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A CPA CALCULATION FOR THE 11-LAYERED THIN FILM*

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The local density of electronic states has been calculated for a film consisting of 11 atomic layers. The standard CPA method has been extended to systems finite in one direction. The tight-binding one band model is used. Both surface and internal density of states are presented as functions of certain physical parameters.

1. *Introduction*

The problem of determining the density of states function is one of the most fundamental in solid state physics. For bulk materials it has been elaborated rather well, especially for pure crystallographic samples. Less progress has been made for alloys and amorphous media although in the last ten years the situation has changed drastically.

Similar problems occur also in thin film physics and its close relative — surface physics. The lack of translational symmetry in the direction perpendicular to the surface essentially complicates theoretical considerations. As a consequence they must have a mainly qualitative character. Thin film alloys represent even more difficult objects for theoretical treatment. Small wonder that only a few papers are devoted to their theoretical aspects.

In this paper we present a method based on the Green function technique, applicable to both pure and alloyed films. The main attention is focussed on the properties of the density of states function. For alloys we extend the conventional CPA method in its simplest version. Apart from the so called natural defect (the existence of the surfaces alone) we admit some differences in comparison with the interior of the film by introducing the surface values of some physical parameters. These differences are assumed to cause a relatively small change in the coherent potential on the surfaces so that one may truncate the appropriate Dyson equation at the linear term in the surface perturbation. Within

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this approximation it became possible to obtain exact formulas for the most important Green functions e.g. their matrix elements in the site representation G_{nn} for the centre and for the surface layers of the film.

In Section 2 we formulate the physical model and give an outline of the Green function method suitable for the CPA for electrons. We also give numerical values of some coefficients characterizing the Green functions in the momentum representation which are necessary for further considerations.

The third Section is devoted to the calculation of the Green functions for more realistic situations including the surface changes of the most important physical quantities. These are expressed by unperturbed Green functions described in the preceding section and then integrated over the appropriate Brillouin zone. Some of these functions are presented at the end of Section 3.

In Section 4 we describe the densities of states for different chemical compositions. First we show the densities for the pure film and then for alloys with a uniform and non-uniform (different at the surfaces) distribution of atoms of both kinds. In both cases we observe some new effects absent in bulk samples, for instance, a redistribution of electrons between the surface and the bulk of the film. A brief discussion of the numerical results is given at the end of the paper.

Despite its qualitative and model character this work indicates essential differences in the behaviour of a film and a bulk sample, which manifest themselves in several subtle effects not occurring in bulk materials.

2. Model. General description

In order to simplify the theoretical considerations we have restricted ourselves to the simplest geometrical structure namely to the simple cubic lattice structure with 001 orientation (the z-axis perpendicular to the surface). The film considered is thus composed of 11 identical atomic planes. We will index them by the Greek letters μ, ν, φ etc. all of them taking on the values: 1, 2, 3, ..., 11. The position of an atom in one plane will be denoted by a two-dimensional vector $\boldsymbol{R}$. Three-dimensional positions will be represented by the letters: i, j, l, m, n.

The reasons for the choice of such a film thickness are of a purely technical nature. Thicker films involve much more elementary but very tedious calculations. The procedure is significantly simplified when the number of atomic planes is odd but still it consumes much time. On the other hand, the properties of thicker films change rather slowly with increasing thickness. It is well known (see, for example, [1]) that typical surface- and thin film behaviour is related to very thin slabs consisting of few atomic planes only. Thus our film seems to be a good representative from this point of view.

The electronic system is described by the hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}, \tag{1}$$

where t_{ij} denote the transfer integrals between the i-th and j-th sites. t_{ii} has the meaning of the electron energy on the i-th site which will be hereafter denoted also by E_i. The operators c and $c^{\dagger}$ have the usual sense. Here we assume the existence of Wannier states for our system first proven by Rehr and Kohn [2] for semi-infinite samples. The hamiltonian (1) is essentially of the one-band type.

Following the similar calculations for bulk crystals we put

$$t_{ij} = \begin{cases} t, & \text{if } i \text{ and } j \text{ are the nearest neighbours} \\ 0, & \text{otherwise } (i \neq j). \end{cases} \tag{2}$$

The difference between atoms is taken into account via the energies E_i. For a two-component alloy $A_{1-c}B_c$ we have

$$E_i = \begin{cases} E_A, & \text{if the } i\text{-th site is occupied by an } A \text{ atom,} \\ E_B, & \text{if the } i\text{-th site is occupied by a } B \text{ atom.} \end{cases} \tag{3}$$

In more detailed considerations we should admit the dependence of E_i on the distance from the surface, at least its surface value may differ from its bulk value. This is in fact built-in into our general theory but in numerical calculations we did not make use of this possibility.

The Green functions, we will use later, is defined by the equation

$$(z-H)G = 1, \tag{4}$$

where z is an arbitrary complex number. In the matrix form one has

$$\sum_m (z\delta_{nm} - H_{nm})G_{ml} = \delta_{nl}. \tag{5}$$

Here, $H_{nm} = t_{nm}$.

If the film has translational symmetry in the xy-plane (a pure system or an averaged alloy) then Eq. (5) may be partially diagonalized by means of the two-dimensional Fourier transformation according to the rule

$$f_n = \frac{1}{N} \sum_k e^{-i\mathbf{k}\cdot\mathbf{n}} f_{\mu k} \quad (\mu = \mu(n)), \tag{6}$$

where N denotes the number of atomic sites in one plane xy and $\mathbf{k}$ is a two-dimensional wave vector. The coefficients $f_{\mu k}$ depend in general on the plane index μ. After applying this formula to Eq. (5) we obtain

$$\sum_{\varphi} (z\delta_{\mu\varphi} - t_{\mu\varphi}(k))G_{\varphi\nu}(k) = \delta_{\mu\nu}, \tag{7}$$

where

$$t_{\mu\varphi}(k) = \begin{cases} 2t \cos ak_x + \cos ak_y, & \text{if } \mu = \varphi \\ t & , \text{if } |\mu - \varphi| = 1 \\ 0 & , \text{otherwise} \end{cases} \tag{8}$$

(a — the lattice constant).

For the sake of simplicity we abbreviate the expression with two cosines by s_k

$$s_k = 2(\cos ak_x + \cos ak_y). \tag{9}$$

This quantity varies from (-4) to $(+4)$; the corresponding two-dimensional band width is then equal to $8\,|t|$.

Let us denote the matrices (with respect to plane indices μ, ν and so on) appearing in Eq. (7) by $\hat{t}$ and $\hat{G}$. In this notation instead of (7) we may write

$$\hat{G}(\boldsymbol{k}) = (z - \hat{t}(\boldsymbol{k}))^{-1}. \tag{10}$$

Here,

$$\hat{t}(\boldsymbol{k}) = \begin{bmatrix} E_1 + ts_k, & t & , 0 & , \ldots\ldots \\ t & , E_2 + ts_k, & t & , \ldots\ldots \\ 0 & , t & , E_3 + ts_k, & \ldots\ldots \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ \ldots\ldots & \ldots\ldots & \ldots\ldots, & E_1 + ts_k \end{bmatrix}. \tag{11}$$

Hence,

$$\hat{G}(\boldsymbol{k}) = \begin{bmatrix} x_1, & t, & 0, & \ldots\ldots \\ t, & x_2, & t, & \ldots\ldots \\ 0, & t, & x_3, & \ldots\ldots \\ \ldots\ldots & \ldots\ldots & \ldots, & \ldots \\ \ldots\ldots & \ldots\ldots & \ldots\ldots, & x_1 \end{bmatrix}^{-1}, \tag{12}$$

where

$$x_\mu = E_\mu + ts_k - z. \tag{13}$$

For convenience we will assume $|t|$ to be unity in the energy scale in all further considerations.

The matrix elements of $\hat{G}(\boldsymbol{k})$ may easily be evaluated for moderate values of the film thickness d. For higher values of d this is also possible but in a form rather useless for practical purposes. The fact that x_μ are in general complex drastically limits effective progress in the whole theory. One is thus forced to make some additional approximations, just at this stage of considerations. The most natural one consists in putting all the x's constant across the film. All the quantities derived within such an approximation will be distinguished by the index "*o*".

All the matrix elements of the Green function $\hat{G}^{(o)}(\boldsymbol{k})$ may be expressed in the following way:

$$G^{(o)}_{\mu\nu}(\boldsymbol{k}) = \sum_{\tau=1}^{11} A^{\tau}_{\mu\nu} \frac{1}{x - r^{\tau}}, \tag{14}$$

where r^{τ} are zeros of the determinant

$$D = \det \begin{bmatrix} x, & 1, & 0, & \dots\dots \\ 1, & x, & 1, & \dots\dots \\ \dots & \dots & \dots & \dots\dots \\ \dots & \dots & \dots, & x \end{bmatrix} . \tag{15}$$

The coefficients $A^{\tau}_{\mu\nu}$ are determined by simple algebraic manipulations. In the next Section we will need four functions only: $G^{(o)}_{1,1}$, $G^{(o)}_{1,6}$, $G^{(o)}_{6,6}$ and $G^{(o)}_{1,11}$. The coefficients $A^{\tau}_{\mu\nu}$ for these matrix elements are collected in Table I.

It is due to its simplicity that we were able to proceed with calculations of form (14) of the unperturbed Green functions much faster than might be suggested by (12).

TABLE I

A^{τ} \ r^{τ}	−1.932	−1.732	−1.414	−1.000	−0.518	0.000	0.518	1.000	1.414	1.732	1.932
$A^{\tau}_{1.1}$	−0.011	−0.042	−0.083	−0.125	−0.156	−0.167	−0.156	−0.125	−0.083	−0.042	−0.011
$A^{\tau}_{1,6}$	−0.043	0.000	0.118	0.000	−0.161	0.000	0.161	0.000	−0.118	0.000	0.043
$A^{\tau}_{6,6}$	−0.167	0.000	−0.167	0.000	−0.167	0.000	−0.167	0.000	−0.167	0.000	−0.167
$A^{\tau}_{1,11}$	−0.011	0.042	−0.083	0.125	−0.156	0.167	−0.156	0.125	−0.083	0.042	−0.011

3. Green functions for films with surface perturbation

Let us now assume that the energy E_1 and E_{11} at surface planes differs from that inside the film by an amount δE. Then we must put

$$x_1 = x + \delta x = x_{11}. \tag{16}$$

At the same time, $x_2 = x_3 = \dots = x_{10} = x$. The difference δx may include the change in the electron energy or in the coherent potential or in other parameters. It seems justified to treat δx as relatively small so that we replace the exact Dyson equation: $\hat{G} = \hat{G}^{(o)} + \hat{G}^{(o)} \cdot \hat{V} \cdot \hat{G}$ by its version linear in the perturbation $\hat{V}$

$$\hat{G}(k) = \hat{G}^{(o)}(k) + \hat{G}^{(o)}(k) \cdot \hat{V} \cdot \hat{G}^{(o)}(k). \tag{17}$$

Here $\hat{G}$ denotes the Green function (12) with x's chosen in the above manner, and

$$\hat{V} = \begin{bmatrix} \delta x, & 0, & 0, & \dots \\ 0\,, & 0, & 0, & \dots \\ 0\,, & 0, & 0, & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots, & \delta x \end{bmatrix} \tag{18}$$

(two elements different from zero). We have assumed that both surface planes are identical which is not always true.

In further considerations we will be interested in two matrix elements only $G_{1,1}$ and $G_{6,6}$. These functions are equal to:

$$G_{1,1} = G^{(o)}_{1,1} + 2\delta x (G^{(o)}_{1,1})^2 \quad \text{for} \quad |G^{(o)}_{1,11}| = |G^{(o)}_{1,1}| \tag{19}$$

and

$$G_{6,6} = G^{(o)}_{6,6} + 2\delta x (G^{(o)}_{1,6})^2 \quad \text{for} \quad |G^{(o)}_{1,6}| = |G^{(o)}_{11,6}|. \tag{20}$$

It is easy to see that

$$(G^{(o)}_{1,1})^2 = \sum_{\tau=1}^{11} B^{\tau}_{1,1} \frac{1}{x-r^{\tau}} + \sum_{\tau=1}^{11} \tilde{B}^{\tau}_{1,1} \left(\frac{1}{x-r^{\tau}}\right)^2 \tag{21}$$

and analogically for $(G^{(o)}_{1,6})^2$. The coefficients B are related to coefficients A in the following way:

$$B^{\tau}_{\mu\nu} = 2A^{\tau}_{\mu\nu} \sum_{\tau'=1}^{11} \frac{A^{\tau'}_{\mu\nu}}{r^{\tau}-r^{\tau'}}, \tag{22a}$$

$$\tilde{B}^{\tau}_{\mu\nu} = (A^{\tau}_{\mu\nu})^2. \tag{22b}$$

Their values are given in Table II.

TABLE II

B^{τ} \ r^{τ}	-1.932	-1.732	-1.414	-1.000	-0.518	0.000	0.518	1.000	1.414	1.732	1.932
$B^{\tau}_{1,1}$	-0.019	-0.063	-0.103	-0.109	-0.070	0.000	0.070	0.109	0.103	0.063	0.019
$\tilde{B}^{\tau}_{1,1}$	0.000	0.002	0.007	0.016	0.024	0.028	0.024	0.016	0.007	0.002	0.000
$B^{\tau}_{1,6}$	0.013	0.000	0.010	0.000	0.004	0.000	-0.004	0.000	-0.010	0.000	-0.013
$\tilde{B}^{\tau}_{1,6}$	0.002	0.000	0.014	0.000	0.026	0.000	0.026	0.000	0.014	0.000	0.002

4. *Densities of states*

The main purpose of this paper is to calculate the density of electronic states g, which is connected with the Green function G by means of the relation

$$g_n(\omega) = -\frac{1}{\pi} \operatorname{Im} G_{nn}(\omega + i0_+). \tag{23}$$

It has the meaning of the local density of states per atom and holds for both pure systems and alloys.

For systems with translational symmetry in each direction, $g(\omega)$ does not depend on the position n. For thin films it is true with respect to the xy plane. Otherwise one should take into account the dependence of g on μ. This may be done in our scheme for every plane separately. However, the differences between internal planes are rather small so that it is reasonable to restrict the calculations to two extreme planes: the surface and the central ones. We will thus consider two densities: g_s (surface) and g_c (centre). The former corresponds to $\mu = 1$, the latter to $\mu = 6$.

In order to evaluate any g-function it is necessary to apply the inverse Fourier transformation which for diagonal matrix elements reduces to the simple summation

$$G_{nn} = \frac{1}{N} \sum_{k} G_{\mu\mu}(k), \qquad \mu = \mu(n). \tag{24}$$

Here, $G_{\mu\mu}(\boldsymbol{k})$ depends on $\boldsymbol{k}$ through s_k only. Thus the sum over $\boldsymbol{k}$ may be replaced by an appropriate integral over (say) s. For this purpose we introduce an additional auxiliary density h, corresponding to the function s_k. In two dimensions for square lattices it resembles rather well a step function with a narrow peak in the middle (cf. Fig. 1, dotted line). We will ignore this peak making thus an analogy with the free electron gas. The more realistic shape of h would drastically complicate numerical calculations. In our model the h-function is equal to

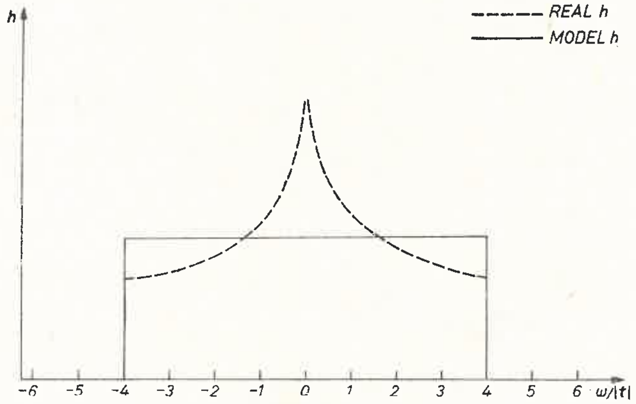

Fig. 1. The two-dimensional density of states h. Full line — model density, dotted line — real density corresponding to two cosines

$$h(\omega) = \begin{cases} \frac{1}{8}, & \omega \in (-4,4), \\ 0, & \text{otherwise}, \end{cases} \tag{25}$$

being normalized to unity.

Within such an approximation we have

$$G_{nn} = \tfrac{1}{8} \int_{-4}^{4} G_{\mu\mu}(s)ds, \qquad (\mu = \mu(n)). \tag{26}$$

As we have seen, every G_{nn}-function is a sum of terms of the type $(x-r)^{-1}$ or of the type $(x-r)^{-2}$. Therefore we need only to integrate these simple fractions. The results are

$$f^{\tau} \equiv \tfrac{1}{8} \int\limits_{-4}^{4} \frac{1}{x-r^{\tau}}\, ds = \tfrac{1}{8}\left(\ln\left(z+r^{\tau}-E-4\right)-\ln\left(z+r^{\tau}-E+4\right)\right),$$

$$\tilde{f}^{\tau} = \tfrac{1}{8} \int\limits_{-4}^{4} \frac{1}{(x-r^{\tau})^{2}}\, ds = \tfrac{1}{8}\left(\frac{1}{z+r^{\tau}-E-4} - \frac{1}{z+r^{\tau}-E+4}\right). \tag{27}$$

The imaginary part of f^{τ}, multiplied by the factor $(-1/\pi)$, will be further denoted by g^{τ} and that of $\tilde{f}^{\tau}$ — by $\tilde{g}^{\tau}$. It is easy to see that for real E, g^{τ} reproduces the step function h, and $\tilde{g}^{\tau}$ is equal to zero. Hence the g-functions play an essential role in alloys, where electronic energies are described by a complex potential Σ.

Note that for large z, all the f-functions are proportional to $\dfrac{1}{z}$, as desired.

According to the results of previous considerations we have the following formulas for the densities $g_{c}^{(o)}$ and $g_{s}^{(o)}$:

$$g_{c}^{(o)} = \sum_{\tau} A_{c}^{\tau} g^{\tau} = \sum_{\tau} |A_{c}^{\tau}| h^{\tau}, \tag{28a}$$

$$g_{s}^{(o)} = \sum_{\tau} A_{s}^{\tau} g^{\tau} = \sum_{\tau} |A_{s}^{\tau}| h^{\tau}, \tag{28b}$$

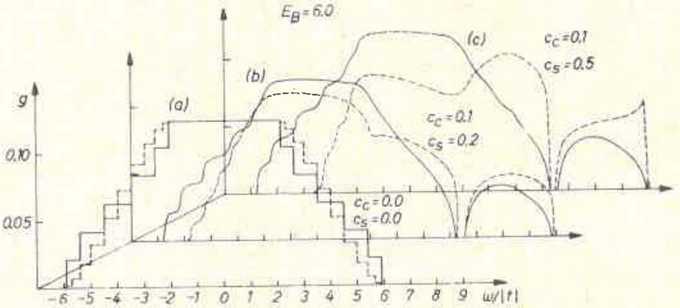

Fig. 2. Surface (dotted line) and central (full line) density of states for small (b) and large (c) difference in the surface concentration of B-atoms. The plot (a) corresponds to the pure A-system

where h^{τ} denotes the step function h shifted by r^{τ}. Both densities are thus compositions of 11 step functions. Their plots are shown in Fig. 2 (a); the full line corresponds to g_{c}, and the dotted line to g_{s} (this convention serves for other figures too).

The presence of steps in the densities for pure systems is very characteristic in our model. They reflect a specific way if quantization of the z-component of the wave vector $\boldsymbol{k}$. k_z is not a good quantum number for electrons in a thin film, but we may imagine a "quantization unit" in the z-direction of the order $(2\pi/d)$ (d — number of atomic planes in a film) which is much larger than $(2\pi/N)$. The "quantity" τ plays the role of k_z in our model.

The dependence of electron energy, and consequently — the density of states on τ, is however much more complicated than the usual parabolic one.

It is worth noting that the band width of both bands is the same and very close to that of a three-dimensional system. For the simple cubic crystal one has the value 12.00 in units of $|t|$. Here, we have 11.93.

The surface density of states is more concentrated around the central energy (original atomic energy, E_A). This is connected with a redistribution of electrons between the surface and bulk in materials with the number of electrons per atom different from 1.0 and 0.5. In alloys this effect may be much greater.

Let us now calculate the two densities of states for an alloy. We consider a two-component system of the type $A_{1-c}B_c$ with a completely random distribution of atoms of both kinds. In contrast to bulk sample theories we admit the surface concentration of B-atoms to be different from that in the bulk of the film. To such a system we apply the most elementary version of the CPA method with the diagonal disorder only.

We use two coherent potentials: one (Σ_c) for the internal planes and one (Σ_s) for the surface planes. The well known (see, for instance, [3]) equation for the coherent potential splits off in our case into two equations

$$\Sigma_c = c_c E_B + \Sigma_c (E_B - \Sigma_c) G_c, \tag{29a}$$

$$\Sigma_s = c_s E_B + \Sigma_s (E_B - \Sigma_s) G_s. \tag{29b}$$

Here,

$$G_c = G_{6,6}, \quad G_s = G_{1,1},$$

both Green functions in the site representation. The subscript "c" refers to the central plane whereas the subscript "s" — to surface planes.

From the results of Section 3 it follows that

$$G = G^{(o)} + 2(\Sigma_s - \Sigma_c)\tilde{G}^{(o)}, \tag{30}$$

where

$$G^{(o)} = \sum_\tau A_c^\tau f^\tau, \quad \tilde{G}^{(o)} = \sum_\tau (B_c^\tau f^\tau + \tilde{B}_c^\tau f^\tau). \tag{30'}$$

Substituting (30) into (29a) one obtains:

$$\Sigma_s = \Sigma_c + \frac{\Sigma_c - c_c E_B - \Sigma_c (E_B - \Sigma_c) G^{(o)}}{2\Sigma_c (E_B - \Sigma_c) \tilde{G}^{(o)}}. \tag{31}$$

Making use of Eq. (29b) we get the equation for Σ_c:

$$\Sigma_s = c_s E_B + \Sigma_s (E_B - \Sigma_s)\,(G^{(o)} + 2(\Sigma_s - \Sigma_c)\tilde{G}^{(o)}) \tag{32}$$

with Σ_s given by (31). This is one non-linear equation for one complex variable Σ_c.

The total density of states is equal to:

$$g_c = \frac{1}{\pi} \operatorname{Im} \frac{\Sigma_c - c_c E_B}{\Sigma_c(\Sigma_c - E_B)}, \tag{33}$$

and analogically for the surface density g_s.

5. *Discussion*

In order to check the validity of the approximation (17) we have calculated the densities g_c and g_s for two distinct situations. The first one corresponds to a small difference between the surface and bulk concentration of B-atoms, e.g. $c_c = 0.1$ and $c_s = 0.2$. The second case represents a larger difference between them: $c_c = 0.1$ and $c_s = 0.5$. In the latter case g_s differs significantly from g_c and cuts off sharply on its right edge. This suggests that such a difference in concentrations may be too high for our model. The plots of g_c and g_s in both cases are given in Fig. 2 where we have also placed both densities for the pure A-system (two curves distinguished by the index "a").

In Fig. 3 we present a comparison of the densities g_c and g_s calculated for an uniform distribution of B-atoms, equal to 0.1 and 0.5. The atomic energy $E_B = 6.0$, and at the same time, $E_A = 0.0$ (in units of $|t|$). We see that the step structure vanishes very quickly with increasing concentration of B-atoms. For $c = 0.5$ it disappears entirely and for $c = 0.1$ it is noticeable on the left parts of the plot only. Simultaneously one observes the existence of a gap between the A-part and the B-part of the total densities of states. For higher values of c this gap becomes smaller but it still occurs. This is a little unexpected as the value $E_B = 6.0$ was chosen to lie very close to the right edge of the densities for the pure A-film, e.g. close to the value 5.93. A narrowing of the original band is also to be underlined here. Another interesting feature of the result is that the B-band is not concentrated around the value $E_B = 6.0$, but is shifted to higher values of energy; we may call it a "repulsion" between two band.

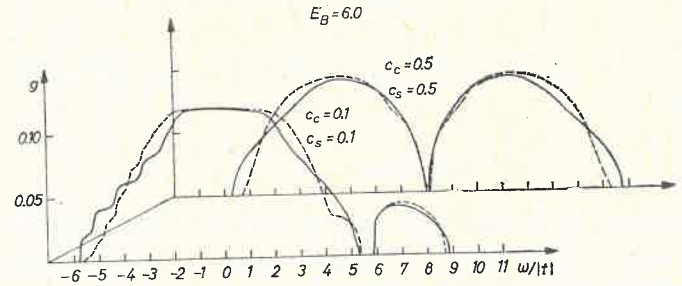

Fig. 3. Surface (dotted line) and central (full line) density of states for two values of concentration of B-atoms: $c = 0.1$ or $c = 0.5$. The surface concentration is the same as in other planes

Fig. 4 shows the densities for two different nonuniform distributions of B-atoms. The left plot corresponds to a surface enriched film ($c_s = 2c_c$), the right one is the opposite case ($c_c = 2c_s$). Both plots reflect these changes very clearly.

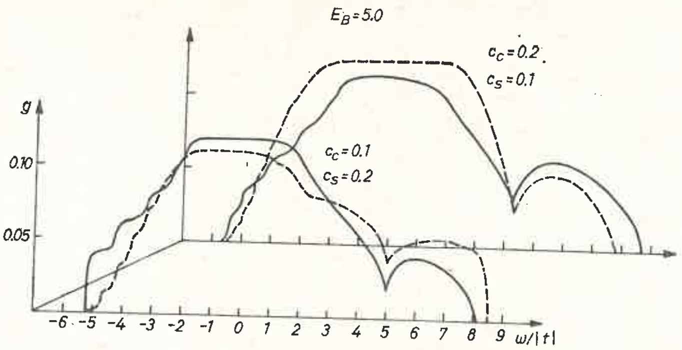

Fig. 4. Density of states for a nonuniform distribution of B-atoms. The surface concentration $c_s = 2c_c$ or $c_s = \frac{1}{2}c_c$. Dotted line — surface density, full line — central density

Finally, in Fig. 5 we compare the results obtained for different values of E_B, namely 3.0, 4.0, 5.0, and 6.0. In all cases we put $c_c = c_s = 0.1$, and $E_A = 0.0$. It is easy to observe the separation of the B-band from the A-band. We want to underline that the surface B-band separates earlier than the bulk B-band. It drops to zero quicker than the central band does. The existence of a surface gap alone might be of some importance in future investigations.

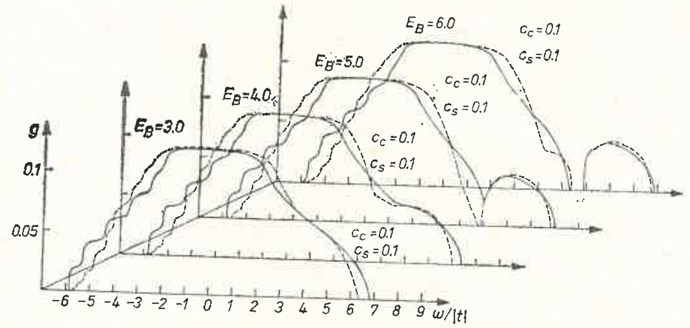

Fig. 5. Surface (dotted line) and central (full line) density of states for several values of E_B

In conclusion we must say that our calculations are only qualitative and based on a model which is not connected with any real sample. Nevertheless it may be easily adopted to more realistic situations. The main purpose of this work was to elaborate a method of calculation suitable for thin films. To our knowledge the problem has not been solved in the literature.

In our subsequent paper we will present the results of similar calculations for three other thicknesses (3,7, and 15 atomic layers) of thin films and a comparison will be made. We will also compare our results with corresponding ones based on the CPA calculations for semi-infinite samples (Refs. [4–7]).

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