written in PLI. Excessively high computer time is necessary to solve the integrals by conventional methods[5]. This problem was overcome by generalizing Gauss' equation[6] to any number of variables. This can be done changing the variables in such a way as to transform the original interval for each variable into another one, ranging from 0 to 1, as required by the Gauss' formula. The integral is then evaluated over n^2 points, each one of them given by the roots of the Legendre polynomials of order n with their respective weight.[7]

The numerical evaluation was carried over $n^2 = 100$ points to obtain an acceptable approximation. Nevertheless, 25 points are enough to maintain error below 1% for the integrals, but their place in the function magnifies the overall error.

In Table I the values of ρ_f/ρ_g vs. k_0 calculated with Eq. (1) are given under the assumption α = a thickness independent constant. Only two values of the specularity parameter p are taken into account, because in general the experimental data fit the theoretical values better by postulating p = 0.

Table II shows the dependence of ρ_f/ρ_o on k_0 calculated with Eq. (2) for the same p-values as in Table I, but with $\alpha = f(d)$, (i.e. D = d and r = thickness

TABLE II

Numerical data according to Eq. (2). p, k_0 and r have the same significance as in Table I.

	$p = 0$				$p = 0.5$			
k_0	$r = 0.1$	$r = 0.22$	$r = 0.42$	$r = 0.62$	$r = 0.1$	$r = 0.22$	$r = 0.42$	$r = 0.62$
0.01	54.8700	81.0040	139.7323	257.4954	32.8003	57.0046	116.2411	236.6560
0.02	28.1572	41.0842	70.3962	129.2758	17.0153	29.0588	58.6566	118.8614
0.03	19.2322	27.7615	47.2602	86.4922	11.7423	19.7326	39.4419	79.5564
0.04	14.7706	21.1111	35.7139	65.1412	9.1070	15.0774	29.8525	59.9413
0.05	12.0376	17.1187	28.7844	52.3278	7.5226	12.2829	24.0975	48.1697
0.06	10.2924	14.4523	24.1581	43.7736	6.4629	10.4166	20.2553	40.3109
0.07	9.0092	12.5500	20.8589	37.6735	5.7056	9.0853	17.5153	34.7068
0.08	8.0442	11.1224	18.3841	33.0978	5.1364	8.0863	15.4599	30.5030
0.09	7.2906	10.0098	16.4563	29.5337	4.6919	7.3078	13.8588	27.2287
0.10	6.6870	9.1207	14.9164	26.6870	4.3361	6.6857	12.5799	24.6133
0.20	3.9367	5.1055	7.9802	13.8682	2.7176	3.8778	6.8190	12.8364
0.30	2.9947	3.7570	5.6658	9.5952	2.1657	2.9360	4.8966	8.9104
0.40	2.5127	3.0775	4.5070	7.4578	1.8846	2.4619	3.9338	6.9463
0.50	2.2180	2.6670	3.8107	6.1749	1.7133	2.1758	3.3551	5.7673
0.60	2.0186	2.3917	3.3459	5.3194	1.5978	1.9840	2.9687	4.9810
0.70	1.8744	2.1940	3.0134	4.7079	1.5144	1.8464	2.6922	4.4189
0.80	1.7652	2.0451	2.7638	4.2492	1.4513	1.7427	2.4844	3.9971
0.90	1.6796	1.9288	2.5694	3.8922	1.4020	1.6617	2.3226	3.6688
1.00	1.6107	1.8356	2.4137	3.6064	1.3622	1.5967	2.1928	3.4060
2.00	1.2972	1.4134	1.7108	2.3174	1.1811	1.3011	1.6053	2.2194
3.00	1.1936	1.2730	1.4753	1.8852	1.1201	1.2014	1.4071	1.8207
4.00	1.1430	1.2034	1.3574	1.6679	1.0898	1.1513	1.3071	1.6199
5.00	1.1132	1.1620	1.2864	1.5370	1.0716	1.1211	1.2467	1.4988
6.00	1.0936	1.1347	1.2391	1.4492	1.0596	1.1010	1.2063	1.4175
7.00	1.0798	1.1152	1.2052	1.3864	1.0510	1.0866	1.1773	1.3592
8.00	1.0696	1.1006	1.1798	1.3390	1.0446	1.0759	1.1555	1.3154
9.00	1.0616	1.0894	1.1600	1.3021	1.0396	1.0675	1.1385	1.2811
10.00	1.0554	1.0803	1.1441	1.2725	1.0356	1.0607	1.1248	1.2536

independent constant). There are more curves given with different r, than with different α because actually the available data fit the former more closely.

In Table I the column corresponding to $\alpha = 0$ is actually the numerical data of the F–S equation. A column with $r = 0$ in Table II would be identical. These values are given in order to estimate the error of the method. For this purpose they should be compared with the data obtained by Soffer[8] with Simpson's rule using 2^{13} subdivisions. The error is less than 0.1% up to $k_0 = 0.05$. However, the first value for $k_0 = 0.01$ has an error of 6%.

The evaluation method is thus justified because the computation time was reduced to 30 seconds per column.

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