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**LOCAL FREQUENCY
DISTRIBUTION FUNCTION
OF A CRYSTAL WITH ADSORBED ATOMS.**

Part I

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1. INTRODUCTION

Different experimental techniques are available in order to measure the characteristics of the surface phonons in the case of adsorbed atoms or adsorbed monolayers. Recently, also the neutron spectroscopy has been extended to these cases^{1,2/} (the frequency distributions of chemisorbed H atoms on Ni-catalysts were determined^{2/}). In order to give a qualitative interpretation of the neutron inelastic scattering experiments from a surface with adsorbed atoms, the local frequency distribution functions of atoms of the adsorbate-substrate system have to be calculated. The previous theoretical work on this subject considered either the semi-infinite crystal (or slab having a thickness of several atomic planes with an adsorbed monolayer^{3/}), or a crystal with various concentrations of impurity atoms in the surface layer^{4/}.

In this paper it is assumed that the adsorbed atoms are randomly distributed on the (001) crystal surface of a simple cubic lattice and are bound to the surface atoms by central and non-central force constants. The calculation of the frequency distribution function is based on the VPA method. The Green function of a crystal with a planar defect is also derived.

2. MODEL

We consider a semi-infinite harmonic simple cubic crystal with (100) surface covered by randomly adsorbed atoms of a given concentration. Each adatom is assumed to be bound to one surface atom only. In the harmonic approximation this bound can be described by the central force constant α and by the non-central one β .

We assume that relaxation and reconstruction of the surface layer take place neither at the clean crystal surface nor due to the presence of adsorbed atoms. Then, by assuming only the nearest neighbour interaction between the crystal atoms and the adatoms, the whole system can be characterized by masses of crystal atoms M_0 , of adatoms M' , and by the force constant matrix F , which is identical to the force constant matrix of an ideal crystal: for all crystal sites but the surface layer,

where the force constant submatrices have the following form^{/6/}

$$\begin{aligned}
 \underline{F}_{\underline{0},\underline{i}} &= - \begin{pmatrix} \alpha & 0 & \pm\eta \\ 0 & \beta & 0 \\ \mp\eta & 0 & \beta \end{pmatrix} & \underline{F}_{\underline{0},\pm\underline{j}} &= - \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & \pm\eta \\ \mp 0 & \eta & \beta \end{pmatrix} \\
 \underline{F}_{\underline{0},-\underline{k}} &= - \begin{pmatrix} \beta & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix} & \underline{F}_{\underline{0},\underline{k}} &= - \begin{pmatrix} \beta' & 0 & 0 \\ 0 & \beta' & 0 \\ 0 & 0 & \alpha' \end{pmatrix}
 \end{aligned} \tag{1}$$

$$\begin{aligned}
 \underline{F}_{\underline{0},\underline{0}} &= -(\underline{F}_{\underline{0},\underline{i}} + \underline{F}_{\underline{0},-\underline{i}} + \underline{F}_{\underline{0},\underline{j}} + \underline{F}_{\underline{0},-\underline{j}} + \underline{F}_{\underline{0},\underline{k}} + \underline{F}_{\underline{0},-\underline{k}}) \\
 \underline{i} &\equiv (1, 0, 0), \quad \underline{j} \equiv (0, 1, 0), \quad \underline{k} \equiv (0, 0, 1), \quad 2\eta = -\beta + \beta'n_0.
 \end{aligned}$$

The origin of the coordinate system is in the surface plane and z-components of coordinates of adsorbed atoms are equal to +1, n_i is the occupation number operator at the site i . It is equal to zero when no adatom is bound at the site i and is equal to one in the opposite case. We assume that the operators acquire their two possible values in a random way and are nonzero only on the surface. Since the goal of our calculations is the frequency distribution function, we shall not take into account the restrictions in the force constants due to the invariance under an infinitesimal rigid body rotation of the crystal, i.e., we put $\eta=0$. It was shown^{/5/} that this approximation has only a small effect on the shape of the frequency distribution function (PDF), all its qualitative features remaining unchanged. On the other hand, the approximation simplifies substantially further calculations.

In order to use the single-site CPA treatment^{/3/}, in the first period of our calculation we also ignore the interaction between the adatoms taking into account only the bond with the surface. Measurements of the coverage dependence of the adsorption heat give us hint that this step may be often justified. In many cases the difference of the adsorption heat at zero coverage and for a monolayer, respectively, is less than 1%^{/7/}. Then, $\underline{F}_{\underline{k},\underline{k}} = -\underline{F}_{\underline{0},\underline{k}}$, $\underline{F}_{\underline{k},\underline{0}} = \underline{F}_{\underline{0},\underline{k}}$ are the only nonzero force constant submatrices of the adsorbed atom.

Having determined the force constant matrix \underline{F} we can write the equation of motion for the Green functions of the system

$$(\underline{M}\omega^2 - \underline{F})\underline{G} = \underline{I}, \quad (2)$$

where

$$\underline{M} = \begin{pmatrix} \underline{M}' & \underline{0} \\ \underline{0} & \underline{M}_0 \end{pmatrix}$$

and \underline{M}' , \underline{M}_0 are diagonal matrices corresponding to the adatom layer and to the crystal atoms, respectively.

$$(\underline{M}')_{\underline{i},\underline{i}} = M' n_{\underline{i}} \delta_{\underline{i},\underline{i}}, \quad (\underline{M}_0)_{\underline{i},\underline{i}} = M_0 \delta_{\underline{i},\underline{i}}.$$

Explicitly, the equation of motion for the diagonal element of the surface Green function has the form

$$M_0 \omega^2 \underline{G}_{\underline{0},\underline{0}} - \underline{F}_{\underline{0},\underline{1}} (\underline{G}_{\underline{1},\underline{0}} - \underline{G}_{\underline{0},\underline{0}}) - \underline{F}_{\underline{0},-\underline{1}} (\underline{G}_{-\underline{1},\underline{0}} - \underline{G}_{\underline{0},\underline{0}}). \quad (3)$$

The first six terms on the left-hand side of Eq.(3) describe dynamics of surface atoms, the last one describes the adatom-surface interaction and contains the nondiagonal adatom-surface element of the Green function $\underline{G}_{\underline{k},\underline{0}}$. However, this element can be easily eliminated from Eq.(2) by means of the equation of motion of an adsorbed atom

$$n_0 M' \omega^2 \underline{G}_{\underline{k},\underline{0}} = \underline{F}_{\underline{k},\underline{0}} \underline{G}_{\underline{0},\underline{0}} + \underline{F}_{\underline{k},\underline{k}} \underline{G}_{\underline{k},\underline{0}} - \underline{F}_{\underline{0},\underline{k}} (\underline{G}_{\underline{0},\underline{0}} - \underline{G}_{\underline{k},\underline{0}}) \quad (4)$$

$$\underline{G}_{\underline{k},\underline{0}} = (M' \omega^2 \underline{I} + \underline{F}_{\underline{0},\underline{k}})^{-1} \underline{F}_{\underline{0},\underline{k}} \underline{G}_{\underline{0},\underline{0}} \quad \text{for } n_0 \neq 0.$$

By applying this relation to the last term of Eq. (3) we get

$$\underline{F}_{\underline{0},\underline{k}} (\underline{G}_{\underline{k},\underline{0}} - \underline{G}_{\underline{0},\underline{0}}) = \underline{F}_{\underline{0},\underline{k}} [(M' \omega^2 \underline{I} + \underline{F}_{\underline{0},\underline{k}})^{-1} \underline{F}_{\underline{0},\underline{k}} - \underline{I}] \underline{G}_{\underline{0},\underline{0}} = n_0 \underline{\Delta\phi} \underline{G}_{\underline{0},\underline{0}},$$

where

$$\underline{\Delta\phi} = \begin{pmatrix} \beta' \frac{\omega^2}{\omega^2 - \delta_1} & 0 & 0 \\ 0 & \beta' \frac{\omega^2}{\omega^2 - \delta_2} & 0 \\ 0 & 0 & \alpha' \frac{\omega^2}{\omega^2 - \delta_3} \end{pmatrix}$$

$$\delta_1 = \delta_2 = \beta' / M', \quad \delta_3 = \alpha' / M'.$$

Since there are no elements of the force constant matrix connecting a subsurface layer with adsorbed atoms due to the assumed short range of forces, the dimensionality of the matrix equation (2) can be reduced to the dimensionality of the equation of motion of the clean crystal

$$(\underline{M}_0 \omega^2 - \underline{\Phi} - \Delta \underline{\Phi}) \underline{G} = \underline{I}, \quad (5)$$

where $\underline{\Phi}$ denotes the force constant matrix of the clean crystal and $(\Delta \underline{\Phi})_{\ell, \ell'} = \Delta \underline{\Phi}_{\ell \ell'} \delta_{\ell \ell'}$ for all surface lattice sites. Knowing the solution of Eq. (5) the adatom Green function can be calculated directly from the diagonal element of the surface Green function $\underline{G}_{0,0}$. Combining the equation of motion for $\underline{G}_{\underline{k}, \underline{k}}$

$$n_0 M' \omega^2 \underline{G}_{\underline{k}, \underline{k}} = \underline{F}_{0, \underline{k}} (\underline{G}_{0, \underline{k}} - \underline{G}_{\underline{k}, \underline{k}}) + \underline{I} = \underline{F}_{0, \underline{k}} (\underline{G}_{\underline{k}, 0} - \underline{G}_{\underline{k}, \underline{k}}) + \underline{I}$$

with Eq. (4), we obtain

$$\underline{G}_{\underline{k}, \underline{k}} = \underline{K} \underline{G}_{0,0} n_0 + \frac{1}{M'} \begin{pmatrix} \frac{1}{\omega^2 - \delta_1} & 0 & 0 \\ 0 & \frac{1}{\omega^2 - \delta_2} & 0 \\ 0 & 0 & \frac{1}{\omega^2 - \delta_3} \end{pmatrix}$$

where

$$K^{\mu \kappa} = \left(\frac{\delta_1}{\omega^2 - \delta_1} \right)^2 \delta_{1, \kappa}$$

(By the Green symbols we denote three coordinate axes).

The frequency distribution function of the lattice vibrations is closely related to the Green function. For the crystal with an infinitely large disordered surface the local frequency distribution function (LFDF) of the surface layer is equal to a configurationally averaged LFDF

$$\rho_s(\omega^2) = - \frac{M_0}{\pi} \lim_{\epsilon \rightarrow 0+} \text{ImTr} \langle \underline{G}_{0,0}(\omega^2 + i\epsilon) \rangle. \quad (6)$$

Similarly LFDF of the adsorbed layer

$$\rho_a(\omega^2) = - \frac{M'}{\pi} \lim_{\epsilon \rightarrow 0+} \text{ImTr} \langle n_0 \underline{G}_{\underline{k}, \underline{k}}(\omega^2 + i\epsilon) \rangle. \quad (7)$$

It follows from Eqs. (6,7) that for the calculation of LFDF's $\rho_s(\omega^2)$ and $\rho_a(\omega^2)$ we need the knowledge of the averaged Green function and the conditionally averaged Green function, respectively. The diagonality of the perturbation $\Delta \underline{\Phi}$ in eq.

(5) allows us to calculate them by using a surface modification of the coherent potential approximation (CPA) ^{14/}.

CPA is a single site approximation and does not take into account the correlation effects in occupation of sites by adsorbed atoms. The averaged Green function is expressed in terms of the diagonal self-energy matrix Σ

$$\langle G \rangle_{\text{CPA}} = [M_0 \omega^2 I - \Phi - \Sigma]^{-1}.$$

The matrix Σ is nonzero only on the surface and due to symmetry of the cubic crystal it has only two nonzero elements.

$$\Sigma_{\underline{\ell}, \underline{\ell}'} = \begin{pmatrix} \Sigma_1 & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & \Sigma_3 \end{pmatrix} \delta_{\underline{\ell}, \underline{\ell}'}$$

They can be calculated from the Soven-Taylor equation

$$\Sigma_{\underline{0}, \underline{0}} (I - (\Delta\Phi_{\underline{0}, \underline{0}} - \Sigma_{\underline{0}, \underline{0}}) \langle G_{\underline{0}, \underline{0}} \rangle_{\text{CPA}}) = c \Delta\Phi_{\underline{0}, \underline{0}},$$

where c is the concentration of adatoms on the crystal surface.

The conditionally averaged Green function of an occupied site can be easily deduced from $\langle G_{\underline{0}, \underline{0}} \rangle_{\text{CPA}}$ by using the Dyson equation

$$\langle n_{\underline{0}, \underline{0}} G_{\underline{0}, \underline{0}} \rangle_{\text{CPA}} = (I - \langle G_{\underline{0}, \underline{0}} \rangle_{\text{CPA}} (\Delta\Phi_{\underline{0}, \underline{0}} - \Sigma_{\underline{0}, \underline{0}}))^{-1} \langle G_{\underline{0}, \underline{0}} \rangle_{\text{CPA}}.$$

To compare our CPA calculation, where we neglect the lateral interaction between adatoms, with the model involving small but nonzero adatom-adatom interactions, we calculate also the LFDF's of a crystal with an adsorbed monolayer with the following non-diagonal interadsorbate force constant matrices:

$$F_{\underline{k}, \underline{k} \pm \underline{i}} = - \begin{pmatrix} a'' & 0 & 0 \\ 0 & \beta'' & 0 \\ 0 & 0 & \beta'' \end{pmatrix} \quad F_{\underline{k}, \underline{k} \pm \underline{j}} = - \begin{pmatrix} \beta'' & 0 & 0 \\ 0 & a'' & 0 \\ 0 & 0 & \beta'' \end{pmatrix}. \quad (8)$$

3. THE GREEN FUNCTION OF A CRYSTAL WITH PLANAR DEFECTS

The force constant matrix of a simple cubic crystal with the nearest neighbour interaction and both with isotopic and force constant planar defects may be written down in the form of the following table

$$\underline{D} \equiv \begin{bmatrix}
 \dots & \dots & \dots & \dots & \dots & \dots \\
 \dots & \underline{M}_{-2} \omega^2 - \underline{F}_{-2,-2} & \underline{F}_{-2,-1} & 0 & 0 & 0 \dots \\
 & \underline{F}_{-1,-2} & \underline{M}_{-1} \omega^2 - \underline{F}_{-1,-1} & \underline{F}_{-1,0} & 0 & 0 \\
 0 & 0 & \underline{F}_{0,-1} & \underline{M}_0 \omega^2 - \underline{F}_{0,0} & \underline{F}_{0,1} & 0 \\
 0 & 0 & 0 & \underline{F}_{1,0} & \underline{M}_1 \omega^2 - \underline{F}_{1,1} & \underline{F}_{1,2} \\
 \dots & 0 & 0 & 0 & \underline{F}_{1,0} & \underline{M}_1 \omega^2 - \underline{F}_{1,2} \dots \\
 \dots & \dots & \dots & \dots & \dots & \dots
 \end{bmatrix} \quad (9)$$

where the indices refer to the respective planes.

This quasideagonal form enables us to calculate easily the diagonal part of the Green function $\underline{G} = \underline{D}^{-1}$ for an arbitrary plane of the crystal:

$$\begin{aligned}
 \underline{G}_{0,0} &= (\underline{M}_0 \omega^2 - \underline{F}_{0,0} - \underline{F}_{0,-1} \underline{Z}_{-1,-1} \underline{F}_{-1,0} - \underline{F}_{0,1} \underline{Z}_{1,1} \underline{F}_{1,0})^{-1}, \\
 \underline{Z}_{-1,-1} &= (\underline{M}_{-1} \omega^2 - \underline{F}_{-1,-1} - \underline{F}_{-1,-2} \underline{Z}_{-2,-2} \underline{F}_{-2,-1})^{-1}, \\
 \underline{Z}_{1,1} &= (\underline{M}_1 \omega^2 - \underline{F}_{1,1} - \underline{F}_{1,2} \underline{Z}_{2,2} \underline{F}_{2,1})^{-1},
 \end{aligned} \quad (10)$$

etc.

For the defects confined to a finite number of planes, this infinite system of equations can be truncated, as the matrices for the ideal planes are all identical.

Only two equations of (10) suffice for evaluation of the diagonal part of the Green function of an ideal crystal

$$\begin{aligned}
 \underline{G}_{0,0} &= (\underline{M}_0 \omega^2 - \underline{F}_{0,0} - 2\underline{F}_{0,-1} \underline{Z}_{-1} \underline{F}_{-1,0})^{-1}, \\
 \underline{Z}_{-1} &= (\underline{M}_0 \omega^2 - \underline{F}_{0,0} - \underline{F}_{0,-1} \underline{Z}_{-1} \underline{F}_{-1,0})^{-1},
 \end{aligned} \quad (11)$$

as

$$\underline{F}_{0,0} = \underline{F}_{-1,-1}, \quad \underline{F}_{0,-1} = \underline{F}_{-1,-2}, \quad \underline{M}_n = \underline{M}_0, \quad \text{etc.}$$

To calculate the Green function of a crystal bounded by the plane "0" with a layer of adsorbed atoms (the plane "1"), we

put

$F_{2,1} = F_{1,2} = 0$, $M_1 = M^T$, $M_n = M_0 I$ for $n \leq 0$
 $F_{0,0}$, $F_{0,-1}$, $F_{0,1} = F_{1,0}$ and $F_{1,1}$ are defined by the expressions (1) and (8), respectively. (The indices which appear repeatedly will be denoted further by one index, e.g., $F_{0,0} = F_0$). In this case the infinite system of equations (10) is reduced to five equations

$$\begin{aligned} G_1 &= (M' \omega^2 - F_1 - F_{1,0} Z_0 F_{0,1})^{-1}, \\ G_0 &= (M_0 \omega^2 - F_0 - F_{0,-1} Z_{-1} F_{-1,0} - F_{0,1} Z_1 F_{1,0})^{-1}, \\ Z_0 &= (M_0 \omega^2 - F_0 - F_{0,-1} Z_{-1} F_{-1,0})^{-1}, \\ Z_{-1} &= (M_0 \omega^2 - F_{-1} - F_{0,-1} Z_{-1} F_{-1,0})^{-1}, \\ Z_1 &= (M' \omega^2 - F_1)^{-1}. \end{aligned} \quad (12)$$

Because all the planes are translationally symmetric, it is advantageous to perform the calculations for Fourier transforms of Eqs. (12). The resulting equations are equations for c -numbers only:

$$\begin{aligned} Z_{-1}^{\kappa\kappa}(\phi_1, \phi_2) &= (M_0 \omega^2 - F_{-1}^{\kappa\kappa}(\phi_1, \phi_2) - Z_{-1}^{\kappa\kappa}(\phi_1, \phi_2) (\gamma^\kappa)^2)^{-1}, \\ \phi_1 &= k_{\parallel 1} a_1, \quad \phi_2 = k_{\parallel 2} a_2, \quad \gamma^{1,2} = \beta, \quad \gamma^3 = \alpha. \end{aligned}$$

These equations yield

$$Z_{-1}^{\kappa\kappa}(\phi_1, \phi_2) = \frac{M_0 \omega^2 - F_{-1}^{\kappa\kappa}(\phi_1, \phi_2) \pm \sqrt{(M_0 \omega^2 - F_{-1}^{\kappa\kappa}(\phi_1, \phi_2))^2 - 4(\gamma^\kappa)^2}}{2(\gamma^\kappa)^2} \quad (13)$$

The sign in (13) should be chosen so that the Green function of the ideal crystal (11) on the real axis would have a negative imaginary part.

$$\lim_{\epsilon \rightarrow 0_+} \text{Im} G_0(\phi_1, \phi_2; \omega^2 + i\epsilon) \leq 0.$$

In the area where the Green function is real, it is to be an analytic contribution from the area with nonzero imaginary part.

Substituting (13) into the Fourier transform of (11) we get

$$G_0^{KK}(\phi_1, \phi_2; \omega^2 + i\epsilon) = \mp [(M_0(\omega^2 + i\epsilon) - F_{-1}^{KK}(\phi_1, \phi_2))^2 - 4(\gamma^K)^2]^{-1}.$$

Denoting $M_0\omega^2 - F_{-1}^{KK}(\phi_1, \phi_2) \equiv \zeta^K$ we can write

$$G_0^{KK}(\phi_1, \phi_2; \omega^2 + i\epsilon) = \mp [(\zeta^K)^2 - 4(\gamma^K)^2 + 2M_0\zeta^K i\epsilon]^{-1}.$$

The aforementioned requirements for the sign in (13) are fulfilled when

$$2(\gamma^K)^2 Z_{-1}^{KK}(\phi_1, \phi_2) = \begin{cases} \zeta^K - \sqrt{(\zeta^K)^2 - 1} & \zeta^K > 2\gamma^K, \\ \zeta^K - i\sqrt{1 - (\zeta^K)^2} & |\zeta^K| < 2\gamma^K, \\ \zeta^K + \sqrt{(\zeta^K)^2 - 1} & \zeta^K < -2\gamma^K. \end{cases} \quad (14)$$

Knowing $Z_{-1}^{KK}(\phi_1, \phi_2)$ we can easily calculate the Fourier transforms of all the quantities in Eqs. (12)

$$Z_0^{KK}(\phi_1, \phi_2) = [M_0\omega^2 - F_0^{KK}(\phi_1, \phi_2) - Z_{-1}^{KK}(\phi_1, \phi_2)(\gamma^K)^2]^{-1},$$

$$Z_1^{KK}(\phi_1, \phi_2) = [M_1\omega^2 - F_1^{KK}(\phi_1, \phi_2)]^{-1},$$

$$G_1^{KK}(\phi_1, \phi_2) = [M_1\omega^2 - F_1^{KK}(\phi_1, \phi_2) - Z_0^{KK}(\phi_1, \phi_2)(\gamma^K)^2]^{-1}, \quad (15)$$

$$G_0^{KK}(\phi_1, \phi_2) = [M_0\omega^2 - F_0^{KK}(\phi_1, \phi_2) - Z_1^{KK}(\phi_1, \phi_2)(\gamma^K)^2 - Z_{-1}^{KK}(\phi_1, \phi_2)(\gamma^K)^2]^{-1},$$

where

$$\gamma'^{1,2} = \beta', \quad \gamma'^3 = \alpha',$$

$$F_{-1}^{11}(\phi_1, \phi_2) = 2\alpha(1 - \cos\phi_1) + 2\beta(1 - \cos\phi_2) + 2\beta,$$

$$F_{-1}^{33}(\phi_1, \phi_2) = 2\beta(1 - \cos\phi_1) + 2\beta(1 - \cos\phi_2) + 2\alpha,$$

$$F_0^{KK}(\phi_1, \phi_2) = F_{-1}^{KK}(\phi_1, \phi_2) + \gamma'^K - \gamma^K,$$

$$F_1^{11}(\phi_1, \phi_2) = 2\alpha''(1 - \cos\phi_1) + 2\beta'(1 - \cos\phi_2) + \beta',$$

$$F_1^{33}(\phi_1, \phi_2) = 2\beta''(1 - \cos\phi_1) + 2\beta''(1 - \cos\phi_2) + \alpha'.$$

To calculate LFDF's, the diagonal elements of the Green functions should be obtained from Eqs.(15) by double integration of the Fourier transforms

$$G_{0,0}^{KK}(\omega^2 + i\epsilon) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} G_0^{KK}(\phi_1, \phi_2; \omega^2 + i\epsilon) d\phi_1 d\phi_2,$$

$$G_{\underline{k}, \underline{k}}^{KK}(\omega^2 + i\epsilon) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} G^{KK}(\phi_1, \phi_2; \omega^2 + i\epsilon) d\phi_1 d\phi_2.$$

In the case when $\alpha/\beta = \alpha''/\beta''$ the double integrals can be reduced to the one-dimensional ones.

Similarly, the diagonal elements of $\langle G \rangle_{CPA}$ may be calculated by substituting in Eqs.(9-15) $\underline{\Phi}$ instead of \underline{F} and $\underline{M}_0 - \underline{\Sigma}/\omega^2$ instead of \underline{M}_0 .

REFERENCES

1. White J.W. In: Dynamics of Solids and Liquids by Neutron Scattering, ed. by S.W.Lovesey, T.Springer. Springer-Verlag, Berlin, 1977.
2. Stockmeyer R. et al. Ber. Bunsenges. Phys.Chem, 1980, 84, p.79.
3. Alldredge G.P., Allen R.E., de Wetter F.W. Phys.Rev., 1971, B4, p.1682.
4. Surda A. Czech.J.Phys., 1979, B29, p.668.
5. Karasova I., Surda A. In: Proc. of the Vth Conf. of Czech. Phys., Kosice, 1977.
6. Ludwig W., Lengeler B. Solid State Comm., 1964, 2, p.83.
7. Schmidt L.D. In: Interactions on Metal Surfaces, ed. R.Gomer, Springer-Verlag, Berlin, 1975.

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