PROCEDURE FOR ESTIMATING THE CONTRIBUTION OF INTERFACE SCATTERING OF ELECTRONS TO THE SPECIFIC RESISTANCE AND THE TEMPERATURE COEFFICIENT OF RESISTANCE OF FILMS

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A procedure, which allows the contribution of electron scattering at the interlayer interface to the specific resistance of Cu-based thin film systems to be estimated, has been proposed. The method of estimation is based on the comparison of the specific resistances and the temperature coefficients of resistance (TCR) measured for single- and two-layer films with identical thicknesses, and provided that the film deposition conditions, the types and the concentrations of defects (monitored by comparing the defect spectra calculated making use of the Vand technique), and the concentrations of grains with crystal structure defects (monitored by the method of transmission microscopy) are identical for both experimental configurations. The interface between two layers was simulated by interrupting the film deposition for some time. It has been demonstrated that the interface scattering increases the specific resistance by 12–21% and simultaneously decreases the TCR by 9–20%, if the thickness of the film system falls within the interval 60–90 nm.

The permanent interest to multilayer film systems is connected with the circumstance that the interfaces between layers give rise to the mechanism of electron scattering, which is additional to the bulk (background), surface, and grain-boundary ones and can essentially affect the physical properties of multilayer film systems and multilayers. At the same time, the passage of electrons through the interface and their scattering at it remain explored insufficiently until now. This circumstance has provoked the assumption, made in a number of works [1, 2, 3, 4], that the transmission coefficients for the interlayer interface (ILI), Q, and the intergrain boundary (IGB), r, are equal to each other. The formal similarity between the crystalline structures of the ILI and the IGB, as well as the results of works, in which the methods for analyzing the grain-boundary scattering [5, 6, 7, 8] and calculating the coefficient r (see, e.g., work [2]) have been developed, serves as some reason for such an assumption.

One of the earliest attempts to evaluate the contribution of the interface scattering in a two-layer film to the magnitude of the specific resistance has been made in work [9]. It has been shown there that, provided $k = \frac{d}{\lambda_0} = 0.1 \div 1$, where d is the film thickness, and λ_0 the electron mean free path in the film bulk, the interface scattering contributes three (at $k = 1$) to five (at $k = 0.1$) times less than the surface or the grain-boundary one does. The contribution of the interface scattering to the specific resistance comes up with that of the grain-boundary scattering only at $k \geq 9$ (this is the case of large thicknesses or high temperatures). The author of work [10] tried to estimate the value of the coefficient Q in two-layer films Au/(Fe, Ni, Co). But the relevant experimental and calculation techniques allowed only the sum $Q + p$ to be estimated, where p is the reflectivity coefficient of the outer surface of the top or bottom film. In the framework of the Fuchs approximation, it has been obtained that $Q + p = 1.3$ for the Au/Fe, 0.8 for the Au/Co, and 1.2 for the Au/Ni film, which falls within the limits of experimental errors. If grain-boundary scattering is taken into account, the value of $Q + p$ diminishes down to 0.6, 0.2, and 0.5, respectively. The authors of work [11], using the multilayer film of the system Ti/Al as an example, have compared the experimental value of the specific resistance with the corresponding theoretical values, calculated if either interface scattering (ρ_{inf}) or grain-boundary one (ρ_{g}) was made allowance for, as well as with the specific resistance of the multilayer system ρ_{ml}. The result obtained testify that only if $k > 7$, the chain of approximate equalities $\rho \simeq \rho_{\text{inf}} \simeq \rho_g \simeq \rho_{\text{ml}}$ is valid, while, at $k < 7$, the ratios ρ_{inf}/ρ and ρ_{inf}/ρ_g decrease from 1 (at $k = 7$) down to 0.2 (at $k = 0.1$).

The analysis of the results of works [9, 10, 11] evidences that the problem of interface scattering, notwithstanding its importance, is far from being resolved, because only the values for relative quantities or the sum $Q + p$ were obtained there.

It was this circumstance that determined the goal of our researches which can be formulated as follows: the development of a method for estimating the contribution of the electron interface scattering to the magnitudes of the specific resistance and the TCR of films.

1. Method for Estimating the Interface Scattering Contribution to the Magnitudes of the Specific Resistance and the TCR

The essence of the method, which is proposed by us, is based on high-precision measurements of the specific resistances or the TCRs [3] of two metal film specimens with identical thickness, one of which is a single-layer film, and the other is a two-layer film system, the internal interface in which has been simulated by interrupting the film deposition for some time (10 min) in the course of the film fabrication. In order that the evaluation of the contribution of the electron interface scattering to the specific resistance or the TCR be correct, the following conditions concerning a single-layer film and a two-layer system must be strictly fulfilled:

— the film thickness has to be measured with an accuracy not less than ±0.5 nm;

— the film deposition rate has to be maintained constant with an accuracy not less than ±0.1 nm/s;

— close values of the concentrations of crystal structure defects of the vacancy and crystal structure types, as well as the close activation energies of the healing of those defects, have to be provided in both configurations; the values concerned are evaluated by constructing the defect spectra following the Vand technique [12];

— the dimension distributions of crystallites have to be identical in each configuration, and the deviation from the average value cannot exceed 10%;

— the concentrations of crystallites with crystal structure defects, which possess relatively high healing activation energies, should be approximately equal.

Analyzing the difference between the values of the specific resistance or the TCR, measured for two configurations under the conditions indicated above, one can draw a conclusion concerning the role of electron interface scattering in electrophysical properties.

The results of our researches for the Cu-based films and film systems 60, 75, and 90 nm in thickness are reported below.

2. Experimental Method and Technique

Film specimens for carrying out the structural researches and studying the electrophysical properties of the films were fabricated in a VUP-5M vacuum installation (the residual atmospheric pressure of 5×10^{-4} Pa) using the film deposition rate $\omega = 1.5$ nm/s and provided the substrate temperature $T_{\mathrm{S}} = 300$ K. The deposition rate and the specimen thickness were monitored, as in work [13], using the quartz resonator method which ensured the thickness measurement error of ±0.1 nm. The electric resistance was measured with the help of an APPA-109 digital voltmeter with an accuracy of ±0.06%. The temperature of the substrate and the annealing temperature were monitored making use of a chromel–alumel thermocouple and a DT-838 multimeter which ensured the corresponding temperature accuracy of ±0.5 K. The TCR was calculated following the recommendations of work [3]. Electron-diffraction and structural researches were carried on making use of a high-resolution TEM-125K electron microscope (the "Selmi" public corporation, Sumy, Ukraine).

Three series of film specimens have been fabricated and studied: Cu(36), Cu(24), Cu(36)/Cu(24)/S and Cu(60); Cu(30), Cu(45), Cu(30)/Cu (45)/S and Cu(75); and Cu(30), Cu(60), Cu(30)/Cu (60)/S and Cu (90). Here, the film or layer thickness, in nanometers, is indicated in the parentheses, and S stands for the substrate.

The calculation of the defect distribution function (the defect spectrum) was carried out following the technique described in work [12]. With this aim in view, the specimens were subjected to the heat treatment within the temperature interval 300–630 K and in the schedule "heating–cooling" at a rate of 3–5 K/min (two annealing cycles were fulfilled). According to the results of work [12], the distribution function $F_0(E)$ is connected to the annealing rates $\frac{\partial \rho}{\partial T}$ (the first heating) and $\left(\frac{\partial \rho}{\partial T}\right)_1$ (the first or the second cooling) by the relation

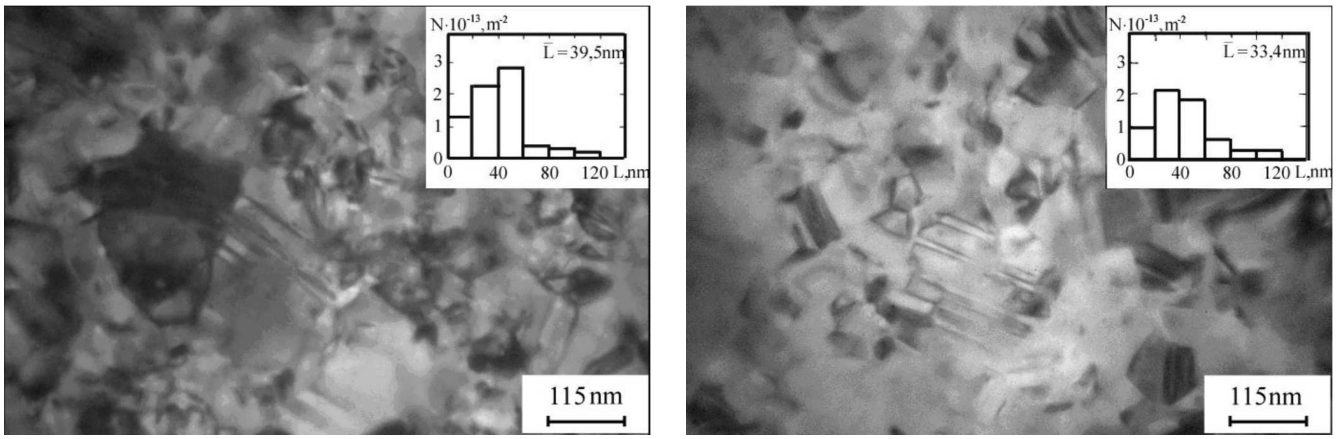
$$F_0(E) = -\left(\frac{1}{kU}\right)\left(\frac{\partial \rho}{\partial T} - \left(\frac{\partial \rho}{\partial T}\right)_1\right), \qquad (1)$$

where k is the Boltzmann constant, $E = nkT$ is the activation energy of the healing of a defect, and $U = u(u+2)/(u+1)$ is the function connected with the number of degrees of freedom u possessed by the system of defects .

The value of u is determined by the logarithmic equation

$$u + \lg u = \lg\left(4nt\omega_{\max}/2\pi\right), \qquad (2)$$

where n is the number of atoms in a defect, t is the time of annealing to a definite temperature, and $\omega_{\max} = k\Theta_{\mathrm{D}}/\hbar$ is the Debye frequency.



a **b**

Fig. 1. Microstructures and corresponding histograms of a single-layer Cu(60) film (a) and a two-layer Cu(36)/Cu(24)/S film system (b)

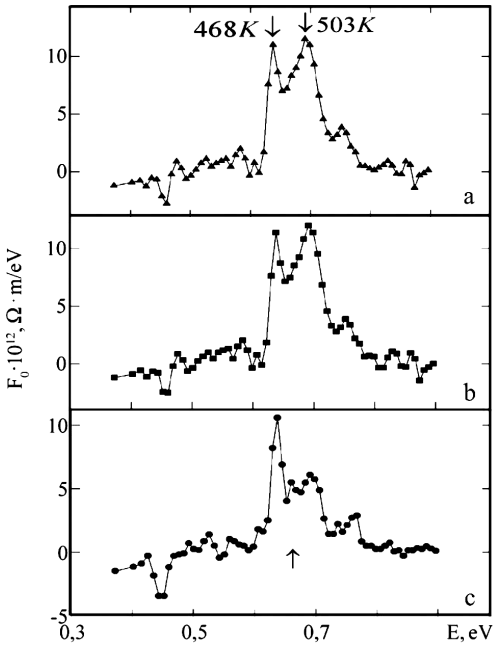


Fig. 2. Defect spectra of the Cu(24) (a) and Cu(36) (b) films and the Cu(24)/Cu(36)/S film system (c). The arrows point at the main maxima in the spectra and the feature induced by the interface

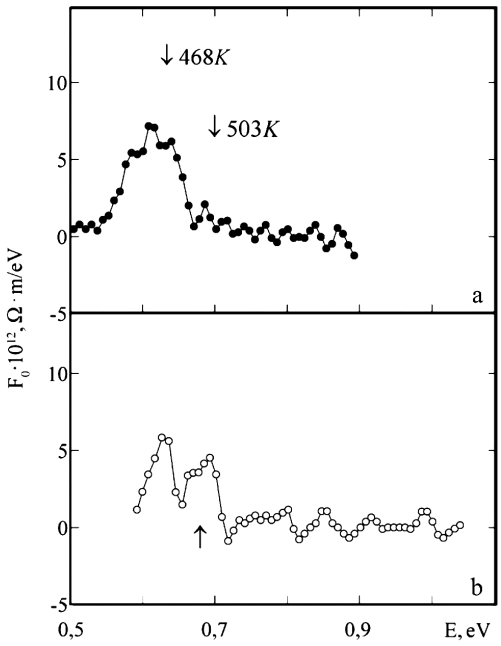


Fig. 3. Comparison of the defect spectra of a Cu(90) film (a) and a Cu(30)/Cu(60)/S film system (b). The arrows fulfill the same functions as in Fig. 2

3. Results of Researches and Their Discussion

3.1. Crystalline structure and the spectrum of defects

Figure 1 exhibits the microstructures and the corresponding histograms for single- (a) and two-layer (b) specimens annealed to $T_A \approx 600$ K, each having the total thickness $d = 60$ nm. The similar characters of the histograms, as well as the close values of both the average dimension L of crystallites and the concentration of crystallites with crystal structure defects ($N_\partial \approx 3.57 \times 10^{13}$ m^{-2} for the Cu(60) and $N_\partial \approx 3.60 \times 10^{13}$ m^{-2} for the Cu(36)/Cu(24)/S specimen), attract attention. We note that if the Cu films were annealed under somewhat different conditions (a higher T_A, a lower rate of heating, etc.), there would appear defects in them [14, 15] with the activation

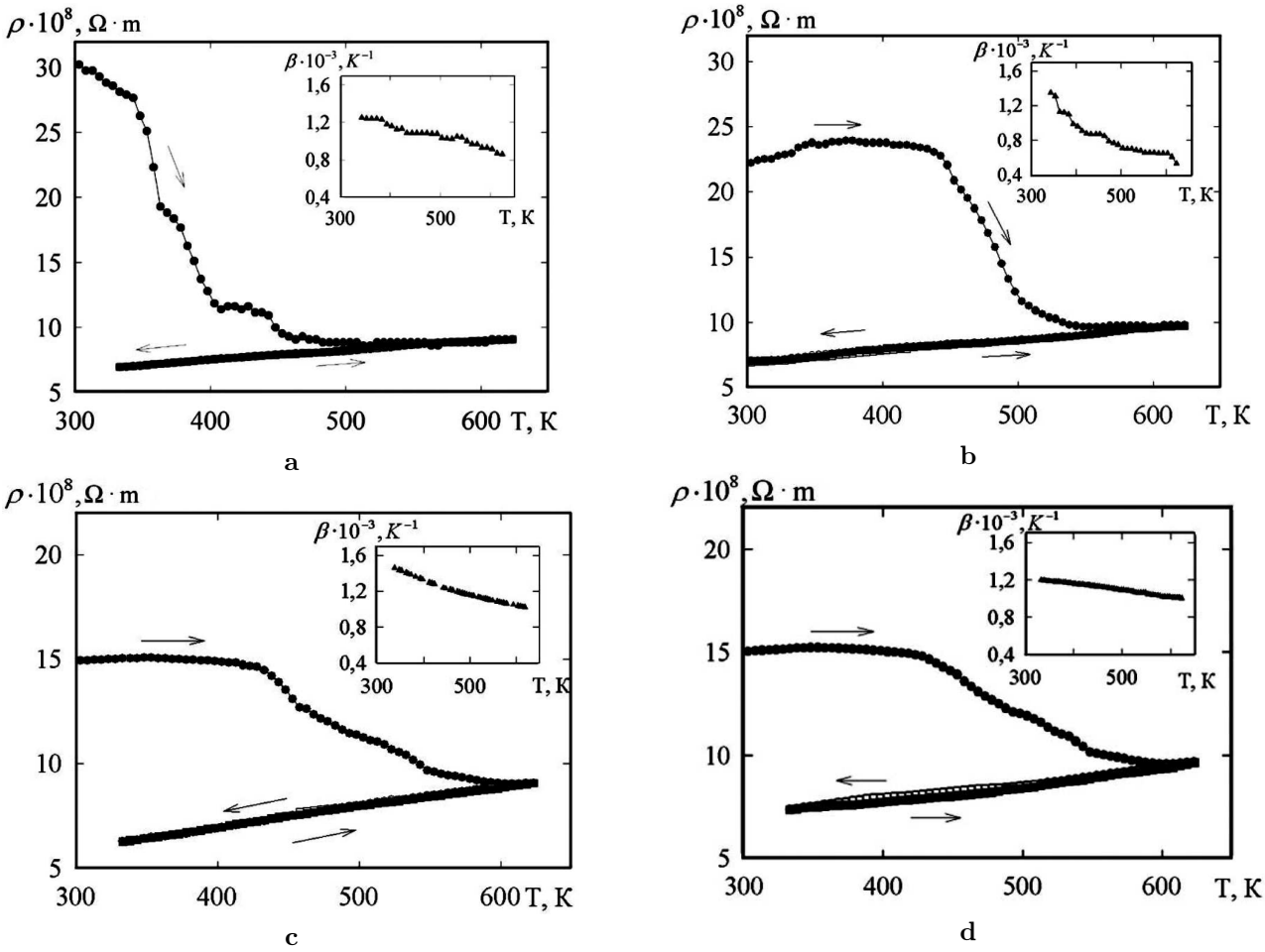


Fig. 4. Temperature dependences of the specific resistance and the TCR (in the insets) for two thermostabilizing cycles and at various thicknesses of the specimens $d = 60$ (a,b) and 75 nm (c,d)

energy of the healing within the interval $E = 0.94 \div 1.59$ eV. But, in our researches, the attained T_A's were lower, which reduced the probability of the diffusion smearing of the interface. The identity of the spectra testifies that the deposition conditions for those specimens were very close. At the same time, the spectrum feature at $E = 0.66$ eV for the specimen with the interface (Fig. 2,b) evidences for a certain contribution of this artificial interface to the defect spectrum. The same feature also reveals itself in the case of the specimen Cu(30)/Cu(60)/S (Fig. 3,b). Figure 2, where those two specimens are used as examples, illustrates the shape of the defect spectrum for the Cu(24) and Cu(36) films, and the Cu(24)/Cu(36)/S film system.

The analysis of the results which are depicted in Figs. 1–3 allows a conclusion to be drawn that the conditions, under which the specimens were fabricated, and the regimes of their heat treatment satisfy, to a great extent, the requirements stated in Section 2. This enables us to assert that the difference between the electrophysical properties of single-layer films and two-layer film systems is connected with the availability of the interface in the latter.

3.2. Electrophysical properties

Figure 4 exhibits the dependences of the specific resistance and the TCR on the temperature for single-layer films Cu(60) and Cu(75), and two-layer film systems Cu(24)/Cu(36)/S and Cu(30)/Cu (45)/S.

The TCR was calculated by the relation $\beta = \rho_0^{-1} \frac{\Delta\rho}{\Delta T}$, where ρ_0 is the initial amplitude of the specific resistance. The calculations gave the values of the

relative increase of the specific resistance $\frac{\rho(\mathrm{Cu/Cu})-\rho(\mathrm{Cu})}{\rho(\mathrm{Cu})}$, which fell within the limits $\Delta\rho/\rho = 0.12 \div 0.21$, and the values of the relative reduction of the TCR $\frac{\beta(\mathrm{Cu})-\beta(\mathrm{Cu/Cu})}{\beta(\mathrm{Cu})}$, which fell within the limits $\Delta\beta/\beta = 0.09 \div 0.20$. Such a variation of the electrophysical quantities can be explained by the additional scattering of electrons at the interface. Our results can be qualitatively confronted with the data of work [2], where the coefficient of longitudinal tensoresistive sensitivity γ_l of a single-layer film of a certain metal and that of a film system $\mathrm{Me_1/Me_2/Me_3/S}$ with identical thicknesses were compared with one another (the difference between our experiment and that of work [2] consisted in that the three-layer system in work [2] included three components). To make a comparison with our data, we cite some results from work [2]. The ratios of $\gamma_l(\mathrm{Cu}(265))$, $\gamma_l(\mathrm{Sc}(265))$, and $\gamma_l(\mathrm{Cr}(265))$ to $\gamma_l(\mathrm{Cr}(120)/\mathrm{Sc}(70)/\mathrm{Cr}(75)/\mathrm{S})$ are equal to 0.16, 0.10, and 0.27, respectively, i.e. they agree rather well with our results.

4. Conclusions

The method proposed allows the calculation of the contribution of the electron interface scattering to the specific resistance and the TCR of film specimens to be carried out. The values of the TCR turned out to lie within the limits 9—21%. This result is in a qualitative agreement with the data of works [2, 11]. Similar researches can be extended further to two- and three-layer film systems, in which the interface is formed as a result of deposition of various metals with low interdiffusion, as it was done in work [2]. An immediate study of the crystalline structure of the interface, both natural and artificial, making use of the high-resolution electron microscopy method, is also of a great interest.

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МЕТОДИКА ОЦІНКИ ВНЕСКУ ІНТЕРФЕЙСНОГО РОЗСІЯННЯ НА МЕЖІ ПОДІЛУ ШАРІВ У ВЕЛИЧИНУ ПИТОМОГО ОПОРУ І ТЕРМІЧНОГО КОЕФІЦІЄНТА ОПОРУ ПЛІВОК

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Р е з ю м е

Запропоновано методику оцінки внеску у питомий опір та термічний коефіцієнт опору (ТКО) розсіяння електронів на межі поділу (МП) шарів (інтерфейсі) плівкової системи на основі Cu, в якій штучно змодельовано межу поділу двох шарів шляхом зупинки конденсації плівки на певний час. Методика оцінки базується на порівнянні питомого опору і ТКО одношарової плівки і двошарової плівкової системи однакової товщини, в яких ідентичні умови конденсації, тип і концентрація дефектів (контролюється шляхом порівняння спектрів дефектів, розрахованих за методикою Венда) та концентрація зерен з дефектами пакування (контролюється методом електронної мікроскопії). Отримано, що інтерфейсне розсіяння приводить до збільшення питомого опору на 12—21% і до зменшення ТКО на 9—20% в інтервалі товщин 60—90 нм.