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The Influence of Electrons Scattering at Grain Boundary and at Surface on Resistivity and Thermal Coefficient of Resistance of Nanocrystalline Silver Films

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The paper describes the method of separation of the share of both surface and grain boundary electron scattering on resistance and thermal coefficient of resistance (TCR). The calculation of ρ_d, β_d and ρ_{gb}, β_{gb} values, which correspond to the surface and grain boundary electron scattering respectively, and their comparative analysis were done based on experimental data of thermal and size dependence of specific resistance (ρ) and TCR (β) for nanocrystalline silver films.

Keywords: Nanocrystolline silver films, Grain boundary electron scattering, Surface electron scattering, Resistance, Thermal coefficient of resistance.

PACS numbers: 61.46. ± w, 72.80. ± r, 73.20. ± r

1. INTRODUCTION

The grate practical and scientific interest to single-layer silver films conditioned both possibility of decision of a number of problems of solid state physics and perspective their application as a component of multilayered film structures in the different areas of technique [1, 2].

At research of external size effect in electro-physical properties of film samples it is necessary to take into account except conduction electron scattering in film bulk on phonons and defects also scattering on the external surfaces of film, grain boundaries and interfaces (in case of two- and multilayered film systems).

For the decision of task of determination of influence of external surfaces and internal dividing boundaries into functional properties (TCR, gauge factor) of sensing element of sensors there is a row of methods [3-5]. With application of one of them there is the possibility to separate the share of both surface and grain boundary electron scattering on specific resistance and thermal coefficient of resistance [3].

2. TECHNIQUE OF EXPERIMENT

Samples were got by method of thermal evaporation in a vacuum setting with pressure of remaining gases 10^{-4} Pa. Condensation of samples was carried out on to the pyroceram substrates with copper contacts. The sample thickness was controlled in situ by method of quartz resonator. Researches of crystalline structure and phase composition were carried out by transmission electron microscopy and electron diffraction methods (apparatus TEM-125K). Thermal annealing to 600-700 K and cooling of samples were carried out in one loop in a vacuum. Control of temperature was carried out by a chromel–alumel thermocouple. The value of TCR was estimated from correlation:

$$\beta = \frac{1}{R}\frac{\Delta R}{\Delta T}\,. \qquad (1)$$

By findings the $\rho(T)$ та $\beta(T)$ dependences were built for different thickness of Ag films.

3. THEORETICAL METHOD OF SEPARATIN DIFFERENT TYPE OF ELECTRON SCATTERING

At research of electrophysical properties of film samples it is necessary to take into account the conduction electron scattering in film bulk on phonons and defects (ρ_0), on the external surfaces of film (ρ_d), on grain boundaries (ρ_{gb}). Considering that contributions of these mechanisms are additive, it is possible to write down such correlation:

$$\rho = \rho_0 + \rho_{gb} + \rho_d\,, \qquad (2)$$

where $\rho_0 + \rho_{gb} = \rho_g$ – the specific resistance of polycrystalline film with infinitive thickness (i.e. $d \to \infty$).

Going out from (1) and taking into account, that $\beta = \frac{d\ln\rho}{dT}$, in work [3] it was got the correlation:

$$\beta = \frac{\rho_0}{\rho}\beta_0 + \frac{\rho_{gb}}{\rho}\beta_{gb} + \frac{\rho_d}{\rho}\beta_d\,. \qquad (3)$$

At the decision of task of determination of influence of grain boundary and surface scattering into of specific resistance and thermal coefficient of resistance on the example of metallic films by authors [3] such basic correlations were offered:

$$\rho_{gb}(T) = (\beta_g\rho_g - \beta_0\rho_0)T + (\rho_{gb})_0\,, \qquad (4)$$

$$\beta_{gb}(T) = \frac{(\beta_g\rho_g - \beta_0\rho_0)}{(\beta_g\rho_g - \beta_0\rho_0)T + (\rho_{gb})_0} \sim \frac{1}{T}\,, \qquad (5)$$

$$\rho_d(T) = \rho(T) - \rho_g(T), \qquad (6)$$

$$\beta_d(T) = \frac{(\beta\rho - \beta_g\rho_g)}{(\beta\rho - \beta_g\rho_g)T + (\rho_d)_0}\,, \qquad (7)$$

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where $(\rho_{gb})_0 \cong \rho_g(0) - \rho_0(0) \cong \rho_g(0)$ is the constant of integration, which is evened $\rho_{gb}(T)$ at $T \to 0$ K;
$(\rho_d)_0 \cong \rho(0) - \rho_g(0) \cong \rho(0)$ is the constant of integration, which is evened $\rho_d(T)$ at $T \to 0$ K.

4. EXPERIMENTAL RESULTS

The results of structural and phase state research for Ag films, which before and after annealing to 600 K, are presented on Fig. 1 on the example of Ag(22) sample (thickness in nm point in brackets). Film samples have a crystalline grate which corresponds to FCC-phase with the grate parameter 0,407±0,001 nm, that is near to the parameter of massive samples a_0(Ag) = 0,408 nm [6]. Annealing of samples to 600 K does not influence on the value of grate parameter and promotes the increasing of crystalline medium size in 5-6 times as a result of intensive recrystallization processes, that correlates with data of work [7], where annealing of samples was conducted in the column of TEM.

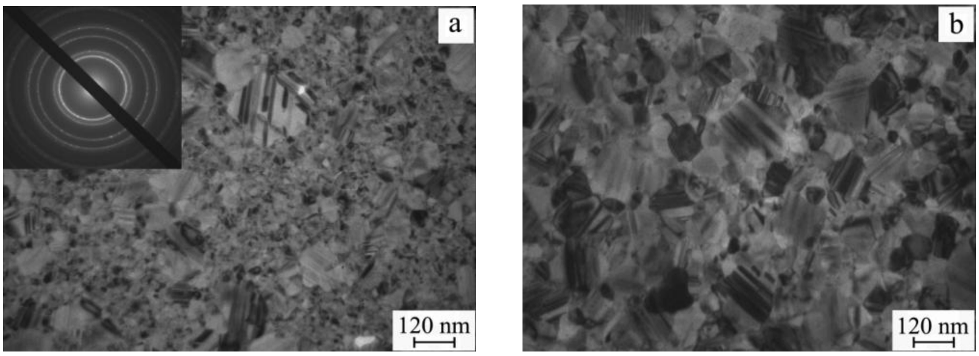

Fig. 1 – Microstructure and diffraction pattern from Ag(22) sample before (a) and after annealing to T_a = 600 K (b)

The temperature dependences of specific resistance and TCR are presented on Fig. 2 on the example of Ag(22) and Ag(40) samples. At the analysis of dependences $\rho(T)$ for single-layer Ag films becomes noticeable, that period, in which healing of defects are occured, at every films is different. It takes place because to specific resistance substantially depends on film thickness: than the film thickness greater, the healing of defects occurs earlier. The reversal cycle (cooling) correspond to typical metallic dependence $\rho(T)$.

On the basis of findings of specific resistance and TCR at a room temperature for thermostabilizate single-layer Ag films (Table 1) there is a possibility to complement the size dependences $\rho(d)$ and $\beta(d)$ (Fig. 3), which got in work [2]. Size dependences $\rho(d)$ and $\beta(d)$ for single-layer Ag films allow to define $\rho_\infty(\rho_g)$ and $\beta_\infty(\beta_g)$ values, that may need in the subsequent at application of method of determination of influence of grain boundary and surface scattering into thermal coefficient of resistance. The finding data for ρ_g and β_g for Ag films and bulks are presented in Table 2.

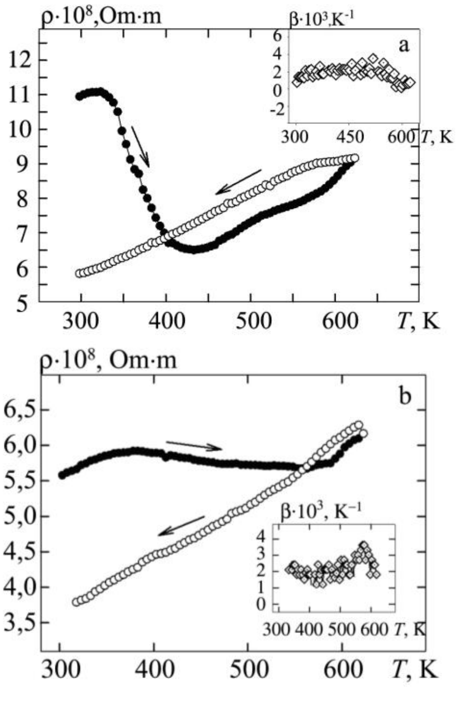

Fig. 2 – Temperature dependences of specific resistance and TCR for Ag(22) (a) and Ag(40) (b) films

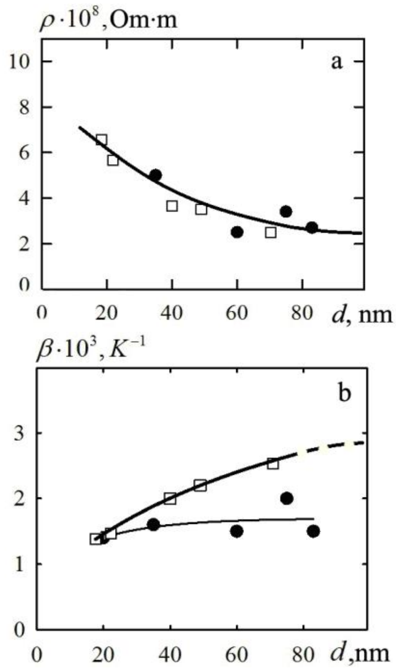

Fig. 3 – Size dependences of specific resistance (a) and TCR (b) for Ag films. □ – our data, ● – data of work [2]

Table 1 – The contribution of grain boundary and surface electron scattering into of specific resistance and thermal coefficient of resistance for Ag films

Film (nm)	$\rho \cdot 10^8$, Ohm·m	$\beta \cdot 10^3$, K^{-1}	$\rho(0) \cdot 10^8$, Ohm·m	$\rho_d \cdot 10^8$, Ohm·m (6)	$\beta_d \cdot 10^3$, K^{-1} (7)	$(\rho_{gb})_0 \cdot 10^8$, Ohm·m	$\rho_{gb} \cdot 10^8$, Ohm·m (4)	$\beta_{gb} \cdot 10^3$, K^{-1} (5)	$\frac{\rho_{gb}}{\rho_d}$	$\left\lvert\frac{\beta_{gb}}{\beta_d}\right\rvert$
Ag(19)	6,50	1,40	2,50	4,10	0,71				0,07	1,73
Ag(22)	5,81	1,42	1,60	3,41	0,69				0,09	1,77
Ag(40)	3,65	2,00	1,10	1,25	0,37	0,20	0,32	1,23	0,25	3,32
Ag(49)	3,50	2,20	0,60	1,10	1,00				0,28	1,23
Ag(70)	2,77	2,50	0,20	0,37	0,37				0,85	3,27

Table 2 – The specific resistance and TCR for infinitive thick films and bulks

Film	$\rho_g \cdot 10^8$, Ohm·m	$\beta_g \cdot 10^3$, K^{-1}	$\rho_0 \cdot 10^8$, Ohm·m [6]	$\beta_0 \cdot 10^3$, K^{-1} [6]
Ag(x)	2,40	2,85	1,60	4,03

The values $\rho(0)$ were got by extrapolation of experimental dependences $\rho(T)$ for samples of different thickness from 300 K on 0 K; $(\rho_{gb})_0 = 0{,}20 \cdot 10^{-8}$ Ohm·m was taken such, as $\rho(0)$ for thicker sample. Values of specific resistance and TCR, which conditioned by grain boundary ρ_{gb} and β_{gb} and surface electron scattering ρ_d and β_d, were calculated after equations (4)-(7). The finding results of calculations for Ag(x) films are presented in a Table 1.

5. DISCUSSION OF RESULTS

The analysis of the finding results shows the following. The value of specific resistance, which is conditioned grain boundary scattering, as known, is determined the degree of dispersion of film crystallites [8]. A value ρ_{gb} is maximal for nanocrystalline samples (Ti, V, Mo and Cr) and has a minimum value in epitaxial samples or polycrystalline with relatively large grain size. For the Ni, Cu and Mo wires, in which grain size is more than at films, value ρ_{gb} is 0,2; <0,1; $0{,}45 \cdot 10^{-8}$ Ohm·m respectively [3, 8]. In our case in Ag films by a result of calculations the value ρ_{gb} is $0{,}32 \cdot 10^{-8}$ Ohm·m, and value β_{gb} – $1{,}23 \cdot 10^{-3}$ K^{-1}.

The role of surface scatering diminish with the increase of film sample thickness, as a result the size of ρ_d diminishes in all interval of silver films thickness (Fig. 4 a).

As a role of scattering at surface falls with growth of samples thickness, the main mechanisms of electrons relaxation in the volume of samples is scattering on phonons, defects of crystalline structure and grain boundaries. Thus, basic contribution in the size of specific resistance will give the grain boundary scattering. It is confirmed by values of ρ_{gb}/ρ_d, which is increased with growth of samples thickness (Fig. 4 b).

Unlike ρ_d, value β_d, and also $\left|\frac{\beta_{gb}}{\beta_d}\right|$ are by a lowdimensional values. This result is explained in [14], coming from determination of TCR (expression (1)), from which it follows, that value β depends both on specific resistance and from temperature dependence $\Delta\rho / \Delta T$. Thus, the product of two values is present, which determine TCR with their different tendency to the change with a thickness.

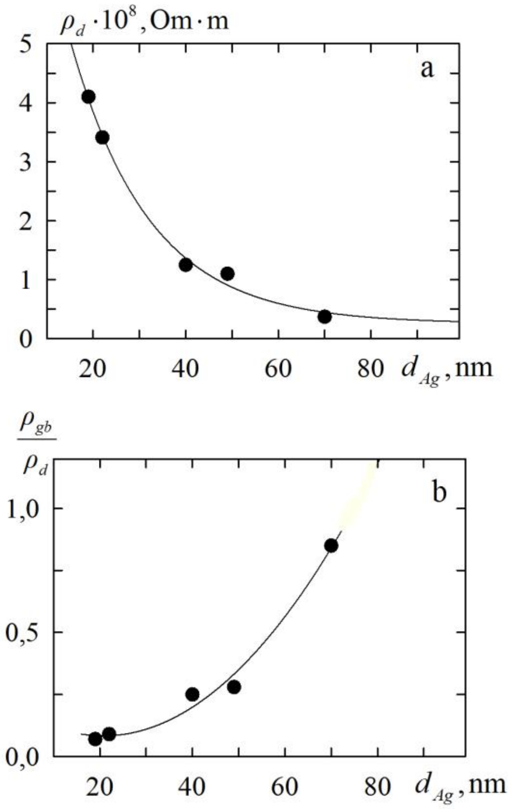

Fig. 4 – Size dependences of specific resistance, which conditioned by surface electron scattering ρ_d (a) and relation the specific resistance, which conditioned by grain boundary electron scattering, to ρ_d (b)

6. CONCLUSION

1. The role of electron scattering at surface diminish with the increase of film sample thickness, as a result the size of ρ_d diminishes in all interval of silver films thickness.

2. The main mechanisms of electrons relaxation in the volume of samples is scattering on phonons, defects of crystalline structure and grain boundaries. The scattering at grain boundary gives the basic contribution in the size of specific resistance. It is confirmed by values of ρ_{gb}/ρ_d, which is increased with growth of samples thickness.

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