

Monte-Carlo Calculations of the Electrical Resistance of Ultra-Thin Metal Films

H.-U. Finzel* and P. Wißmann

Institut für Physikalische und Theoretische Chemie der Universität Erlangen-Nürnberg

Z. Naturforsch. **40 a**, 161–163 (1985); received December 7, 1984

The thickness dependence of the electrical resistance of ultra-thin metal films is calculated under the assumption that atoms or clusters of equal shape and size impinge and stick upon the substrate with statistical equipartition. The deposition process is simulated with the aid of a random generator. By network analysis an initially strong and then weaker decrease of the resistance with increasing film thickness is found.

Ultra-thin metal films show strong peculiarities in the electrical properties. For example, the electrical resistance is strongly enhanced for films with a discontinuous structure [1]. Coutts and Hopewell [2] were the first who tried to describe this behaviour by means of a statistical model. The high standard of the present computer generation enables us to further refine the models including detailed assumptions on the contact resistance between different film areas.

Starting point for our calculation is the assumption that atoms or clusters of equal shape and size impinge and stick upon the surface with a statistical equipartition. For reasons of simplification a quadratical substrate is considered and divided into 10×10 equal unit cells. Each cell can be occupied by one or several atoms or by clusters. The sectioning is characterized by the column index i and the row index j (Figure 1).

With the aid of a random generator real number couples (i, j) are produced. Each couple corresponds to a well-defined cell to be occupied. The process is repeated until the desired number of atoms or clusters is reached. Figure 1 shows the simulation of the precipitation process achieved by this procedure. The number of condensed atoms or clusters is counted in fractions of a reference thickness d_0 which is assumed to correspond with 100 real number couples. For $d \geq 0.2 d_0$ certain cells are

doubly occupied (cell 4, 10 in Fig. 1 b) while the majority of cells is still empty. For $d = 0.4 d_0$ an already coherent structure is detectable characterized in Fig. 1 c by connecting lines. For $d = 0.7 d_0$ the first closed current path develops (Figure 1 d).

In order to calculate the electrical resistance of the film the following simplifications are introduced:

(a) The current only flows between neighbouring occupied cells. Since each cell (i, j) is surrounded by eight neighbours only eight current paths must be taken into account when starting from an arbitrary cell. This assumption is based on the experience that quantum mechanical tunnelling of the electrons is ineffective for large distances between metal islands [3, 4].

(b) The resistance between two neighbouring cells is still dependent on the degree of occupation. If a cell (i, j) is occupied by k and the neighbouring cell by l atoms or clusters, then the effective resistance is assumed to be

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

This formulation represents the most simple possibility to take into account that for sufficiently high thickness the resistance of the film should vary inversely proportional to d . The square root can be interpreted as the geometrical average of the thicknesses of both cells participating in the current flow. Crystallite boundary scattering [5] is excluded from the consideration in the present case.

(c) The resistance between two occupied cells in the diagonal, i.e. from (i, j) to $(i + 1, j \pm 1)$, is assumed to be larger by a factor of α than the

* Present address: DIEHL, Fischbachstr. 16, 8505 Röthenbach.

Reprint requests to Prof. Dr. P. Wißmann, Institut für Physikalische und Theoret. Chemie der Universität, Egerlandstraße 3, 8520 Erlangen.

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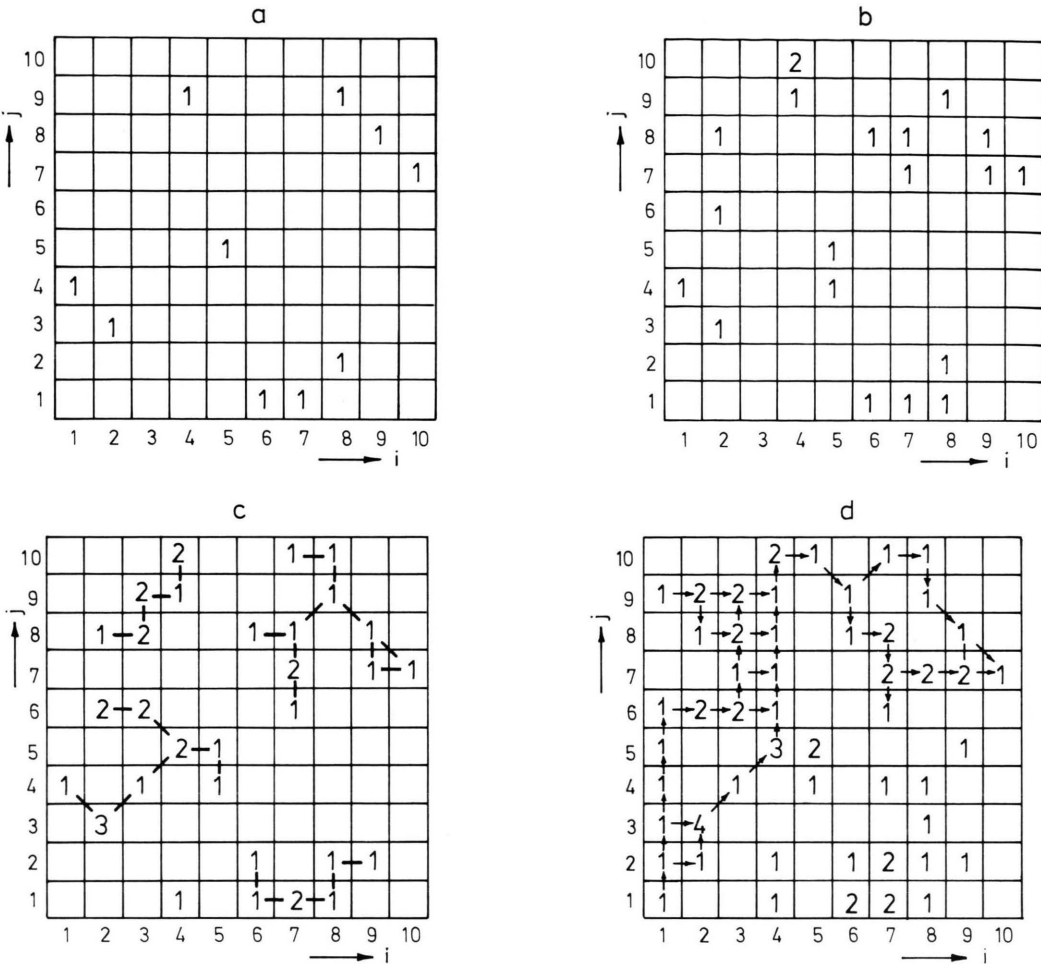


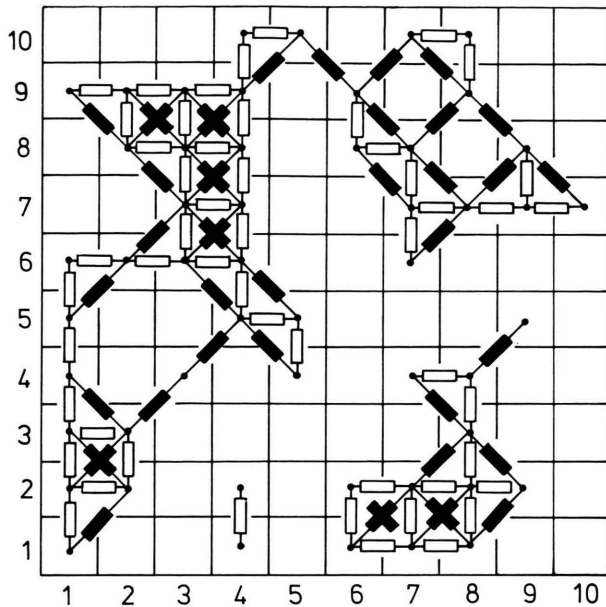
Fig. 1. Examples for the simulation of the deposition process. The occupation of the unit cells is
 a) $d = 0.1 d_0$, b) $d = 0.2 d_0$, c) $d = 0.4 d_0$, d) $d = 0.7 d_0$.

resistance between directly neighbouring cells. By this procedure a possible formation of highly ohmic bridges between the metal islands [6] is taken into account.

In the frame-work of these assumptions the formation of a conducting layer must be originated by at least *one* current path of occupied cells from $i = 1$ to $i = 10$ without interruption. Obviously this case only happens for $d \geq 0.7 d_0$ as can be seen from Fig. 1 d, where the path between the cells (1, 1) and (10, 7) is closed for the first time.

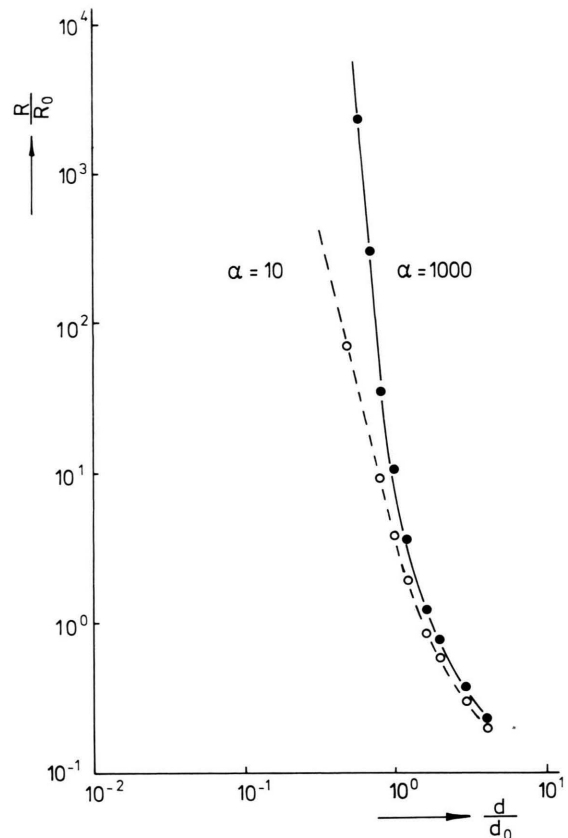
The network with the current paths of Fig. 1 d is shown in Figure 2. Note that the island area between (6, 1) and (9, 5) does not contribute to the electron transport. The network is reduced to the

total resistance R with the aid of a specially developed computer program on the basis of classical network analysis [7]. By evaluating the quantity R/R_0 it is guaranteed that the description is nearly independent of the number of cells under consideration. The result is shown in Fig. 3 where R/R_0 is plotted against d/d_0 in a doubly logarithmic scale. Such a scale is advantageous in order to cover the whole resistance range and to read out the characteristic parameters d_0 and R_0 from a comparison with experimental data. The smooth trace of the curves was achieved by simulating each point ten times and averaging. A simple simulation was proved to be insufficient to avoid statistical scattering of the calculated values.

Fig. 2. Network and current paths for $d = 0.7 d_0$.

The parameter α describing the enhancement of the resistance in the diagonal is considered to be distinctly higher than unity. The value $\alpha = 1000$ stands for the most simple behaviour that the diagonal practically does not at all contribute to the conductivity. It is easily seen from Fig. 3 that the resistance decreases with increasing thickness in all cases. For $\alpha = 1000$, however, the slope is steeper than for $\alpha = 10$. The simulation is restricted to thicknesses smaller than $4 d_0$. The calculation of R values for a higher thickness requires a drastically increasing consumption of computing time which seemed to be no more justified.

The mathematical model presented here can be applied, for example, to the interpretation of the growth of metal films on isolating single-crystal substrates suggesting that the cell dimensions are those of the adsorbing atoms or clusters. The highly

Fig. 3. Thickness dependence of the electrical resistance R (full curve calculated with $\alpha = 1000$ and dashed curve with $\alpha = 10$).

ohmic bridges characterized by the amount of α , then, may stand for a contribution of electron hopping via substrate surface states [8]. Unfortunately, corresponding measurements have not been reported until now in the literature.

In a refined model the discussion should also include coagulation processes at the substrate surface [1] and a possible size distribution of the impinging clusters.

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