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The effect of linear thermal expansion on the temperature coefficient of resistance of double-layer thin metallic films

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A general theoretical expression for the temperature coefficient of resistance of double-layer thin metallic films, based on the well known Fuchs–Sondheimer model, is derived. This expression includes the linear thermal expansion coefficients and Poisson's ratios of the double layers and the substrate, also the film dimensions and temperature coefficient of resistance of the double-layer thin film, with and without the thermal expansion of both the film layers and the substrate. Numerical calculations are carried out for gold–silver double-layer films deposited on a glass substrate, where variations in the temperature coefficient of resistance depending on thermal expansion are studied as a function of reduced film thickness. The computed numerical results, using the derived new expression for the temperature coefficient of resistance of the double-layer thin metallic films, show that the thermal expansion decreases the value of the temperature coefficient of resistance.

1. Introduction

The temperature coefficient of resistance of single-layer thin metallic films has been studied theoretically [1–6] as well as experimentally [7–15]. All these studies are based on the well known Fuchs–Sondheimer model [16, 17] and its developments. The temperature coefficient of resistance, β_f, is a very important parameter which is specified for high-performance thin-film resistors [18]. The Fuchs–Sondheimer model for electrical conductivity was developed and modified for application to double-layer thin metallic films [19, 20]. A general theoretical expression for the temperature coefficient of resistance of double-layer thin metallic films has been derived [21] based on the Fuchs–Sondheimer model for electrical conductivity [16, 17] for single-layer and double-layer films [19, 20], taking into consideration the bulk conductivity, β_f, and dimensions of the double layers. In these previous studies [21] for β_f, the linear thermal expansion of the substrate and the film layers were neglected for simplicity, by assuming that the linear thermal expansion coefficients of the film layers and the substrate are nearly the same. When the thermal expansion of each film layer differs from that of the substrate and from each other, then thermal strains cannot be neglected [22], and must be taken into account to derive a more exact expression for the temperature coefficient of resistance.

The aim of this study is to derive a more exact general expression for the temperature coefficient of resistance of double-layer thin metallic films, taking into account the linear thermal expansion and the thermal strains, as well as all the other parameters which were taken into consideration during the previous derivation of the temperature coefficient of resistance β_{RF} for negligible thermal expansions.

2. Preliminary definitions

Consider a double-layer thin metallic film consisting of a base layer and a superimposed overlayer from two different metals deposited on a non-metallic substrate, S, as shown in Fig. 1. The surface of the film is parallel to the plane $z = 0$, the base layer with surfaces at $z = 0$ and $z = -t_1$ containing metal 1, while the overlayer at $z = 0$ and $z = t_2$ contains metal 2, where t_1 and t_2 are the thickness of the base and overlayer respectively. The film layers are supposed to have the same length l and width w. If the interface between the two layers is ideally smooth, the conduction electrons impacting on the interface have two options – reflection or refraction. The impacting electrons may be reflected back according to the law of reflection, with a probability 0, and/or passed through the interface according to the law of refraction, with a probability Q. Suppose that the conduction electrons in the layers

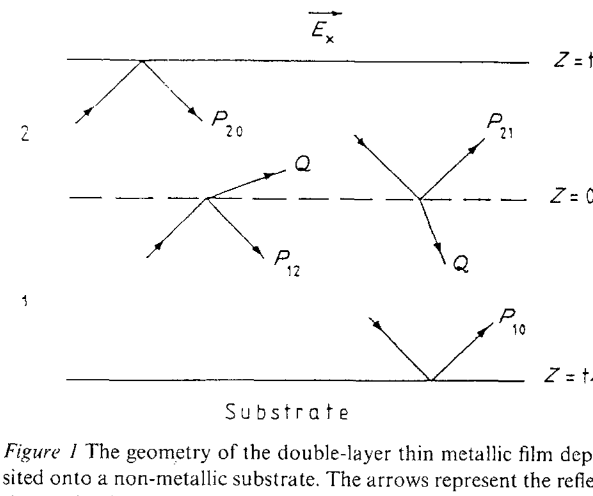

Figure 1 The geometry of the double-layer thin metallic film deposited onto a non-metallic substrate. The arrows represent the reflection and refraction of the impacting electrons on the surface and interface.

have two different effective masses, m_1 and m_2, Fermi velocities. Fermi velocities v_{F1} and v_{F2}, bulk mean free paths λ_{01} and λ_{02} and densities n_1 and n_2.

For a firmly attached film-substrate system, it is assumed that the thermal expansion of the substrate χ_s and the thermal expansion of the film length and width are identical and determined by the expansion coefficient of the substrate χ_s and given by the relation:

$$\frac{dl}{l} = \frac{dw}{w} = \chi_s dT \tag{1}$$

where dT is the differential variation in temperature.

The differential variation in temperature dT induces a differential variation in the film length, width and thickness beside the thermal strains induced in the length ε_{T1}, width ε_{T2} and thickness ε_{T3} of the film, which are given by the following relations as:

$$\frac{dl}{l} = \chi_f dT + \varepsilon_{T1} = (\chi_s - \chi_f) dT \tag{2}$$

$$\frac{dw}{w} = \chi_f dT + \varepsilon_{T2} = (\chi_s - \chi_f) dT \tag{3}$$

$$\frac{dt}{t} = \varepsilon_{T3} = 2\mu_f \frac{\chi_f - \chi_s}{1 - \mu_f} dT \tag{4}$$

where χ_f and χ_s; μ_f and μ_s are the linear thermal expansion and the Poisson's ratio of the film and substrate respectively. The temperature coefficient of resistance β_{RF} and of resistivity β_F of the film and β_{R0} and β_0 of the bulk are represented, respectively, as:

$$\beta_{RF} = \frac{1}{R_F}\frac{dR_F}{dT} \qquad \beta_F = \frac{1}{\varrho_F}\frac{d\varrho_F}{dT} = -\frac{1}{\sigma_F}\frac{d\sigma_F}{dT} \tag{5}$$

$$\beta_{R0} = \frac{1}{R_0}\frac{dR_0}{dT} \qquad \beta_0 = \frac{1}{\varrho_0}\frac{d\varrho_0}{dT} = -\frac{1}{\sigma_0}\frac{d\sigma_0}{dT} \tag{6}$$

where R_F, R_0; ϱ_F, ϱ_0 and σ_F, σ_0 are the resistance, resistivity and conductivity of the film and the bulk material, respectively.

3. Effect of thermal expansion

The electrical conductivity of a double-layer thin metallic film [20] is given by:

$$\sigma_F = \frac{t_1}{t_1 + t_2}\sigma_{01}F_1(K, P, Q) + \frac{t_2}{t_1 + t_2}\sigma_{02}F_2(K, P, Q) \tag{7}$$

where σ_{01}, σ_{02} and t_1, t_2 are the bulk electrical conductivity and the thickness of the base and overlayer films, respectively. The functions $F_1(K, P, Q)$ and $F_2(K, P, Q)$ are defined in [20, 21] and for simplicity can be written as F_1 and F_2, respectively. Equation 7 can be rewritten as follows:

$$R_F^{-1} = \frac{w}{l} t_1\sigma_{01}F_1\left(1 + \frac{t_2\sigma_{02}F_2}{t_1\sigma_{01}F_1}\right) \tag{8}$$

Taking the logarithmic differentiation of Equation 8 with respect to temperature, then the temperature coefficient of resistance of the double-layer thin metallic film β_{RFTS}, when taking into account the thermal strains or thermal expansions of the film layers and the substrate, respectively, can be written as:

$$\beta_{RFTS} = \frac{t_1\sigma_{01}F_1\beta_{01}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\times\left(1 - \frac{d\ln F_1}{\beta_{01}dT} + \frac{2\mu_1}{\beta_{01}}\frac{\chi_1 - \chi_s}{1 - \mu_1}\right) + \frac{t_2\sigma_{02}F_2\beta_{02}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\times\left(1 - \frac{d\ln F_2}{\beta_{02}dT} + \frac{2\mu_2}{\beta_{02}}\frac{\chi_2 - \chi_s}{1 - \mu_2}\right) \tag{9}$$

But

$$\frac{d\ln F_1}{dT} = \frac{d\ln F_1}{d\ln K_1}\cdot\frac{d\ln K_1}{dT} + \frac{d\ln F_1}{d\ln K_1}\cdot\frac{d\ln K_1}{d\ln K_2}\cdot\frac{d\ln K_2}{dT} \tag{10}$$

and

$$\frac{d\ln K_1}{d\ln K_2} = \frac{\left(\beta_{01} - 2\mu_1\frac{\chi_1 - \chi_s}{1 - \mu_1}\right)}{\left(\beta_{02} - 2\mu_2\frac{\chi_2 - \chi_s}{1 - \mu_2}\right)} \tag{11}$$

where $K_1 = t_1/\lambda_{01}$ and $K_2 = t_2/\lambda_{02}$ are the reduced thickness of the base and overlayer. In the same way, $d\ln F_2/dT$ and $d\ln K_2/d\ln K_1$ can be given by changing in Equations 10 and 11 the index 2 by 1 and the index 1 by 2, respectively. Substituting for $d\ln F_1/dT$ and $d\ln K_1/d\ln K_2$ from Equations 10 and 11, and for $d\ln F_2/dT$ and $d\ln K_2/d\ln K_1$ into Equation 9, β_{RFTS} can be written as:

$$\begin{aligned}\beta_{RFTS} = {} & \frac{2t_1\sigma_{01}F_1\beta_{01}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\left(1 - \frac{d\ln F_1}{d\ln K_1}\right) + \frac{2t_2\sigma_{02}F_2\beta_{02}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\left(1 - \frac{d\ln F_2}{d\ln K_2}\right)\\ & + \frac{t_1\sigma_{01}F_1\beta_{01}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\times\left[\left(1 + 2\frac{d\ln F_1}{d\ln K_1}\right)\frac{2\mu_1}{\beta_{01}}\frac{\chi_1 - \chi_s}{1 - \mu_1} - 1\right]\\ & + \frac{t_2\sigma_{02}F_2\beta_{02}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\times\left[\left(1 + 2\frac{d\ln F_2}{d\ln K_2}\right)\frac{2\mu_2}{\beta_{02}}\frac{\chi_1 - \chi_s}{1 - \mu_2} - 1\right]\end{aligned} \tag{12}$$

Using the general expression for the temperature coefficient of resistance, when the thermal expansion was negligible as derived before [21], β_{RF} takes the form:

$$\beta_{RF} = \frac{t_1\sigma_{01}F_1\beta_{01}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\left(1 - \frac{d\ln F_1}{d\ln K_1}\right) + \frac{t_2\sigma_{02}F_2\beta_{02}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2}\left(1 - \frac{d\ln F_2}{d\ln K_2}\right) \tag{13}$$

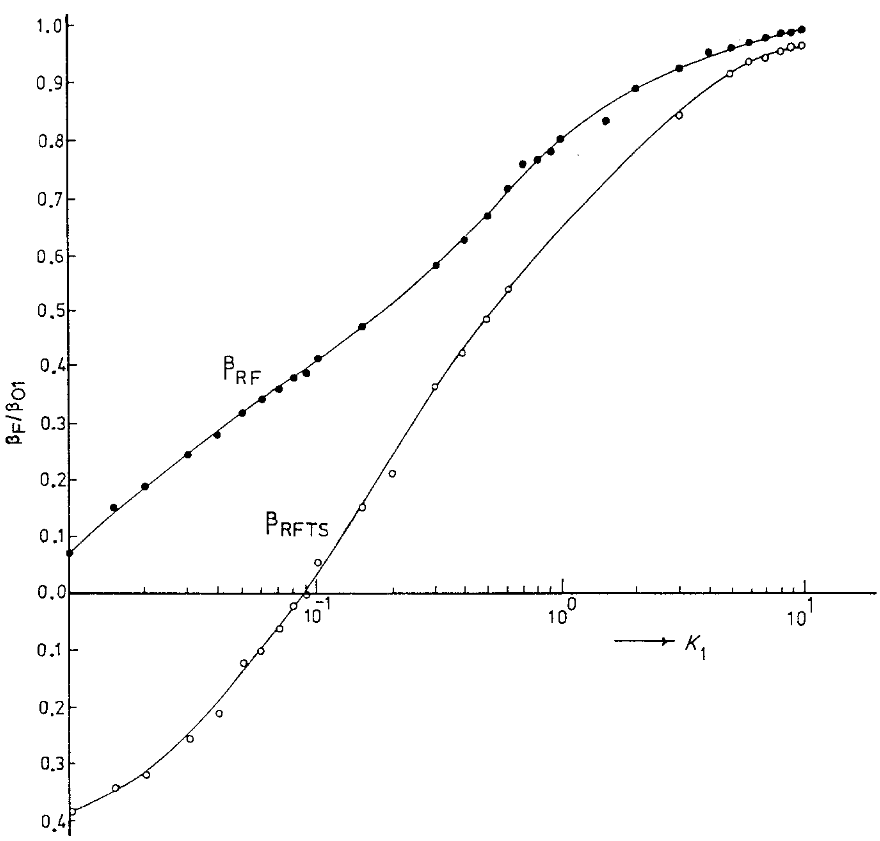

Figure 2 The reduced temperature coefficient of resistance with thermal expansion β_{RFTS}/β_{01} and without thermal expansion β_{RF}/β_{01} as a function of the reduced film thickness K_1 for $K_2 = 0.1$.

and

$$\frac{d \ln F_1}{d \ln K_1} = \frac{1 - F_1 - W_1}{F_1}$$

and

$$\frac{d \ln F_2}{d \ln K_2} = \frac{1 - F_2 - W_2}{F_2} \tag{14}$$

where

$$W_1 = \frac{3}{4}\int_0^1 dx_1(x_1 - x_1^3)\frac{\partial}{dK_1}[(1 - A)\{(1 - P_{10}) + D^{-1}(1 + P_{10}A)(X_1 + CQY_1)\}] \tag{15}$$

As defined in [21]; W_2 can be defined by changing the index 2 by 1 and 1 by 2 in Equation 15. Using Equations 12, 13, 14 and 15:

$$\begin{aligned}\beta_{RFTS} = {} & 2\beta_{RF} - \frac{t_1\sigma_{01}F_1\beta_{01}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2} \\ & \times \left\{1 + \frac{2\mu_1}{\beta_{01}}\frac{\chi_1 - \chi_s}{1 - \mu_1}\left[1 - \frac{2(1 - W_1)}{F_1}\right]\right\} \\ & - \frac{t_2\sigma_{02}F_2\beta_{02}}{t_1\sigma_{01}F_1 + t_2\sigma_{02}F_2} \\ & \times \left\{1 + \frac{2\mu_2}{\beta_{02}}\frac{\chi_2 - \chi_s}{1 - \mu_2}\left[1 - \frac{2(1 - W_2)}{F_2}\right]\right\}\end{aligned} \tag{16}$$

4. Numerical results

The gold overgrowth film deposited onto the glass substrate, which was predeposited by silver films, forms the double-layer thin metallic film which is considered for these numerical calculations. Gold and silver have the same crystal structure, and the interface between these layers has a negligible effect on the specularity reflection scattering of the conduction electrons, which means most of them are transmitted through the interface. That is, the reflection specularity parameters P_{12} and P_{21} are both nearly equal to zero, and the refraction parameter Q is nearly equal to unity. The parameters P_{10} and P_{20} are taken to be totally specular ($P_{10} = 1$) and totally diffuse ($P_{20} = 0$), respectively.

For numerical analysis, the following constant parameters are used as listed in [23], where the subscripts 1, 2 and s are related mainly to the over-layer gold, base-layer silver and the substrate, respectively:

linear thermal expansion

$$\chi_1 = 18.9 \times 10^{-6},\ \chi_2 = 13.9 \times 10^{-6},\ \chi_s = 6 \times 10^{-6}$$

Poisson's ratio $\mu_1 = 0.38$, $\mu_2 = 0.42$, $\mu_s = 0.3$

bulk conductivity

$$\sigma_{01} = 4.55 \times 10^5,\ \sigma_{02} = 6.21 \times 10^5$$

bulk mean free path $\lambda_{01} = 523\,\text{A}$, $\lambda_{02} = 390\,\text{A}$

bulk temperature coefficient of resistivity

$$\beta_{01} = 41 \times 10^{-4},\ \beta_{02} = 34 \times 10^{-4}$$

The numerical results of the temperature coefficient of resistance β_{RFTS}/β_{01} as a function of the reduced thickness K_1, as calculated from Equation 16, are shown in Fig. 2 for $K_2 = 0.1$ and in Fig. 3 for $K_2 = 0.01$. In Figs 2 and 3, β_{RFTS}/β_{01} was compared with β_{RF}/β_{01} to show the role of thermal expansion for the temperature coefficient of resistance of double-layer thin metallic films. It is clear that β_{RFTS} has the same character as β_{RF}, but with smaller values.

5. Conclusion

The curves of Figs 2 and 3 exhibit the following features.

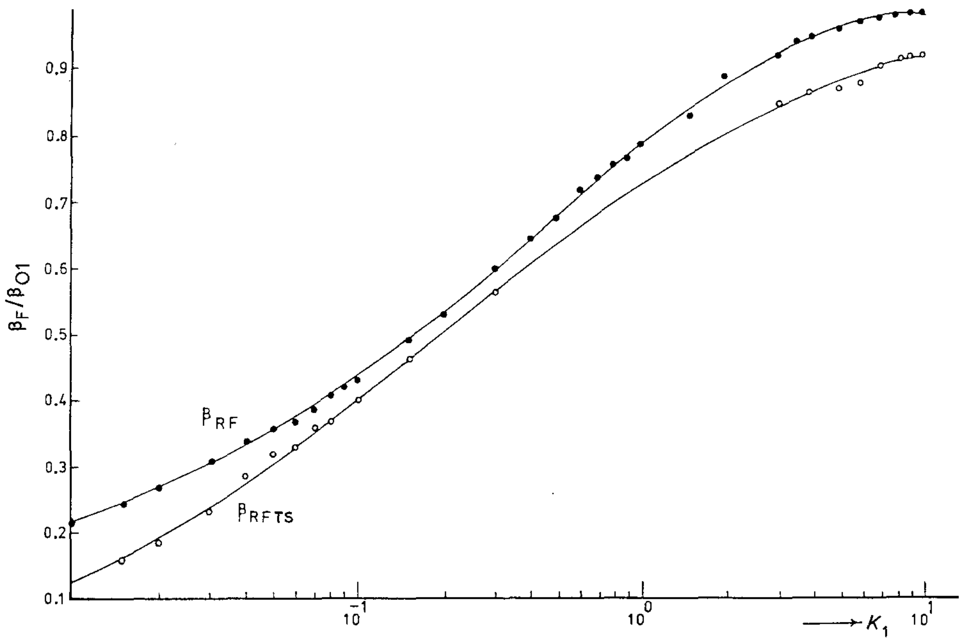

Figure 3 As Fig. 2, for $K_2 = 0.01$.

1. The deposition of an overlayer of gold onto a base layer of silver reduces the values of β_{RF} and β_{RFTS}, and this decrease is markedly dependent on the thickness of the overlayer. This result is in good agreement with other theoretical and experimental results [21, 24].

2. The temperature coefficient of resistance with effective thermal strains β_{RFTS} exhibits a size effect such as β_{RF}, without thermal strains. But this size effect is nearly vanishing for large values of the reduced thickness K_1 independent of K_2.

3. The introduction of the effect of thermal strains as a result of the difference in thermal expansions of the film layers and the substrate reduces the value of the temperature coefficient of resistance of the double-layer thin metallic film β_{RF} to become β_{RFTS}.

4. β_{RFTS} is positive and increases with the reduced thickness of the overlayer K_1 for a reduced thickness of the base layer $K_2 = 0.01$. This behaviour is the same as β_{RF}.

5. β_{RFTS} is negative for $K_1 < 0.1$, approaches zero at $K_1 = 0.1$, and becomes positive for $K_1 > 0.1$. This occurs for $K_2 = 0.1$. The occurrence of a negative β_{RFTS} can be related to many causes such as oxidation, trapped impurities, insulation of the grain boundaries and small islands, defects, and the variation in thermal expansion of the film materials and the substrate. The occurrence of negative β_{RFTS} here is related mainly to the difference in thermal expansions or thermal strains of the double layers of the film and substrate as studied for thin films of one material [4, 13, 22, 25, 26, 27]. It is clear that negative β_{RFTS} occurs for small values of film thickness. Therefore it is thought [28] that the temperature coefficient of resistance TCR is positive and approaches the bulk value for thickness of 100 nm. For 10 nm, TCR decreases with thickness and finally approaches zero, becoming negative for film thicknesses of few nanometres.

6. Thus we conclude that Equation 16 is an acceptable theoretical expression for the temperature coefficient of resistance of the double-layer thin metallic film when the variations in resistance with strain are temperature-dependent.

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