THICKNESS DEPENDENCE OF CPA DENSITIES OF STATES FOR ELECTRONS IN THIN FILM ALLOYS*

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The local electronic density of states has been calculated for three values of film thickness d: 3, 7, and 15 atomic layers. This function if found to depend little on d, except for the left edge of the majority band. Different alloy compositions have been considered.

Following the method presented in our previous paper [1] we have calculated the local density of states for electrons in thin films as a function of the film thickness. The procedure has been repeated for three values of the thickness d: 3, 7, and 15 atomic layers (the case $d = 11$ is discussed in detail in [1]). In our simple model all the films considered have the simple cubic lattice structure with 001 orientation. The electrons are described by the one-band tight binding hamiltonian. We have introduced two different coherent potentials: one for the surface layers and one for the internal part. They are built into the standard CPA-theory with a completely random distribution of atoms of both kinds. The single site version of the CPA has been used.

Our energy unit is the hopping integral $|t|$ between the nearest neighbours, taken as independent of the kind of atoms. The electron energy for A-atoms is chosen to be zero, and the corresponding energy for B-atoms, $E_B = 6.0$ (in this unit). These values ensure a splitting of two bands, belonging to these levels. The separation persists for the whole range of concentration of B-atoms, examined in our work. For $E_B = 5.0$ the bands may join into one band as was established in [1]. The former case seemed more interesting for us (more band edges).

The results of numerical calculations are collected in Figs. 1–4. The first two figures correspond to the uniform concentration of B-atoms (0.1 and 0.5). In the next two figures the bulk concentration c is kept equal to 0.1, whereas the surface concentration c_s is 0.2 (Fig. 3) or 0.5 (Fig. 4). In all figures, the full lines represent the internal density of states, and the dotted lines — the surface density of states.

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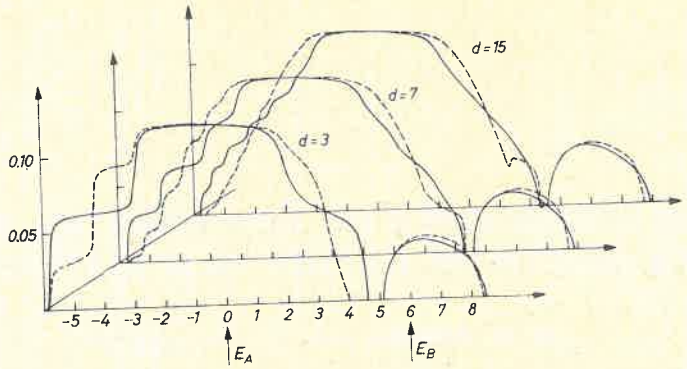

Fig. 1. Surface (dotted line) and internal (full line) density of states for $c = c_s = 0.1$

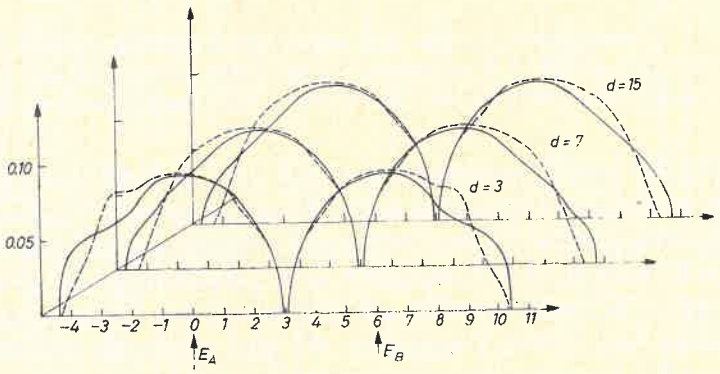

Fig. 2. Surface (dotted line) and internal (full line) density of states for $c = c_s = 0.5$. The plot is symmetric with respect to the energy $E = 3.0 = \frac{1}{2}(E_A + E_B)$

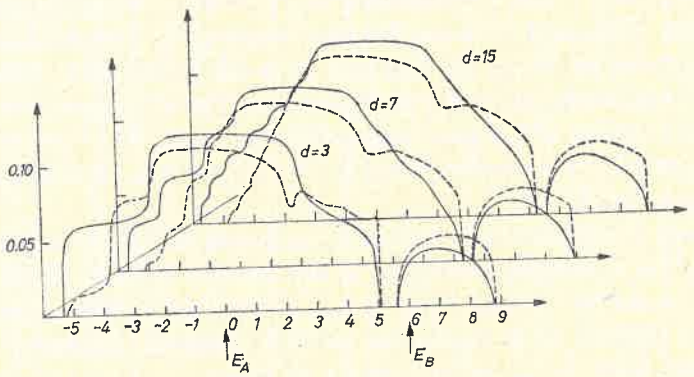

Fig. 3. Surface (dotted line) and internal (full line) density of states for $c = 0.1$, and $c_s = 0.2$. The two surface bands are significantly influenced by the change in the surface concentration c_s, whereas the internal bands remain almost the same as in Fig. 1

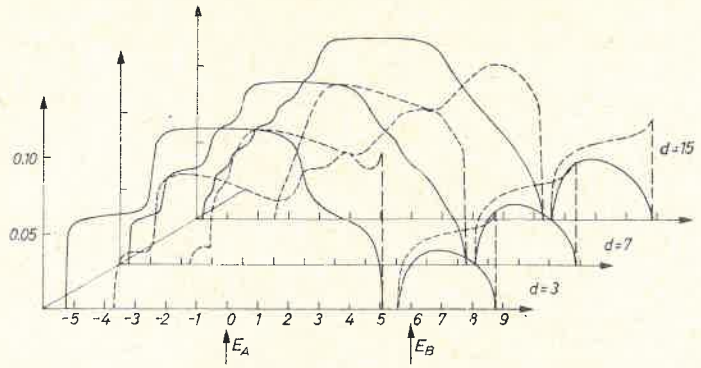

Fig. 4. Surface (dotted line) and internal (full line) density of states for $c = 0.1$, and $c_s = 0.5$. Two peaks are observed at both upper edges of the two surface bands

A striking feature of these plots is a relatively weak dependence of the density considered on the film thickness d. The minority bands (B-bands) are almost identical. Some differences occur in the left part of the A-band where a step structure, characteristic for pure films in our model, persists in alloys with not too high a concentration of B-atoms; the number of steps is equal to $(d+1)/2$ (cf. [1]). The surface density of states is a little more sensitive to the variation of d. We observe details (tails or other irregularities) vanishing with increasing d.

This work leads thus to the conclusion that the local density of states is essentially independent of the presence of other atomic layers, at least in our model. The thickness influences slightly the shape of the density curve mainly on its left side. Hence the examination of various surface phenomena may be restricted to very thin slabs and the thin film theoretical techniques seem to be a convenient tool for describing their behaviour.

Our results and conclusions agree with similar ones obtained for semi-infinite systems [2–4]. Berk [2] was the first who applied the CPA-method for crystals with one surface. His densities are very similar to ours except for the step structure mentioned above. For a small concentration of B-atoms he got a peak on the surface density cuvre typical for the two-dimensional tight binding method. In our model such peaks were ignored [1] in order to make the theory tractable; this approximation favours, however, the free electron behaviour.

The papers [3] and [4] deal with similar physical problems but are based on methods better than the CPA. The authors have found some details on the density curve absent in the CPA. On the other hand they confirm our qualitative features discussed in [1]; in particular a characteristic narrowing of the surface band leading to a charge transfer between the surface and the bulk of a sample.

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