

**DYNAMICS AND ADIABATIC POTENTIAL OF IMPURITY DEFECTS IN NEAR-SURFACE
LAYER OF AB_2 -TYPE STRUCTURES
PART II. INTERACTION OF IMPURITY DEFECTS IN BOUNDARY LAYER WITH SURFACE MODES
OF LATTICE VIBRATION**

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1. Introduction

One of the chief methods of investigating the dynamic properties of crystals are the spectroscopic measurements of impurified crystals. The point is to make use of the polaron effect, that is the relationship between the mechanical properties of the crystal vicinity of the impurity and its electron state. What offers here special experimental possibilities is the optical analogue of the Mossbauer's effect, i.e. the occurrence of a sharp line in the absorption spectrum, that corresponds to the phononless transition; both the frequency and the intensity, corresponding to this line, depend directly upon the parameter that characterizes the interaction of the impurity valence-electrons with the crystal lattice. Measurements of this parameter within various ranges of temperature permit, through the use of dispersion relationships for the frequency, the basis dynamic parameters of a crystal to be determined as well as the changes in the state of equilibrium of the atoms adjacent to the impurity—that is a static deformation-of the crystal in the vicinity of the impurity [5].

The aim of the present work is to construct a semiphenomenological model of interactions of the impurities of both the surface and the boundary layer, with the surface modes of lattice vibration, the model being based on the adiabatic approximation. This model will be employed for determining the dependence of the interaction energy of the above mentioned impurities with the lattice, upon the dynamic parameters of the surface modes. An effort will be made, using the CaF_2 type structure as an example, to plot the curves in the plane k (in the, vicinity of a point of the plane Brillouin's zone), these curves corresponding to the extreme values of the interaction energy. This type analysis is of primary importance to the research practice, both in the field of applications of acoustic resonance to, among other things, determining the optimal parameters of phonon amplifiers, and in quantum electronics, under conditions where, in view of the form of the active element (e.g. wafers) as well as the nature of amixturing, the major role is played by the dynamics of both the surface and the boundary layer of the crystal [9].

In the domain of research on the mechanical properties of the point defects of the impurity type, this analysis permits the deformation to be determined of the admixture ambience depending upon

the temperature (by taking account of the statistics of the phonon distribution). The linear term of the energy of interaction, with the single mode generated in the sample, defines the change in the state of equilibrium of vibration of the lattice points. It is in this sense that the actual interaction depends also upon the dynamic parameters of a stimulated disturbance [6,7].

In order to concretize our considerations we will confine ourselves to the case where the electron state of the impurity is nondegenerate, which means that the deformation of the vicinity of the substitutional impurity is fully symmetrical. We shall assume as well that the actual electron/ion interactions are central.

The description of the dynamic aspect of the problem will be based on the results obtained in Ref. [1].

Section 2 of the present paper contains the construction of the above mentioned semiphenomenological model of interactions. The vibrations on the acoustic and the optical branch are dealt with separately. In view of the applications, the case of the long waves is given a particular consideration in the analysis. In each variant the description of the interactions is obtained through a single phenomenological parameter only.

In Sects. 3 and 4 the analysis is presented along with the results of numerical calculations, as well as with the application to an actual structure and to the cutting of the surface.

2. Semi-Phenomenological Description of Interaction

The energy of interaction of the substitutional admixture with any deformation of its crystal environment in the linear and adiabatic approximation, may be written down in the form [6-7]:

$$(2.1) \quad V^L = \sum_{\bar{l}, \kappa, \alpha} V_{\alpha}(\bar{l}, \kappa) [u_{\alpha}(\bar{l}, \kappa) - u_{\alpha}(\bar{L}, 0)],$$

where l —lattice vector of lattice points in a local coordinates system connected with the impurity $l' = L+l$, L —position vector of the unit cell containing the impurity in crystal coordinates-system (for surface lattice-points $L_3=0$), k —numbers atoms (ions) of various sublattices, α —component.

The energy (2.1) is generated by the interaction of the valence electrons of the impurity with the lattice, in the model of point ions [6]:

$$(2.2) \quad V_{\alpha}(\bar{l}, \kappa) = \int \frac{\partial}{\partial u_{\alpha}(\bar{l}, \kappa)} \left[\frac{ee_{\kappa}}{|\bar{r} - \bar{R}_{\bar{l}}^{\kappa}|} \right] |\Psi(\bar{r})|^2 d\bar{r} = ee_{\kappa} \int \frac{[\bar{r}_{\alpha} - \bar{R}_{\alpha}(\bar{l}, \kappa)]}{|\bar{r} - \bar{R}(\bar{l}, \kappa)|^3} |\Psi(\bar{r})|^2 d\bar{r},$$

where

$$|\Psi(\bar{r})|^2$$

being the charge density of valency electron shell, e_{κ} —actual ion charge, $ee_{\kappa}/|\bar{r}-\bar{R}_i|$ defines the potential of electron/ion interaction

In the case where the deformations are stimulated by the surface wave, one obtains for (2.1)

$$(2.3) \quad V^L = \sum_{j, \kappa, \alpha} [v_\alpha(\bar{k}, g_j; \kappa) u_\alpha(\bar{k}, q_j; \kappa) - v_\alpha(0, 0; \kappa) u_\alpha(\bar{k}, q_j; \kappa)] e^{i\bar{k}\bar{L} - q_j L_3},$$

where \bar{k} — disturbance wave-vector, q — decaying decrements, $u(\bar{k}, q_j; \kappa)$ — amplitude of j -th wave component, $\mathbf{l} = (l_1, l_2)$, $\mathbf{L} = (L_1, L_2)$ —vector projections from (2.1) upon the surface plane, while:

$$(2.4) \quad v_\alpha(\bar{k}, q; \kappa) = \sum_{\bar{l}, l_3} V_\alpha(\bar{l}, l_3; \kappa) e^{i\bar{k}\bar{l}^\kappa - q l_3^\kappa}, \quad (\bar{l}^\kappa = \bar{l} + \kappa \bar{k}),$$

In the long-wave region for the waves on the acoustic branch (where $q(\bar{k} \rightarrow 0) \rightarrow 0$), the relationship (2.3) takes the form:

$$(2.5) \quad V^L = \sum_{\bar{l}, l_3, \kappa, \alpha} V_\alpha(\bar{l}, l_3; \kappa) (i\bar{k}\bar{l}^\kappa - q_j l_3^\kappa) u_\alpha(\bar{k}, q_j; \kappa) e^{i\bar{k}\bar{L} - q_j L_3}.$$

It should be noted that in the limit of $\bar{k} \rightarrow 0$, V^L vanishes. For the vibration on the optical branch $q_j(\bar{k} \rightarrow 0) \rightarrow C_j > 0$ and in the long-wave approximation, for the case under consideration below, where the impurity is at the centre of symmetry of the cluster one obtains:

$$(2.6) \quad v_\alpha(\bar{k}, q; \kappa) = i \sum_{\bar{l}, l_3} \bar{k} \cdot \bar{l}^\kappa V_\alpha(\bar{l}, l_3; \kappa) e^{-q l_3^\kappa}.$$

Hence it follows, in particular, that the optical vibration within the boundary $\bar{k} \rightarrow 0$ yields no polaron effect either. In the case where $C_j > 1$ for the impurity of the boundary layer, the main contribution to V^L comes from the lattice-points of the complex, that are in the region between the impurity and the crystal surface, and so, for the face (110) under consideration in [1], this contribution is defined by the geometrical configuration of the lattice points with the symmetry C_{2v} ; the relationship (2.1) becomes:

$$(2.7) \quad V^L = i \sum_{\alpha, j, \kappa, \bar{l}, l_3 > 0} V_\alpha(\bar{l}, l_3; \kappa) \bar{k} \bar{l}^\kappa e^{q_j |l_3^\kappa|} u_\alpha(\bar{k}, q_j; \kappa),$$

while the concrete relationships between the components of the amplitudes follow from the solution (see [1]) to the dynamic problem for the surface modes of the lattice vibration.

On the above assumptions, the relationship (2.3) may be expressed in a more concrete form; one obtains in the presence of:

$$\bar{R}(\bar{l}^\kappa, l_3^\kappa; \kappa) = \bar{l}^\kappa + j l_3^\kappa, \quad (j = (0, 0, 1)),$$

$$\begin{aligned} \sum_{\bar{l}^\kappa} \bar{k} \bar{l}^\kappa V_\alpha(\bar{l}, l_3; \kappa) &= e e_\kappa \int \sum_{\bar{l}^\kappa} \frac{[\bar{r}_\alpha - \bar{R}_\alpha(\bar{l}, l_3; \kappa)] \bar{k} \bar{l}^\kappa}{|\bar{r} - \bar{R}(\bar{l}, l_3; \kappa)|^3} |\Psi(\bar{r})|^2 d\bar{r} \\ &= -e e_\kappa \sum_{\bar{l}^\kappa} R_\alpha^2(\bar{l}, l_3; \kappa) k_\alpha \int \frac{|\Psi(\bar{r})|^2 d\bar{r}}{|\bar{r} - \bar{R}(\bar{l}, l_3; \kappa)|^3}, \end{aligned}$$

consequently:

$$(2.8) \quad V^L = -ee_x \sum_{j, \bar{l}, l_3} [ik_1 R_1^2(\bar{l}, l_3; \kappa) u_1^j(\bar{k}, q_j; \kappa) + ik_2 R_2^2(\bar{l}, l_3; \kappa) u_2^j(\bar{k}, q_j; \kappa) - q_j R_3^2(\bar{l}, l_3; \kappa) u_3^j(\bar{k}, q_j; \kappa)] \int \frac{|\Psi(\bar{r})|^2 d\bar{r}}{|\bar{r} - \bar{R}(\bar{l}, l_3; \kappa)|^3} e^{i\bar{k}\bar{L} - q_j L_3}.$$

By confining ourselves to the first coordination zone ($\mathbf{k} = 1$ denote then the structural equivalents of the ions F^- in CaF_2 [3]), on consideration of the fact that the factor

$$\int \frac{|\Psi(\bar{r})|^2 d\bar{r}}{|\bar{r} - \bar{R}|^3}$$

is the same for the equidistant lattice points, in the case of the complex in question we ultimately obtain:

$$(2.9) \quad V^L = \varphi_a e^{i\bar{k}\bar{L}} \sum_j [ik_1 u_1^j(\bar{k}, q_j; 1) + ik_2 u_2^j(\bar{k}, q_j; 1) - q_j u_3^j(\bar{k}, q_j; 1)] e^{-q_j L_3},$$

where the notation is used:

$$\varphi_a = -\frac{ee_x a^2}{2} \int \frac{|\Psi(\bar{r})|^2 d\bar{r}}{|\bar{r} - \bar{R}|^3}$$

The coefficient \mathbf{f}_a may be regarded as the phenomenological parameter, while φ_a in (2.9) depends solely upon the parameters of the surface wave.

V^L is a scalar in the group of the cluster (of its symmetry), consequently the above relationships may be expressed by symmetrized coordinates that are transformed according to the irreducible representations of this group. This permits the analysis to be simplified, in the contribution to V^L comes only from the representation \mathbf{G} that satisfy the condition $\mathbf{G} [\mathbf{G}^2]_g$ where \mathbf{G} is the representation of the electron state (basic or excited) of the impurity.

In particular, when the electron level of the impurity is not degenerated, the contribution to V^L is given only by the full-symmetry representations A_1 [6], so that one obtains

$$(2.10) \quad V^L = P_{A_1} \sum_{\alpha} V_{\alpha}(\bar{l}, l_3; \kappa) u_{\alpha}(\bar{l}, l_3; \kappa) = V_{A_1} Q_{A_1}$$

The concrete forms of (2.10) are presented below.

3. Application of the Model to the CaF_2 - Type Structure. Results of Numerical Calculations

The numerical calculations for V^L have been performed for the immediate vicinity of the point $\mathbf{k} = 0$ (in a square (0.05; .005)). The equations from Ref. [1] lead (with the notation adopted therein) to the following relationships between the amplitude ratios:

$$(3.1) \quad \frac{u_j^1(0)}{w_j^1(0)} \equiv \tilde{u}_j^1; \quad \frac{v_j^1(0)}{w_j^1(0)} \equiv \tilde{v}_j^1; \quad g = \left[2 \left(1 - \frac{m_2 \omega^2}{4\alpha} \right) \right]^{-1},$$

$$\frac{u_j^2(0)}{w_j^2(0)} \equiv \tilde{u}_j^2 = g [\tilde{u}_j^1 (e^{-ik_1/4} \cos k_2 \sqrt{2}/4 + e^{ik_1/4} \text{ch } q_j \sqrt{2}/4) - i \sqrt{2} \tilde{v}_j^1 e^{-ik_1/4} \sin k_2 \sqrt{2}/4 - \sqrt{2} e^{ik_1/4} \text{sh } q_j \sqrt{2}/4],$$

$$\begin{aligned}
 (3.1) \quad \frac{v_j^2(0)}{w_j^1(0)} &\equiv \tilde{v}_j^2 = g[-i\sqrt{2} \tilde{u}_j^1 e^{-ik_1/4} \sin k_2 \sqrt{2}/4 + 2\tilde{v}_j^1 e^{-ik_1/4} \cos k_2 \sqrt{2}/4], \\
 \frac{w_j^2(0)}{w_j^1(0)} &\equiv \tilde{w}_j^2 = g[-\sqrt{2} \tilde{u}_j^1 e^{ik_1/4} \operatorname{sh} q_j \sqrt{2}/4 + 2e^{ik_1/4} \operatorname{ch} q_j \sqrt{2}/4], \\
 \frac{u_j^3(0)}{w_j^1(0)} &\equiv \tilde{u}_j^3 = g[\tilde{u}_j^1 (e^{ik_1/4} \cos k_2 \sqrt{2}/4 + e^{-ik_1/4} \operatorname{ch} q_j \sqrt{2}/4) \\
 &\quad + i\sqrt{2} \tilde{v}_j^1 e^{ik_1/4} \sin k_2 \sqrt{2}/4 + \sqrt{2} e^{-ik_1/4} \operatorname{sh} q_j \sqrt{2}/4], \\
 \frac{w_j^3(0)}{w_j^1(0)} &\equiv \tilde{w}_j^3 = g[i\sqrt{2} \tilde{u}_j^1 e^{ik_1/4} \sin k_2 \sqrt{2}/4 + 2\tilde{v}_j^1 e^{ik_1/4} \cos k_2 \sqrt{2}/4], \\
 \frac{v_j^3(0)}{w_j^1(0)} &\equiv \tilde{v}_j^3 = g[\sqrt{2} \tilde{u}_j^1 e^{ik_1/4} \operatorname{sh} q_j \sqrt{2}/4 + 2e^{-ik_1/4} \operatorname{ch} q_j \sqrt{2}/4], \\
 \bar{k} &= (k_1, k_2); \quad i = \sqrt{-1},
 \end{aligned}$$

The symmetrization is performed in the point group C_{2v} (corresponding to the operations parallel to the crystal surface). By calculating the characters for the respective transformation classes on the strength of the relationship:

$$\chi(R) = n_g(\pm 1 + 2\cos\varphi),$$

where n_g — number of lattice points that do *not* change their position during the group operations (\mathbf{f} — angle of rotation, corresponding to the operation R , and making use of the relationship $(R) = n_{\mathbf{G}} \Gamma(R)$ as well as of the character tables of the irreducible representations of the group C_{2v} , one obtains the following distribution of the reducible representation D defined by the plane configuration of the lattice points (i.e. in the plane of the impurity):

$$(3.2) \quad D = 4A_1 + 3A_2 + 4B_1 + 4B_2,$$

The symmetrized functions of the displacements of atoms in this configuration, these functions being transformed according to the irreducible representation \mathbf{G} are determined from the general dependence:

$$(3.3) \quad Q(\Gamma^s) = N \cdot \sum_R [\Gamma(R)]_{ii}^* R u^s,$$

where s is numbers the various functions corresponding to the same representation, N — normalizing coefficient determined from the condition of transformation unitarity. Writing down (3.3) in the form

$$(3.4) \quad Q_m(\Gamma^s) \equiv Q^\sigma(\Gamma) = \sum_{\alpha, \bar{l}} S(\Gamma, \sigma, \alpha, \bar{l}) u_\alpha(\bar{l}); \quad (\bar{Q} = \hat{S} \cdot \bar{u}),$$

one obtains in the case under consideration

$$\hat{S} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ d & 0 & 0 & 0 & d & 0 & 0 & d & 0 & 0 & 0 & d & 0 \\ 0 & d & 0 & 0 & 0 & d & 0 & 0 & d & 0 & 0 & 0 & d \\ 0 & 0 & d & 0 & 0 & 0 & d & 0 & 0 & 0 & d & 0 & 0 \\ d & 0 & 0 & 0 & -d & 0 & 0 & -d & 0 & 0 & 0 & d & 0 \\ 0 & -d & 0 & 0 & 0 & d & 0 & 0 & d & 0 & 0 & 0 & -d \\ 0 & 0 & d & 0 & 0 & 0 & -d & 0 & 0 & 0 & -d & 0 & 0 \\ -d & 0 & 0 & 0 & -d & 0 & 0 & d & 0 & 0 & 0 & d & 0 \\ 0 & -d & 0 & 0 & 0 & -d & 0 & 0 & d & 0 & 0 & 0 & d \\ 0 & 0 & d & 0 & 0 & 0 & d & 0 & 0 & 0 & -d & 0 & 0 \\ -d & 0 & 0 & 0 & d & 0 & 0 & -d & 0 & 0 & 0 & d & 0 \\ 0 & d & 0 & 0 & 0 & -d & 0 & 0 & d & 0 & 0 & 0 & -d \\ 0 & 0 & d & 0 & 0 & 0 & -d & 0 & 0 & 0 & 0 & d & 0 \\ 0 & 0 & d & 0 & 0 & 0 & -d & 0 & 0 & 0 & d & 0 & 0 \end{bmatrix}, \quad d = 1/2.$$

The relationship (3.4), for full-symmetry deformations defined by the surface mode of vibrations [1]:

$$(3.6) \quad u_{\alpha}^i(\bar{l}) = \sum_{j=1}^4 u_{\alpha\sigma}^j \exp[ik\bar{l} - q_j l^3],$$

after a number of transformations, takes ultimately the form:

$$(3.7) \quad \begin{aligned} Q^{(1)}(A_1) &= 2d \cos k_2 \sqrt{2} / 4w_4^1 \sum_{j=1}^4 [(\bar{u}_j^2 e^{ik_1/4} - \bar{u}_j^3 e^{-ik_1/4}) w_j], \\ Q^{(2)}(A_1) &= 2id \sin k_2 \sqrt{2} / 4w_4^1 \sum_{j=1}^4 [(\bar{v}_j^2 e^{ik_1/4} + \bar{v}_j^3 e^{-ik_1/4}) w_j], \\ Q^{(3)}(A_1) &= 2d \cos k_2 \sqrt{2} / 4w_4^1 \sum_{j=1}^4 [(\bar{w}_j^2 e^{ik_1/4} + \bar{w}_j^3 e^{-ik_1/4}) w_j], \\ Q^{(4)}(A_1) &= w_4^1 \sum_{j=1}^4 w_j. \end{aligned}$$

For the configuration of the lattice points of the first coordination zone, one obtains from the subsequent lattice plane, respectively:

$$(3.8) \quad \begin{aligned} Q^{(1)}(A_1) &= d_1 w_4^1 \sum_{j=1}^4 \{[\exp(-q_j \sqrt{2} / 4) (\bar{u}_j^2 e^{ik_1/4} - \bar{u}_j^3 e^{-ik_1/4})] w_j\}, \\ Q^{(2)}(A_1) &= d_1 w_4^1 \sum_{j=1}^4 \{[\exp(-q_j \sqrt{2} / 4) (\bar{v}_j^2 e^{ik_1/4} + \bar{v}_j^3 e^{-ik_1/4})] w_j\}, \\ Q^{(3)}(A_1) &= d_1 w_4^1 \sum_{j=1}^4 \{[\exp(-q_j \sqrt{2} / 4) (\bar{w}_j^2 e^{ik_1/4} + \bar{w}_j^3 e^{-ik_1/4})] w_j\}, \\ d_1 &= 2^{-1/2}. \end{aligned}$$

On the basis of Sect. 2, we have for $V_{A_1}^S$:

$$(3.9) \quad V_{A_1}^\sigma = \sum_{\alpha, \bar{l}^\alpha} V_\alpha(\bar{l}^\alpha) \frac{\partial u_\alpha(\bar{l}^\alpha)}{\partial u_{A_1}^\sigma} = -\varphi_a^1 \sum_{\alpha} R_\alpha(\bar{l}^\alpha, l_3) \left(\frac{\partial u_{A_1}^\sigma}{\partial u_\alpha(\bar{l}^\alpha)} \right)^{-1},$$

where:

$$\varphi_a^1 = ee_x \int \frac{|Y_a(\bar{r})|^2 d\bar{r}}{|\bar{r} - \bar{R}(\bar{l}^\alpha, l_3)|^3},$$

and finally

$$(3.10) \quad \begin{aligned} V_{A_1}^{(1)} &= -a\varphi_a^1, & V_{A_1}^{(2)} &= -a\sqrt{2}\varphi_a^1, & V_{A_1}^{(3)} &= 0, \\ V_{A_1}'^{(1)} &= -\frac{a}{2}\varphi_a^1; & V_{A_1}'^{(2)} &= 0, & V_{A_1}'^{(3)} &= -\frac{a\sqrt{2}}{2}\varphi_a^1, \end{aligned}$$

By putting (3.7) - (3.8) and (3.10) into the expression (2.10) one obtains, after simple transformations, the interaction energy for the surface impurity:

$$(3.11) \quad \begin{aligned} V^L &= F_a \sum_{j=1}^4 \left\{ \left[\tilde{u}_j^2 \left(e^{ik_1/4} \cos k_2 \sqrt{2}/4 - \frac{1}{4} e^{-ik_1/4 - q_j \sqrt{2}/4} \right) + \right. \right. \\ &+ \tilde{u}_j^3 \left(\frac{1}{4} e^{ik_1/4} e^{-q_j \sqrt{2}/4} - e^{ik_1/4} \cos k_2 \sqrt{2}/4 \right) + (\tilde{v}_j^2 e^{ik_1/4} + \tilde{v}_j^3 e^{-ik_1/4}) i \sqrt{2} \sin k_2 \sqrt{2}/4 + \\ &\left. \left. + (\tilde{w}_j^3 e^{ik_1/4} + \tilde{w}_j^2 e^{-ik_1/4}) \frac{\sqrt{2}}{4} e^{-q_j \sqrt{2}/4} \right] w_j \right\}, \end{aligned}$$

where: $F_a = -2a\varphi_a^1 w_4^1$,

The above expression concerns the case where the substitutional impurity is in the plane of the geometrical surface (point 0 Fig. 2). Whereas in the situation where the above impurity takes the position corresponding to the point 7, that is when it is positioned in

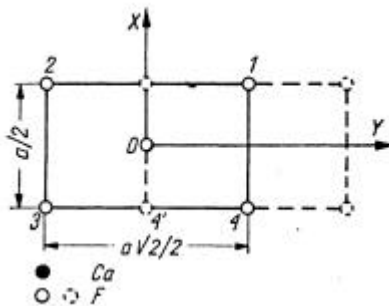


FIG. 1. Configuration of the environment of the surface impurity at (110) face.

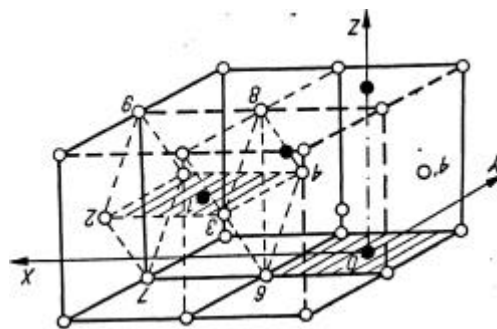


FIG. 2. Spatial ion-arrangement in the impurity's environment.

the subsequent lattice plane, the effect is to be additionally taken into account of the surface lattice-points 6 and 7 in Fig. 2, as well as an appropriate change in the amplitudes of the vibration mode. Proceeding as above one obtains then:

$$\begin{aligned}
Q^{(1)}(A_1) &= 2dw_4^1 \cos k_2 \sqrt{2}/4 \cdot \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \\
&\quad \times \sum_{j=1}^4 [e^{-q_j \sqrt{2}/4} (\tilde{u}_j^2 e^{ik_1/4} - \tilde{u}_j^3 e^{-ik_1/4}) w_j], \\
(3.12) \quad Q^{(2)}(A_1) &= 2diw_4^1 \sin k_2 \sqrt{2}/4 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \\
&\quad \times \sum_{j=1}^4 [e^{-q_j \sqrt{2}/4} (\tilde{v}_j^2 e^{ik_1/4} + \tilde{v}_j^3 e^{-ik_1/4}) w_j], \\
Q^{(3)}(A_1) &= 2dw_4^1 \cos k_2 \sqrt{2}/4 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \\
&\quad \times \sum_{j=1}^4 [e^{-q_j \sqrt{2}/4} (\tilde{w}_j^2 e^{ik_1/4} + \tilde{w}_j^3 e^{-ik_1/4}) w_j], \\
Q^{(4)}(A_1) &= w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 (e^{-q_j \sqrt{2}/4} w_j); \\
Q'^{(1)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [e^{-q_j \sqrt{2}/2} (\tilde{u}_j^3 e^{ik_1/4} - \tilde{u}_j^2 e^{-ik_1/4}) w_j], \\
(3.13) \quad Q'^{(2)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [e^{-q_j \sqrt{2}/2} (\tilde{v}_j^3 e^{ik_1/4} + \tilde{v}_j^2 e^{-ik_1/4}) w_j], \\
Q'^{(3)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [e^{-q_j \sqrt{2}/2} (\tilde{w}_j^3 e^{ik_1/4} + \tilde{w}_j^2 e^{-ik_1/4}) w_j]; \\
Q''^{(1)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [(\tilde{u}_j^3 e^{ik_1/4} - \tilde{u}_j^2 e^{-ik_1/4}) w_j], \\
(3.14) \quad Q''^{(2)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [(\tilde{v}_j^3 e^{ik_1/4} + \tilde{v}_j^2 e^{-ik_1/4}) w_j], \\
Q''^{(3)}(A_1) &= d_1 w_4^1 \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 [(\tilde{w}_j^3 e^{ik_1/4} + \tilde{w}_j^2 e^{-ik_1/4}) w_j];
\end{aligned}$$

where $Q(\mathbf{G})$ —coordinates symmetrized from the configuration of atoms in the plane of surface, $Q'(\mathbf{G})$ —from the configuration (8,9), $Q''(\mathbf{G})$ —from the configuration (6,7).

Appropriate magnitudes of V_G and V'_G are identical to those presented in (3.9), while $V''_\Gamma = V'_\Gamma$. Finally, instead of (3.11) one obtains here:

$$(3.15) \quad V_L \equiv V^L = F_a \exp [i(k_1/2 - k_2 \sqrt{2}/4)] \sum_{j=1}^4 \left\{ \tilde{u}_j^2 \left(e^{ik_1/4 - q_j \sqrt{2}/4} \cos k_2 \sqrt{2}/4 \right. \right.$$

(3.15) [cont.]

$$\begin{aligned}
 & -\frac{1}{4} e^{-ik_1/4 - q_j \sqrt{2}/4} \Big) + \tilde{u}_j^3 \left(\frac{1}{4} e^{ik_1/4 - q_j \sqrt{2}/4} - e^{-ik_1/4 - q_j \sqrt{2}/4} \cos k_2 \sqrt{2}/4 \right. \\
 & \left. - \frac{1}{4} \tilde{u}_j^2 e^{-ik_1/4} + \frac{1}{4} \tilde{u}_j^3 e^{ik_1/4} + (\tilde{v}_j^2 e^{ik_1/4} + \tilde{v}_j^3 e^{-ik_1/4}) i \sqrt{2} \sin k_2 \sqrt{2}/4 \right. \\
 & \left. + (\tilde{w}_j^3 e^{ik_1/4} + \tilde{w}_j^2 e^{-ik_1/4}) \frac{\sqrt{2}}{4} e^{-q_j \sqrt{2}/4} - (\tilde{w}_j^3 e^{ik_1/4} + \tilde{w}_j^2 e^{-ik_1/4}) \frac{\sqrt{2}}{4} \right] w_j \Big\}.
 \end{aligned}$$

4. Results of Numerical Calculations. Conclusions

The results, presented below, of calculations based on dependences (3.11)-(3.15), concern the optical branch of the surface mode in the interval (0 - 0.05) k_1 and k_2 since the acoustic branch yields in this region k no perceptible changes in V^L .

Figures 1 and 2 illustrate the appropriate configurations of the ambience of the surface impurity at (110) face, the displacement of this impurity in the subsequent lattice plane being marked, and the spatial arrangement of ions of the impurity's environment for both cases under consideration.

Figures 3 and 4 represent the sections of the surface $v_L(k_1, k_2)$ for a few planes $k_2 = \text{const.}$ while Figs. 5 and 6—the values of v_L in function of k_2 , calculated for the optimal k_1 .

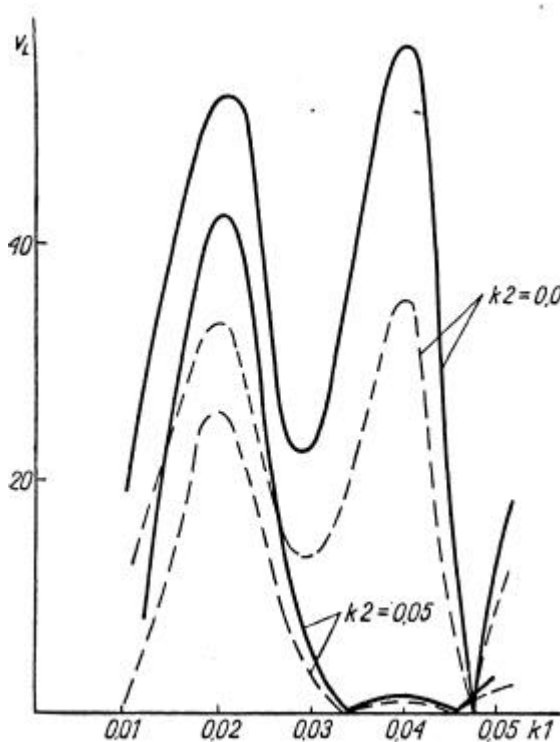


FIG. 3. The section of the surface $v_L(k_1, k_2)$ for $k_2 = \text{const.}$ Solid curves—impurity on geometrical surface, pecked curves—impurity in the near-surface layer.

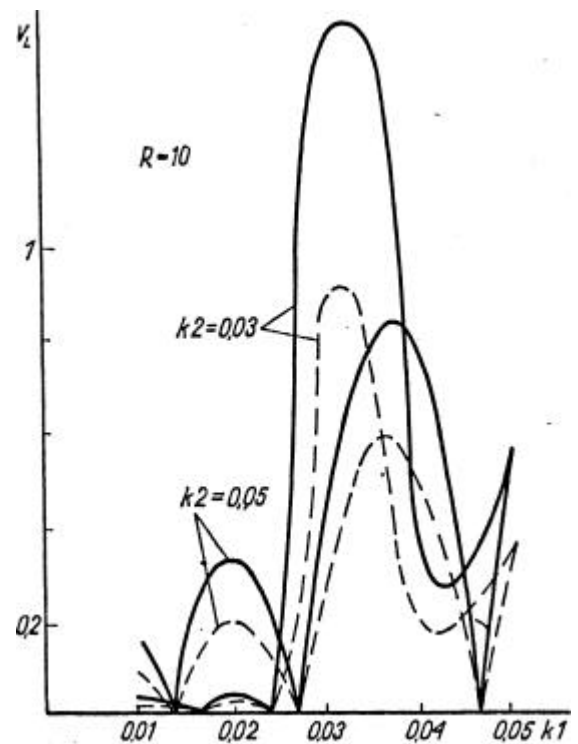


FIG. 4. The section of $v_M(k_1, k_2)$ surface for $k_2 = 0.03; 0.05$ and $R = 10$.

The curves $k_2(k_1)$ in Figs. 7-11, define the vectors k that correspond to the maximum values of v_L (the solid line denotes the main maximum, while the pecked lines—the local minima and maxima).

The calculation results presented lead to the following general conclusions:

1. There are curves in the plane k , for which v_L assumes extreme values.
2. The values of v_L for the antifluorite structure are appreciably higher then the corresponding values for the fluorite structure.

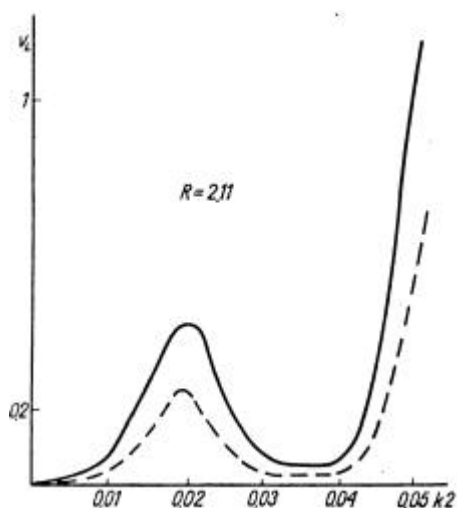


FIG. 5. v_L value in function of k_2 for the optimal k_1 ; $R=2.11$

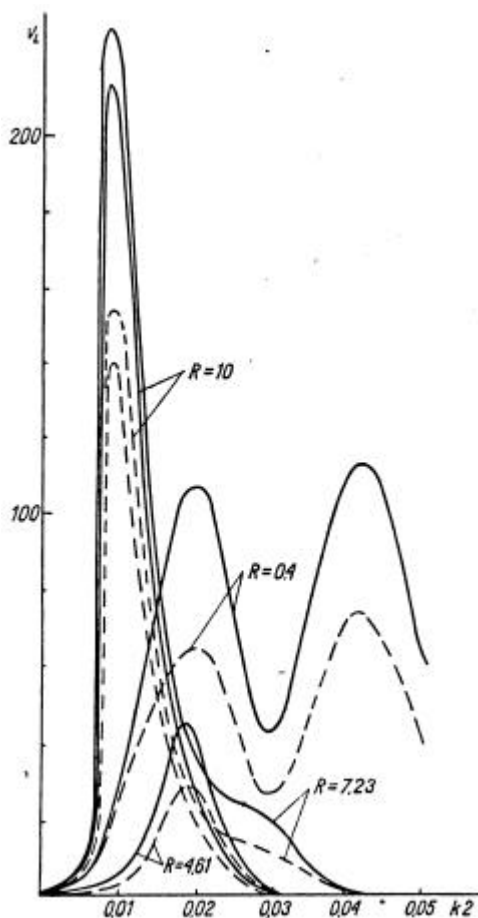


FIG. 6. v_L value in function of k_2 for the optimal k_1 ; $R=4.61$; 7.23 ; 10 ; 0.4 .

3. In the explored region k there are two local maxima of the same order of magnitude for the antifluorite structure, while for the fluorite structure one of the local maxima clearly exceeds the other ones.

4. The v_L values that are maximum in the near-surface layer correspond to the impurities that are placed on the geometrical surface. We have demonstrated that:

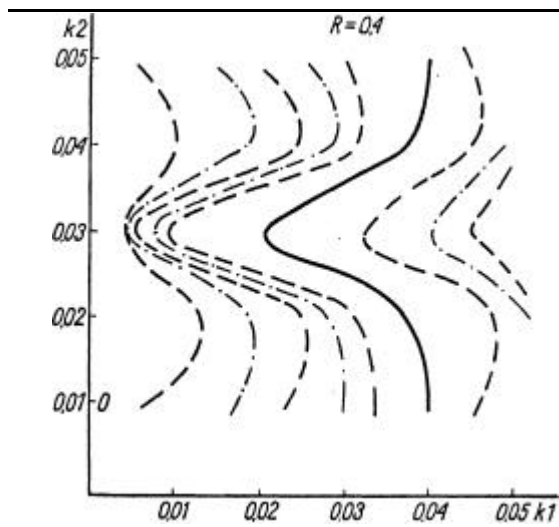


FIG. 7. Curves in the plane k , corresponding to the extreme values of the interaction energy for $R = 0.4$.

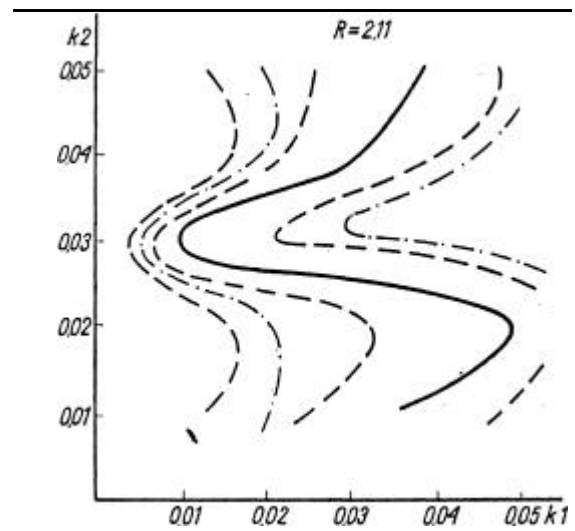


FIG. 8. Curves in the plane k , corresponding to the extreme values of the interaction energy for $R = 2.11$.

- a) There is the possibility of controlling the effect of acoustic resonance in order to obtain the maximum coupling between the surface mode and the electrons of the impurity.
- b) The most intensive interaction with the surface modes of the lattice vibration is that of the impurities on the very surface (also within the first periodicity-layer).
- c) In the case of the surface under analysis the coupling is the greatest for the anti-fluorite structure.

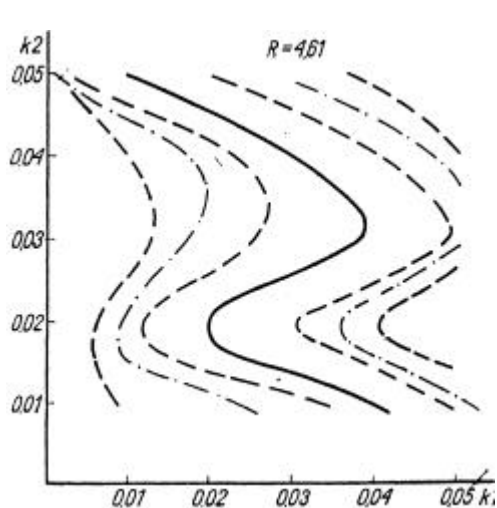


FIG. 9. Curves in the plane k , corresponding to the extreme values of the interaction energy $R = 4.6$.

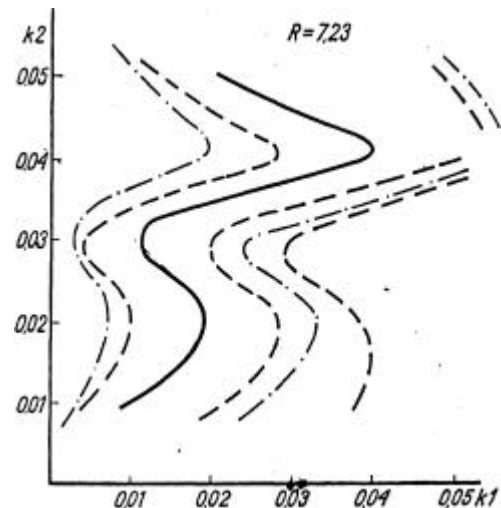


FIG. 10. Curves in the plane k , corresponding to the extreme values of the interaction energy $R = 7.23$.

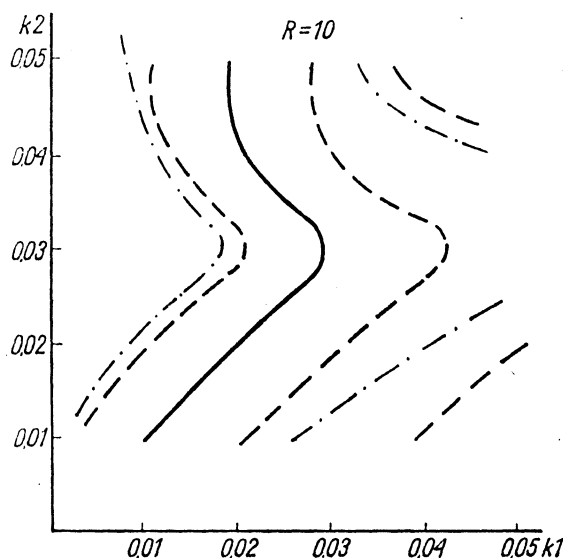


FIG. 11. Curves in the plane k , corresponding to the extreme values of the interaction energy for $R = 10$.

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Streszczenie

DYNAMIKA I POTENCJAŁ ADIABATYCZNY DEFEKTÓW DOMIESZKOWYCH W WARSTWIE PRZYPOWIERZCHNIOWEJ STRUKTUR TYPU AB_2

CZ. II ODDZIAŁYWANIE DEFEKTÓW DOMIESZKOWYCH W WARSTWIE BRZEGOWEJ Z POWIERZCHNIOWYMI MODAMI DRGAŃ SIECI

Praca zawiera analizę wpływu powierzchniowych modów drgań sieci na mechaniczne własności domieszek substytucyjnych warstwy brzegowej. Jej przedmiotem jest konstrukcja modelu półfenomenologicznego, opisującego zależność liniowego cząstka energii oddziaływania od wektora falowego drgań.

Obliczenia numeryczne wykonane dla kryształów o strukturze fluorytu o powierzchni (110) wykazują rezonansowy charakter oddziaływania modów na gałęzi optycznej w obszarze długofalowym.

Uzyskano krzywe w płaszczyźnie A' , odpowiadające maksymalnej oraz minimalnej energii oddziaływania.

Received May 14, 1978

7 J. Techn. Phys. 2/79
