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Microscopic Theory of Tensosensibility of Multi-Layer Polycrystalline Films

The microscopic theory for the coefficient of longitudinal tensosensibility of multi-layer polycrystalline metal films has been developed. The theory takes into consideration as the scattering of conductivity electrons on external and internal surfaces of separate layers and crystalline boundaries, so as the dependence of specular reflection coefficient and coefficient of transmission of crystalline boundaries and boundaries between separate layers on deformation. The experimental verification of the theory done on three-layer film systems Cr/Co/Cr, Cr/Cu/Cr and Ni/Co/Cr given as the quality correspondence.

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Microscopic Theory of Tensosensibility

The theoretical investigations of the effect of tensosensibility in the double-layer films (bi-plates) were firstly presented in the work by Khater and El-Hiti. PROTSENKO and CHORNOUS was proved that the theory KHATER and EL-HITI may be applied to the polycrystalline metal films Me1/Me2/S (where S - substrate) or to double-layer systems a- Me1/Me2/S (where a is the amorphous phase) as boundary case. So, the problem of tensosensibility effect in multi-layer films is of great importance even nowadays, the macroscopic model that gives the opportunity to estimate the coefficients of longitudinal (γl) and transverse (γt) tensosensibility was suggested by PROTSENKO, ODNODVORETZ and CHORNOUS. The results of the experiments are presented in the works by PROTSENKO, ODNODVORETZ and CHORNOUS and show the difference in correspondence of experimental data to computation data for different film systems. For the case with the microscopic model, the relation of $|\gamma l\mathrm{exp}-\gamma l\mathrm{com}|/\gamma l\mathrm{exp}$ constitutes the value from 0.20 – 0.30 (films Co/Ni/S, Cr/Mo/S, Cr/Co/S) to 0.70 (Ni/Co/S). The difference in correspondence of respective values according to the macroscopic model is from 0.02 – 0.07 (films Cr/Co/Cr/S, Cr/Co/Ni/S and Co/Cr/Co/S) to 0.42 (films Ni/Co/Cr/S). Though the macroscopic model is rather simple in general and it permits to obtain the perfect correspondence to the experimental value γl, it can be used only for preliminary estimation of the tensosensibility coefficients. It gives no imagination about the influence of the interior and exterior dimensional effects and the layer interfaces of tensosensibility phenomenon. The analysis we done points on the cause of poor correspondence of the microscopic model to the experimental data in respect to the perfect correspondence of the macroscopic one. This cause depends on the fact that in the last case the macroscopic values are used. These values are measured experimentally with perfect accuracy. In case we use the microscopic model, such the microscopic parameters are used like value of an effective mean free path ($\lambda 0$), the coefficient of it deformation

($\eta_{\lambda 0} = -\frac{1}{\lambda_0}\frac{\partial \lambda_0}{\partial \varepsilon}$), the effective coefficient of specular reflection (p*), the transmission coefficient at grain boundary (r) and at interfaces of separate layers (Q). In this connection we provided the further development and tested the microscopic model for the tensosensibility effect in multi-layer polycrystalline film systems on the base of the approach KHATER and EL-HITI by considering the analytical dependence of the coefficients p*, r and Q on deformation (ε). However, as in the previous sources, we do not take into consideration the processes of interdiffusion of the elements. The processes have the great influence on the values p* and r. But this condition will be of no importance, if we take the parameters calculated from the experimental data to compare the theory and the experiment. The experimental data were obtained under the condition of interdiffusion, and we realized that.

The features of the theory are in the following assumptions. Firstly, on the electrical properties of the i-layer exert their influence electrons of the i±1, i±2 and other layers, if an effective mean free path λg which is limited with the crystallites, is commensurable with thickness $d_1+d_{i\pm1}$, $d_1+d_{i\pm1}+d_{i\pm2}$, and so on. Then, it is assumed that conductivity electrons take part in independent scattering processes (see Fig.) on the external layer surfaces (is characterized with the coefficient p^{i}*) on grain boundaries and on interfaces of layers (is characterized with r^i and Q^i). Besides, as it was mentioned above, the input of external and internal dimensional effects is estimated not only by means of given coefficients, but also with the help of corresponding coefficients of deformation: $\eta_{Qgi} = -\frac{1}{Q_i}\frac{\partial Q_i}{\partial \varepsilon}$, $\eta_{rgi} = -\frac{1}{r_i}\frac{\partial r_i}{\partial \varepsilon}$, $\eta_{p*gi} = -\frac{1}{p_i^*}\frac{\partial p_i^*}{\partial \varepsilon}$ and derivatives $\frac{\partial \ln k_i}{\partial \ln Q_i}, \frac{\partial \ln k_i}{\partial \ln p_i^*}$ and $\frac{\partial \ln k_i}{\partial \ln r_i}$ ($k_i = \frac{d_i}{\lambda_{g_i}}$ where index g corresponds the meaning of the respective parameter, when di→∞; and ε - is longitudinal deformation). To obtain the correlation for the coefficient γ1 the standard methods are used: we write down the inverse resistance formula for the parallel connection of n layers and the logarithmic derivative for the longitudinal deformation:

$$\frac{1}{R} = \frac{a}{l}\left(d_1\sigma_{g_i}F_1 + d_2\sigma_{g_2}F_2 + \cdots + d_n\sigma_{gn}F_n\right) \tag{1}$$

or

$$\frac{d\ln R}{d\ln l} = 1 + \mu_s - A_1\left(\frac{d\ln d_1}{d\ln l} + \frac{d\ln\sigma_{g_1}}{d\ln l} + \frac{d\ln F_1}{d\ln l}\right) - \cdots - A_n\left(\frac{d\ln d_n}{d\ln l} + \frac{d\ln\sigma_{g_n}}{d\ln l} + \frac{d\ln F_n}{d\ln l}\right), \tag{2}$$

where $\frac{d\ln d_i}{d\ln l} = -\mu_{f_i}\frac{1-\mu_s}{1-\mu_{f_i}} \cong -\mu_i^*$ (*l*, *a* – are the values of the initial length and width of the film correspondingly; μ_f, μ_s – are the Poisson's coefficient for the film and the substrate; σ - is the specific conductivity); $A_i = \frac{d_i\sigma_{g_i}F_i}{\sum_{i=1}^{n} d_i\sigma_{g_i}F_i}$ ($F_i = F_i(k_i, L_i, p_i^*, Q_i, r_i)$, L_i – is average grain size in *i*-layer).

As far as $\frac{d\ln\sigma_{g_i}}{d\ln l} = 1 + \eta_{g_i} = \gamma_{g_i}\left(\eta_{g_i} = -\frac{d\ln\lambda_{g_i}}{d\ln\varepsilon}\right)$, so the expression (1) transforms and can formulated in the form of:

$$\gamma = A_1\left(1+\eta_{g1}+\mu_1^* - \frac{d\ln F_1}{d\ln l}\right)+A_2\left(1+\eta_{g_2}+\mu_2^* - \frac{d\ln F_2}{d\ln l}\right)+\cdots+A_n\left(1+\eta_{g_n}+\mu_n^* - \frac{d\ln F_n}{d\ln l}\right)+1+\mu_s\,. \qquad (3)$$

To simplify the expression we represent it for $\frac{d\ln F_1}{d\ln l}$ in the case of doulble-layer film system:

$$\frac{d\ln F_1}{d\ln l}=\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln l}+\frac{d\ln F_1}{d\ln D_1}\frac{d\ln D_1}{d\ln l}+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln Q_1}\frac{d\ln Q_1}{d\ln l}+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln p_1^*}\frac{d\ln p_1^*}{d\ln l}+$$
$$+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln r_1}\frac{d\ln r_1}{d\ln l}+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln k_2}\frac{d\ln k_2}{d\ln l}+\frac{d\ln F_1}{d\ln D_1}\frac{d\ln D_1}{d\ln D_2}\frac{d\ln D_2}{d\ln l}+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln k_2}\frac{d\ln k_2}{d\ln Q_2}\frac{d\ln Q_2}{d\ln l}+ \qquad (4)$$
$$+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln k_2}\frac{d\ln k_2}{d\ln r_2}\frac{d\ln r_2}{d\ln l}+\frac{d\ln F_1}{d\ln k_1}\frac{d\ln k_1}{d\ln k_2}\frac{d\ln k_2}{d\ln p_2^*}\frac{d\ln p_2^*}{d\ln l},$$

where $D=\frac{L}{\lambda_g}$ - the reduced averaged size of grain.

Considering that $\frac{d\ln k_i}{d\ln k_{(i+1)}}=\frac{\beta_{g_i}}{\beta_{g(i-1)}}$, $\frac{d\ln F_i}{d\ln k_i}=\left(1-\frac{\beta_i}{\beta_{g_i}}\right)$ and assuming that $\frac{d\ln F_i}{d\ln k_i}\cong\frac{d\ln F_i}{d\ln D_i}$, it is possible to express the correlation for γ_l on any number of layers. When the electrical properties of *i*-layer depend only on the electrons of *i* and *i±1* layers, the above mentioned correlation can be expressed by the formula:

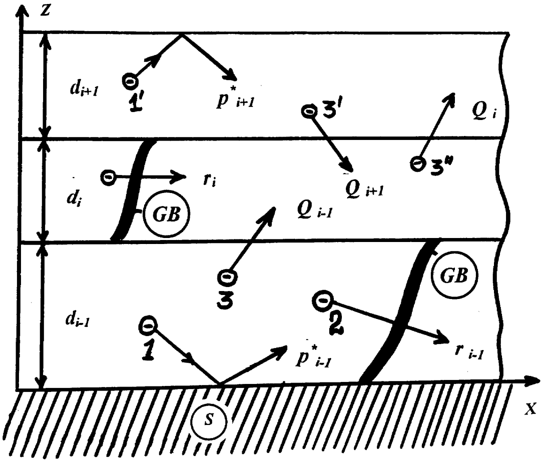
$$\gamma_l=\sum_{i=1}^{n}\frac{A_i}{\sum_{i=1}^{n}A_i}\left\{\left(\gamma_{g_i}+\mu_i^*\right)+\left(1-\frac{\beta_i}{\beta_{g_i}}\right)\left[\left(2\eta_{g_i}+1-\mu_i^*-\eta_{Q_{gi}}\frac{\partial\ln k_i}{\partial\ln Q_i}-\eta_{r_{gi}}\frac{\partial\ln k_i}{\partial\ln r_i}-\eta_{p^*_{gi}}\frac{\partial\ln k_i}{\partial\ln p^*_i}\right)+\right.\right.$$
$$+\left(2\eta_{g_{(i-1)}}+1-\mu_{(i-1)}^*-\eta_{Q_{g(i-1)}}\frac{\partial\ln k_{(i-1)}}{\partial\ln Q_{(i-1)}}-\eta_{r_{g(i-1)}}\frac{\partial\ln k_{(i-1)}}{\partial\ln r_{(i-1)}}-\eta_{p^*_{g(i-1)}}\frac{\partial\ln k_{(i-1)}}{\partial\ln p^*_{(i-1)}}\right)\frac{\beta_{g_i}}{\beta_{g_{(i-1)}}}+ \qquad (5)$$
$$\left.\left.+\left(2\eta_{g_{(i+1)}}+1-\mu_{(i+1)}^*-\eta_{Q_{g(i+1)}}\frac{\partial\ln k_{(i+1)}}{\partial\ln Q_{(i+1)}}-\eta_{r_{g(i+1)}}\frac{\partial\ln k_{(i+1)}}{\partial\ln r_{(i+1)}}-\eta_{p^*_{g(i+1)}}\frac{\partial\ln k_{(i+1)}}{\partial\ln p^*_{(i+1)}}\right)\frac{\beta_{g_i}}{\beta_{g_{(i+1)}}}\right]\right\}+1+2\mu_s$$

(under the condition that *i-1≠0 and i+1≤n*).

Though the formula (5) is complex, the resulting values can be compared easily with the experimental data, because all the values in the right hand part of formula (5) are either defined experimentally, or obtained after proper computation of the experimental data. So, γ_{gi}, β_{gi}, β_i one can obtain from the dimensional dependence for the tensosensibility coefficient or for the thermal coefficient of resistivity. The value of deformation coefficients for η_{Qgi}, η_{rgi} *and* η_{p^*gi}, as well as the derivatives $\frac{\partial\ln k_i}{\partial\ln Q_i}=\frac{Q_i}{k_i}\frac{dk_i}{dQ_i}$ can be defined within the framework of isotopic model by Tosser, Tellier and Pichard of dimensional dependence $\beta_i(d)$, obtained on one and the same series of single-layer films on $\varepsilon=0$ and $\varepsilon_l=const$ (as for our experiments, $\varepsilon=0.06\%$). It should be noted that we assume $Q_i \approx r_i$, because the experimental data are not enough to calculate Q_i, and consequently $\frac{dk_i}{dQ_i} \approx \frac{dk_i}{dr_i}$. For the three-layer film system *Cr/Co/Cr/S* and *Ni/Co/Cr/S* we obtained that on $T = 300\ K$, the parameters of electric transferring are of the such order: $\Delta p^* \sim 10^{-1}$, $\Delta Q \approx \Delta r \sim -10^{-2}$; $\Delta\lambda_g \cong (5\text{-}10)nm$; $\eta_{p*} \sim -10^2$, $\eta_Q \approx \eta_r \sim 10$; $\frac{\partial \ln k_i}{\partial \ln p_i^*} \sim -10^{-1}$, $\frac{d \ln k_i}{d \ln Q_i} \approx \frac{\partial \ln k_i}{\partial \ln r_i} \sim 10^{-2}$.

So, the most sensitive to the film deformation is the coefficient of specular reflection. The item p^* contributes to the total tensosensibility on the level of one unit that is almost 10 times more in comparison with the items $\eta_r \frac{d \ln k}{d \ln r}$ and $\eta_Q \frac{d \ln k}{d \ln Q}$.

It is evident that influence of the three items in total should be more considerable in the condition of low temperatures. But even in the condition of room temperature, we obtain rather good correspondence of the experimental and computation data.



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