The Temperature Coefficient of the Resistance of Ultra-Thin Metal Films from Computer Simulations

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Z. Naturforsch. **40 a**, 1066–1067 (1985);
received August 3, 1985

The thickness dependence of the absolute temperature coefficient of the resistance of ultra-thin metal films is calculated with the help of Monte-Carlo calculations already successfully applied to the simulation of the electrical resistance. An initially strong increase and then a weaker decrease of the ATCR with increasing thickness is found.

In a previous paper we have reported on Monte-Carlo calculations of the electrical resistance of ultra-thin metal films [1]. The model was based on the assumption that clusters of definite size are statistically distributed on the substrate surface. The substrate was divided into cells each of which was open for occupation by one or several clusters. The resistance then was calculated using the relation

$$R_{kl} = R_0 \frac{1}{\sqrt{k\,l}}\,, \tag{1}$$

where k and l are numbers of clusters in two neighbouring cells, respectively, and R_0 is the reference resistance of a hypothetical layer with all cells singly occupied with a cluster of height d_0. A typical Monte-Carlo simulation for $d = 0.7\,d_0$ is shown in Fig. 1 a, and the corresponding network is illustrated in Fig. 1 b. It should be emphasized that the resistance between two occupied next nearest cells (black rectangles in Fig. 1 b) has also been included. This resistance was assumed to be greater by a factor α than that between nearest cells in order to take into account that for a limited range of distances the formation of highly ohmic conducting bridges between the clusters [2] or an electron hopping via surface traps [3] cannot be neglected.

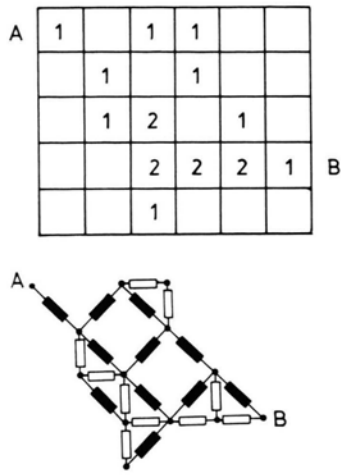

Fig. 1. Examples of the simulation process for $d = 0.7\,d_0$ (a) and the corresponding network (b).

The aim of the present paper is to point out that such a model can also be applied to the description of the absolute a temperature coefficient of the resistance (ATCR) and its correlation with the mean thickness d of the discontinuous film.

The ATCR is defined as [4]

$$\beta = \mathrm{d}R/\mathrm{d}T\,. \tag{2}$$

Obviously we have to sum up the various transitions between occupied cells analogously to the approved resistance treatment. The only modification is that we count the ATCR for two neighbouring crystallites positively and for the next neighbouring crystallites negatively. All other simplifications are similar to those used in the resistance calculation [1]:

(a) The positive ATCR between neighbouring cells is still dependent on the degree of occupation according to (1) and (2),

$$\beta_{kl} = \beta_0\,(1/\sqrt{k\,l})\,, \tag{3}$$

where β_0 is the ATCR for a film with all cells singly occupied. Note that the normalization by β_0 leads to a description which is independent of the number of cells to a first approximation.

(b) The negative ATCR between occupied next neighbouring cells is enhanced by a factor of γ as compared to the prediction of (3). The parameter γ is arbitrarily chosen to be 10 or

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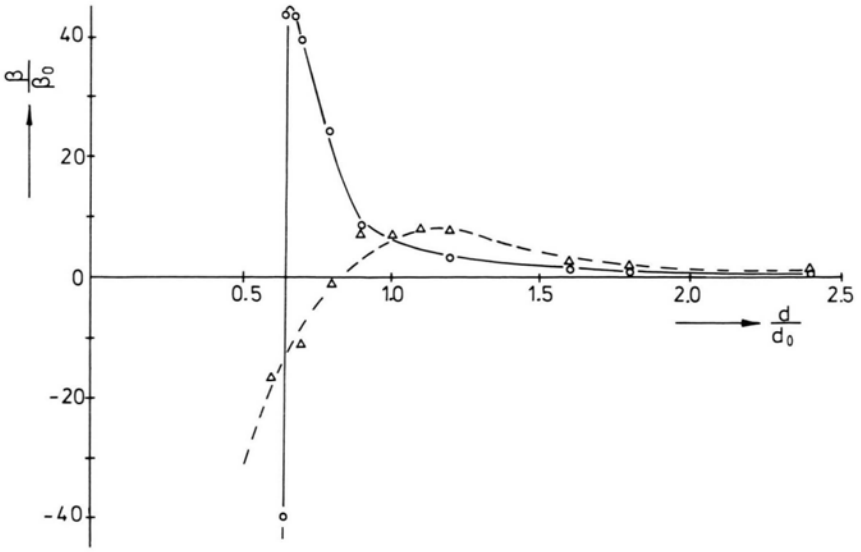

Fig. 2. Thickness dependence of the ATCR calculated according to (3). Full curve with $\gamma = 1000$ and dashed curve with $\gamma = 10$.

1000. This assumption is based on the experience that the highly ohmic bridges [2] or the electron hopping [3] cause the discontinuous films to behave semiconductor-like with respect to the temperature dependence of resistance.

The network analysis [5] has been performed for a quadratic substrate divided into 10×10 cells as described previously [1]. Each simulation was repeated ten times and averaged in order to obtain a smooth curve. The result of the calculation is shown in Figure 2. Obviously the ATCR starts with strongly negative values, runs through a relatively sharp maximum near $d = d_0$ an then decreases towards zero level. The half width of the maximum peak is higher with smaller values of γ.

It would be desirable to check these predictions with experimental data. Unfortunately, only very few measurements of the ATCR of thin films are available in the literature. Some early data on Na [4] and Ni [6, 7] films seem to confirm qualitatively the shape of the curves of Figure 2. It should be mentioned, however, that deviations are to be expected if the films do not show a definite cluster size but rather a smeared cluster size distribution. Moreover, coagulation processes have been excluded from the present consideration.

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