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by

B. Lengeler and W. Ludwig

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D2. LOCALIZED MODES AT EXTENDED DEFECTS IN CRYSTALS

B. LENGELER and W. LUDWIG

Institut für Physikalische Grundlagen der Reaktorwerkstoffe der T.H. Aachen
und Institut für Reaktorwerkstoffe der Kernforschungsanlage Jülich

Abstract—Perturbations in the homogeneity of a crystal can give rise to localized modes of vibration. We have discussed the simplest cases of extended defects, namely planes of impurity atoms with special directions (001, 011, etc.) in a simple cubic crystal with nearest neighbour interaction. Extended defects, such as planes of impurity atoms, will have localized modes with exponentially decreasing amplitudes in the direction perpendicular to the planes and wave-like character in directions parallel to them. The different modes of localized vibrations have been analyzed group-theoretically. It comes out that there will be in general an acoustical and an optical branch of localized modes for a plane defect, the occurrence of which and the frequencies relative to the band of the ideal lattice frequencies depend on the defect-parameters (changes in mass and force constants). In the limit of vanishing coupling between defect plane and "host" lattice we get a free surface, which has been considered by Wallis *et al.* This limiting case has only an acoustical branch, which is identical with the Rayleigh-surface modes for long waves (provided the force-constants fulfill the conditions allowing localized states at all). Also lines of defects can have two branches of modes. The details depend as in other cases on the defect-parameters.

If the homogeneity of a crystal lattice is disturbed by a defect, some of the eigenvibrations can be localized modes, i.e. modes the vibration amplitudes of which decrease exponentially with increasing distance from the defect. The occurrence of such localized modes at point defects has been investigated in a large number of cases.[1–5] A free surface can be considered as a perturbation of the infinite lattice and localized modes can occur; this has been discussed in some cases too.[6–8] But in lattices there might be other sorts of defects (e.g. stacking faults, dislocations, etc.) of one and two dimensions. As an attempt to study the localized modes at such defects we have investigated the simplest cases, namely a plane and a line of impurity atoms in a simple cubic lattice; we will explain here only the results concerning the plane defects, the calculation of which is very simple. Line defects are somewhat more involved, but show in general the same features.[9]

1. MODEL

WE CONSIDER a monatomic infinite simple cubic lattice of masses M and lattice constant a, with interaction between nearest neighbours only. The atoms of one plane of this lattice are to be substituted by impurities, the masses of which are $M' = M(1 + \varepsilon)$ and the coupling parameters (cp) between these atoms and their nearest neighbours are changed; also the cp's in the impurity plane are different from those of the ideal lattice. For the sake of simplicity we do not consider modifications in the structure of the lattice. Here we present the discussion of a (001)- and a (011)-plane only. It is convenient to choose the coordinate system in such a way, that one axis (z) is perpendicular to these planes (Fig. 1). As basis vectors of the lattice we choose in the case

(a) (001)-plane (Fig. 1a)

$$a_k^{(i)} = A_{ki} = a\delta_{ki}. \qquad (1.1)$$

The general equlibrium positions are $X_k^{\mathrm{m}} = A_{ki}m_i$ with integer m_i. We put $(m_1, m_2, m_3) = (m,n,l)$.

(b) (011)-plane (Fig. 1b).

To have an orthogonal basis we choose

$$a_k^{(i)} = A_{ki} = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}. \quad (1.2a)$$

This corresponds to a non-primitive description

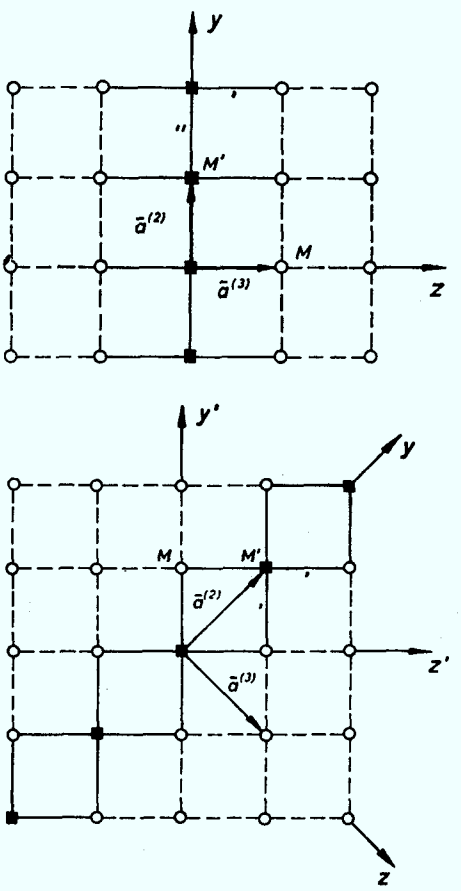

FIG. 1. Position of impurity planes in simple cubic lattice. Choice of coordinate system and basis vectors. Changed cp's full lines, unchanged cp's broken lines.

of the lattice. Every unit-cell contains two atoms ($\mu = 1, 2$), the cell vectors being

$$\mathbf{R}_1 = (0, 0, 0); \quad \mathbf{R}_2 = \frac{a}{\sqrt{2}}(011). \quad (1.2b)$$

It would not be necessary to take such a non-primitive description, but it turns out to be convenient. The equilibrium positions here are given by

$$X_{\mu\,k}^{\mathbf{m}} = A_{ki} m_i + X_k^{\mu}$$

The form of the cp's $\varphi_{i\,j}^{\mu\,\nu\,\mathbf{mn}}$ is determined by the symmetry of the lattice. They must be invariant under all symmetry operations, which transform the perturbed lattice into itself and leave **m, n** unchanged. This gives the following general matrices (with respect to the lower indices) for the cp's:

$$\varphi_{i}^{mno\;m\pm1\;no} = -\begin{pmatrix} \alpha'' & 0 & 0 \\ 0 & \beta'' & 0 \\ 0 & 0 & \gamma'' \end{pmatrix};$$

$$\varphi_{i}^{mno\;m\;n\pm10}_{j} = -\begin{pmatrix} \beta'' & 0 & 0 \\ 0 & \alpha'' & 0 \\ 0 & 0 & \gamma'' \end{pmatrix} \quad (1.3)$$

$$\varphi_{i}^{mno\;m\;n\pm1}_{j} = -\begin{pmatrix} \beta' & 0 & 0 \\ 0 & \beta' & 0 \\ 0 & 0 & \alpha' \end{pmatrix}.$$

All the other cp's are assumed to be those of the ideal lattice:

$$\varphi_{i}^{mnl\;m\pm1\;nl}_{j} = -\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \beta \end{pmatrix}; \quad \text{cyclic} \quad (1.3a)$$

This is an additional assumption, which does not follow from symmetry considerations. From symmetry alone there can be derived, for example, only the form

$$\varphi_{i}^{mnl\;mn\;l+1}_{j} = -\begin{pmatrix} \hat{\beta}_{l+1} & 0 & 0 \\ 0 & \hat{\beta}_{l+1} & 0 \\ 0 & 0 & \hat{\alpha}_{l+1} \end{pmatrix}$$

where the $\hat{\beta}_{l+1}$ must be not equal for different $|l| \geqq 2$. If we would take into account any

"structure effect", we had to consider these cp's as different from each other.

(b) (011)-plane (Fig. 1b).

Because of the lower symmetry of a crystal with a (011)-impurity plane, there are non-diagonal elements in the cp-matrices of the perturbated region, and because of our choice of the coordinate system the cp's outside the perturbed region do not have the usual form. They are

$$\varphi_{\substack{i\\j}}^{\substack{mno\\mno}}{}^{\substack{1\\2}} = \varphi_{\substack{i\\j}}^{\substack{mno\\m\,n-1\,-1}}{}^{\substack{1\\2}} = -\begin{pmatrix} \gamma' & 0 & 0 \\ 0 & \delta' & -\eta' \\ 0 & -\vartheta' & \zeta' \end{pmatrix}$$

$$\varphi_{\substack{i\\j}}^{\substack{mno\\mn-1}}{}^{\substack{1\\2}} = \varphi_{\substack{i\\j}}^{\substack{mno\\m\,n-1\,0}}{}^{\substack{1\\2}} = -\begin{pmatrix} \gamma' & 0 & 0 \\ 0 & \delta' & \eta' \\ 0 & \vartheta' & \zeta' \end{pmatrix} \quad (1.4)$$

$$\varphi_{\substack{i\\j}}^{\substack{mno\\m\pm1\,no}}{}^{\substack{1\\2}} = -\begin{pmatrix} \alpha'' & 0 & 0 \\ 0 & \gamma'' & 0 \\ 0 & 0 & \beta'' \end{pmatrix}$$

All the other cp's shall be unperturbed. They follow from (1.4) by dropping the primes and equating $\delta = \zeta$; $\vartheta = \eta$; $\beta = \gamma$. In the usual frame (x', y', z'-axis parallel to cube edges) the cp's between the same atoms as in (1.4) would be (Fig. 1b)

$$-\begin{pmatrix} \gamma' & 0 & 0 \\ 0 & \beta' & \chi' \\ 0 & \varphi' & \alpha' \end{pmatrix}; \quad -\begin{pmatrix} \gamma' & 0 & 0 \\ 0 & \alpha' & \varphi' \\ 0 & \chi' & \beta' \end{pmatrix};$$

$$-\begin{pmatrix} \alpha'' & 0 & 0 \\ 0 & \hat{\beta} & \hat{v} \\ 0 & \hat{v} & \hat{\beta} \end{pmatrix} \quad (1.5)$$

and the relations between those of (1.4) and (1.5)

$$\delta' = \tfrac{1}{2}(\alpha' + \beta' + \varphi' + \chi');$$
$$\zeta' = \tfrac{1}{2}(\alpha' + \beta' - \varphi' - \chi'); \quad \gamma'' = \hat{\beta} + \hat{v}; \quad (1.6)$$
$$\eta' = -\tfrac{1}{2}(\alpha' - \beta' - \varphi' + \chi');$$
$$\vartheta' = -\tfrac{1}{2}(\alpha' - \beta' + \varphi' - \chi'); \quad \beta'' = \hat{\beta} - \hat{v};$$

and between the unperturbed cp's [$\varphi = \chi = v = 0$]

$$\delta = \zeta = \tfrac{1}{2}(\alpha + \beta); \quad \vartheta = \eta = -\tfrac{1}{2}(\alpha - \beta);$$
$$\beta = \gamma. \quad (1.7)$$

The cp's have to satisfy certain invariance relations:

(i) The potential must be invariant toward infinitesimal translations. This connects the cp's in the following way:

$$\sum_{\mathbf{n},\nu} \varphi_{ij}^{\mathbf{mn}\,\mu\nu} = 0 \quad (1.8)$$

The cp's $\varphi_{i\,j}^{\mathbf{mm}\,\mu\,\mu}$ with $\mathbf{m} = \mathbf{n}$ *and* $\mu = \nu$ are determined by this relation.

(ii) The potential must be invariant toward infinitesimal rotations. This is expressed in the symmetry of $\sum_{\mathbf{n},\nu} \varphi_{i\,j}^{\mathbf{mn}\,\mu\,\nu} \varkappa_{j'}^{\mathbf{n}\,\nu}$ in j and j'. It follows in case

$$\text{(a) } \beta' = \beta; \quad \text{(b) } \gamma' = \beta$$
$$\textit{and} \quad \delta' + \eta' = \beta = \beta' + \chi'. \quad (1.9)$$

We will not insert (1.9) into (1.3,4,6) for the moment. We will calculate the eigenfrequencies with the general cp's as given in (1.3,4,6) because it is not difficult to satisfy the invariance conditions at the end of the calculations (see the discussion in Section 3).

2. EQUATION OF MOTION AND SOLUTION

From the cp's given in Section 1 it is not difficult to write down the equations of motion. Since this would take too much space, we will omit the explicit form of these equations. In case

(a) the equations are separated just as in the ideal lattice because of the diagonality of the cp's. The frequencies of the ideal lattice are given by ($\lambda = M\omega^2$)

$$\lambda(k_t, r = 1) = 4\alpha \sin^2 \frac{k_1 a}{2} + 4\beta \sin^2 \frac{k_2 a}{2} + 4\beta \sin^2 \frac{k_3 a}{2} \quad (2.1)$$

$\lambda(k_i, r = 2)$; $\lambda(k_i, r = 3)$ cyclic;

$$-\pi < k_i a \leqq \pi,$$

and the polarization vectors are $e_i(\mathbf{k}, r) = \delta_{ir}$.

(b) In this case only vibrations with displacements in x-direction are separated from the others, giving for the ideal lattice

$$\lambda(k_i, \sigma) = 4\alpha \sin^2 \frac{k_1 a}{2} + 4\beta\left(1 + \sigma \cos \frac{k_2 a}{\sqrt{2}} \cos \frac{k_3 a}{\sqrt{2}}\right) \tag{2.2a}$$

with

$$(e_1^1, e_1^2) = (1, -\sigma); \quad -\pi < k_1 a \leqq \pi$$

$$-\pi < k_2 a \sqrt{2}, \quad k_3 a \sqrt{2} \leqq \pi.$$

For $\sigma = +1$ (optical branch) the vibrations of the planes $z = al$ and $z = a(l+1)$ are parallel whereas they are antiparallel for $\sigma = -1$ (acoustical branch). This depends on the nonprimitive description of the lattice. Vibrations with displacements in the y–z-plane have frequencies

$$\lambda(k_i; \sigma, \tau) = 4\beta \sin^2 \frac{k_1 a}{2} + 4\delta + 4\sigma \cdot \delta \cos \frac{k_2 a}{\sqrt{2}} \cos \frac{k_3 a}{\sqrt{2}} + 4\tau \cdot \vartheta \sin \frac{k_2 a}{\sqrt{2}} \sin \frac{k_3 a}{\sqrt{2}} \tag{2.2b}$$

with the polarization-vectors

$$(e_2^1, e_2^2, e_3^1, e_3^2) = (1, -\sigma, \sigma\tau, -\tau).$$

$\sigma = \pm 1$ distinguishes optical and acoustical branches, $\tau = \pm 1$ the two branches in the optical resp. acoustical band.

If there is introduced an impurity plane, the translational invariance of the lattice in the x–y-plane is conserved and therefore the components k_1 and k_2 of the wave vectors must be real. But as we will study localized modes, we have to allow for complex z-components of the wave vectors:

$$k_3 \to k_3 + \varkappa i, \quad \varkappa > 0. \tag{2.3}$$

Nevertheless, for stationary states λ must be real, giving in case (a)

$$\sin k_3 a \cdot \sinh \varkappa a = 0.$$

(i) $\varkappa = 0$ describes modes without localized character

$$\varkappa \neq 0, \quad k_3 = 0 \quad \text{or} \quad k_3 = \pi/a$$

$$\lambda(k_i, r = 1; \sigma) = 4\alpha \sin^2 \frac{k_1 a}{2} + 4\beta \sin^2 \frac{k_2 a}{2} + \beta\left[2 + \sigma\left(t + \frac{1}{t}\right)\right] \tag{2.4}$$

$$\lambda(k_i, r = 3, \sigma) = 4\beta \sin^2 \frac{k_1 a}{2} + 4\beta \sin^2 \frac{k_2 a}{2} + \alpha\left[2 + \sigma\left(t + \frac{1}{t}\right)\right] \tag{2.5}$$

$t = \mathrm{e}^{-\varkappa a}$ describes the exponential decrease of the waves perpendicular to the impurity plane. Since $\varkappa > 0$, hence $0 < t < 1$. $\sigma = -1$ corresponds to $k_3 = 0$ and $\sigma = +1$ to $k_3 a = \pi$ here. $\lambda(r = 2)$ is degenerate with $\lambda(r = 1)$.

(b) With displacements parallel x only:

$$\sin \frac{k_3 a}{\sqrt{2}} \cdot \sinh \frac{\varkappa a}{\sqrt{2}} = 0.$$

(i) $\varkappa = 0$, see above

(ii) $\varkappa \neq 0$, $k_3 = 0$ ($k_3 = \pi/a$) is not a vector of the first Brillouin zone in this case), here

$$t = \mathrm{e}^{-\varkappa a/\sqrt{2}}, \tag{2.6}$$

$$\lambda(k_i, \sigma) = 4\alpha \sin^2 \frac{k_1 a}{2} + 2\beta\left[2 + \sigma\left(t + \frac{1}{t}\right) \cos \frac{k_2 a}{\sqrt{2}}\right]. \tag{2.7}$$

With displacements parallel to the y–z-plane only, we get in an analogous way

(i) $\varkappa = 0$, see above

$$\text{(ii)}\quad \sigma\delta \tan\frac{k_3 a}{\sqrt{2}} = \tau \tan\frac{k_2 a}{\sqrt{2}} \tag{2.8}$$

showing that k_2 and k_3 are not independent from each other. This is the most interesting case. The frequencies are (here $t = \mathrm{e}^{-\varkappa a/\sqrt{2}}$)

$$\lambda(k_i;\sigma,\tau) = 4\beta \sin^2\frac{k_1 a}{2} + 4\delta + 2\sigma\left(t + \frac{1}{t}\right)\sqrt{\delta^2 \cos^2\frac{k_2 a}{\sqrt{2}} + \vartheta^2 \sin^2\frac{k_2 a}{\sqrt{2}}}. \tag{2.9}$$

The vibrational states can be classified according to the eigenvalues of the reflection operator Σ (reflection at the impurity plane). States with $\langle\Sigma\rangle = +1$ are denoted by A' and with $\langle\Sigma\rangle = -1$ by A'', hence

$$s^{m\,n-l}_{1\;j} = \pm s^{m\,n\,l}_{1\;j}; \quad s^{m\,n-(l+1)}_{2\;j} = \pm s^{m\,n\,l}_{2\;j}; \quad j = 1, 2 \tag{2.10}$$

$$s^{m\,n-l}_{1\;3} = \mp s^{m\,n\,l}_{1\;3}; \quad s^{m\,n-(l+1)}_{2\;3} = \mp s^{m\,n\,l}_{2\;3},$$

where the upper sign holds for the A'-states, the lower signs for the A''-states.

The eigenstates for the localized modes can be written in A'-state

$$\text{(a)}\quad s^{m\,n\,l}_{1} = e_1\, t^{|l|}(-\sigma)^l \exp ia(k_1 m + k_2 n)$$

$$s^{m\,n\,l}_{3} = e_3 \frac{l}{|l|}\, t^{|l|}\cdot(-\sigma)^l \exp ia(k_1 m + k_2 n) \quad l \neq 0 \tag{2.11}$$

$$= 0 \quad l = 0$$

$$\text{(b)}\quad s^{m\,n\,l}_{1} = e^{\mu}_1(-\sigma)^l \cdot g$$

$$s^{m\,n\,l}_{2} = e^{\mu}_2 \cos k_3 a\sqrt{2}\left(l + \frac{\delta_{\mu_2}}{2}\right)\cdot g$$

$$s^{m\,n\,l}_{3} = e^{\mu}_3\, i \sin k_3 a\sqrt{2}\left(l + \frac{\delta_{\mu_2}}{2}\right)\cdot g$$

$$g = t^{2|2l+\delta_{\mu_2}|} \exp ia\left[k_1 m + k_2\sqrt{2}\times\left(n + \frac{\delta_{\mu_2}}{2}\right)\right] \tag{2.12}$$

The amplitudes of the impurity atoms are different from those in the remaining lattice.

Case (a) (001)-plane. Displacements $\|\varkappa$, A'-state

$$0 = \begin{vmatrix} \beta' - \beta(1+\sigma/t) & \beta'\sigma/t \\ 2\beta'\sigma t & 4(\alpha'' - \alpha - \alpha\varepsilon)\sin^2\frac{k_1 a}{2} + 4(\beta'' - \beta - \beta\varepsilon)\sin^2\frac{k_2 a}{2} \\ & + 2(\beta' - \beta - \beta\varepsilon) - \sigma\beta(1+\varepsilon)(t + 1/t) \end{vmatrix}. \tag{2.13}$$

From this equation t can be determined. Inserting t in (2.5a) we will get λ.

A''-state. Here

$$t = \frac{\sigma\beta}{\beta' - \beta} \quad \text{and} \quad \lambda = \frac{\beta'^2}{\beta' - \beta} + 4\alpha \sin^2\frac{k_1 a}{2} + 4\beta \sin^2\frac{k_2 a}{2} \tag{2.14}$$

for $\sigma = +1$. $\sigma = -1$ would give positive λ only if $\beta' < 0$, which is not compatible with the stability of the lattice.

Displacements $\|z$, A'-state and A''-state. We can get the corresponding equations from (2.13) resp. (2.14) with the following replacements:

$$\alpha'' \to \gamma''; \quad \alpha \to \beta; \quad \beta \to \alpha \quad \text{if } \beta \textit{ is not} \text{ a factor of } \sin\frac{k_2 a}{2} \tag{2.15}$$

$$\beta'' \to \gamma''; \quad \beta' \to \alpha'; \quad \beta \to \beta$$

if β *is* a factor of $\sin \frac{k_2 a}{2}$.

Case (b) (011)-plane. Displacements $\|x$, A'-state

$$0 = \begin{vmatrix} -(1+\varepsilon)\lambda + 4\gamma' + 4\alpha'' \sin^2 \frac{k_1 a}{2} & -4\gamma' t \cos \frac{k_2 a}{\sqrt{2}} \\ -2\gamma' \frac{1}{t} \cos \frac{k_2 a}{\sqrt{2}} & -\lambda + 2\beta + 2\gamma' + 4\alpha \sin^2 \frac{k_1 a}{2} + 2\sigma\beta t \cos \frac{k_2 a}{\sqrt{2}} \end{vmatrix}. \tag{2.16}$$

Here λ has to be substituted by (2.7), then t can be calculated and with t we have λ.

A''-state.

$$t = \frac{\sigma\beta}{\gamma' - \beta} \cos \frac{k_2 a}{\sqrt{2}};$$

$$\lambda = 4\alpha \sin^2 \frac{k_1 a}{2} + \frac{2}{\gamma' - \beta}\left[\gamma'^2 - \beta^2 \sin^2 \frac{k_2 a}{\sqrt{2}}\right]. \tag{2.17}$$

Displacements $\|y$–z-plane, A'-state.

$$0 = \begin{vmatrix} -(1+\varepsilon)R\lambda + 4R\left(\delta' + \gamma'' \sin^2 \frac{k_1 a}{2}\right) & -4t\delta\delta' \cos^2 \frac{k_2 a}{\sqrt{2}} & -4\sigma\tau\vartheta t\eta' \sin^2 \frac{k_2 a}{\sqrt{2}} \\ -\frac{2}{t}\delta' R^2 & \left[-\lambda + 4\beta \sin^2 \frac{k_1 a}{2} + 2\delta + 2\delta'\right] R\delta + 2\sigma t\delta\left[\delta^2 \cos^2 \frac{k_2 a}{\sqrt{2}} - \vartheta^2 \sin^2 \frac{k_2 a}{\sqrt{2}}\right] & +4\tau t\delta\vartheta^2 \sin^2 \frac{k_2 a}{\sqrt{2}} \\ -\frac{2}{t}\eta' R^2 & -2\sigma t\vartheta\left[\delta^2 \cos^2 \frac{k_2 a}{\sqrt{2}} - \vartheta^2 \sin^2 \frac{k_2 a}{\sqrt{2}}\right] & \left[-\lambda + 4\beta \sin^2 \frac{k_1 a}{2} + 2\delta + 2\zeta'\right] \sigma\tau R\vartheta + 4\tau t\vartheta\delta^2 \cos^2 \frac{k_2 a}{\sqrt{2}} \end{vmatrix} \tag{2.18}$$

with λ according to (2.9) and

$$R = \left\{\delta^2 \cos^2 \frac{k_2 a}{\sqrt{2}} + \vartheta^2 \sin^2 \frac{k_2 a}{\sqrt{2}}\right\}^{\frac{1}{2}}.$$

From this t and λ can be determined. The corresponding secular equation for the A''-states follows from (2.18) by the replacements:

$$\delta' \to \zeta'; \quad \vartheta' \to \eta'; \quad \gamma'' \to \beta'';$$
$$\zeta' \to \delta'; \quad \eta' \to '. \tag{2.19}$$

3. DISCUSSION

Because of the translational invariance in the directions of the impurity plane we have a dependence on k_1 and k_2, and therefore the frequencies of the localized modes are distributed in bands. In the figures these bands are shown as functions of the relative changes in mass and cp's. As is seen from Figs. 2–4 (only changes in mass) there is an optical branch and an acoustical one. The optical branch only occurs for negatice ε ($M' < M$) and is in a certain sense similar to the behaviour of the localized mode of an isotopic point defect. But in the case of an isotopic impurity plane there is a partial overlap of the localized band with the frequency band of the ideal lattice, which is not possible for a point defect. Further it is possible to have an acoustical branch if $\varepsilon > 0$ ($M' > M$), which naturally does not occur for a point defect. It should be mentioned that a line defect would give similar dependences on ε, only the breadth of the localized bands (optical *and* acoustical) being smaller in general. Also, in other types of lattices one can guess that the dependence on ε is not very different from this, differences arising mainly in the quantitative statements.

Figures 5–7 show the dependence on the changes in the cp's, where the condition for rotational invariance (1.9) have been taken into account. Again there might be an optical and acoustical band of localized modes. The upper limit of the optical band coincides qualitatively with the frequency dependence on changed cp's for point defects. The occurrence of the acoustical modes is possible only for planes or lines of defects.

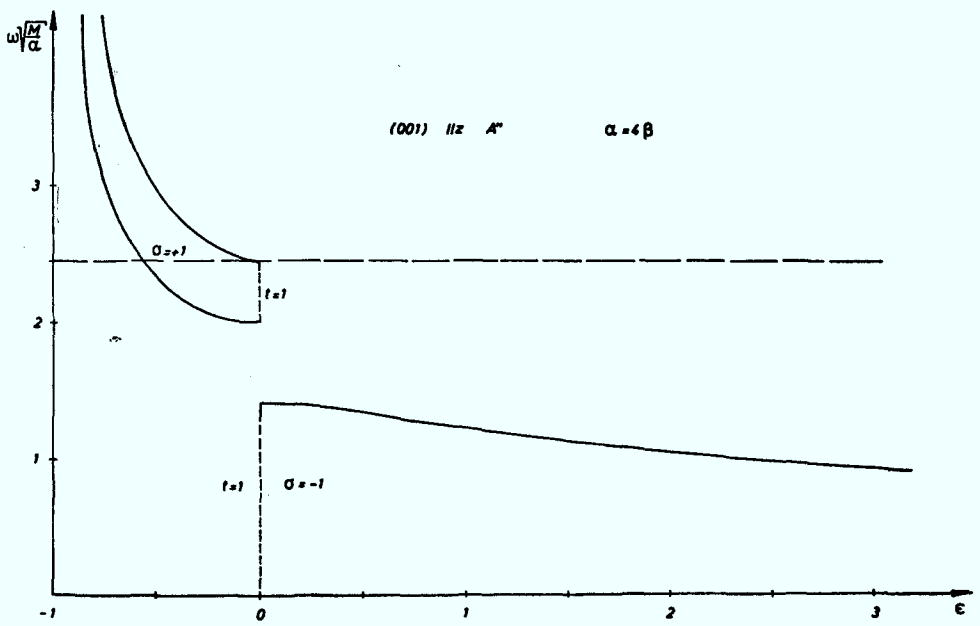

FIG. 2. Optical and acoustical band of localized modes as function of $\varepsilon = (M' - M)/M$. No change in cp's. (001)-plane, displacements $\|z$, A''-state.

The most interesting case is that of the (011)-impurity plane. There is a true dependence [Eq. (2.8)] of k_3 on k_2. This means that to the exponential decrease of amplitudes in z-direction there is superposed an oscillation of the amplitudes determined by the direction of the prop-

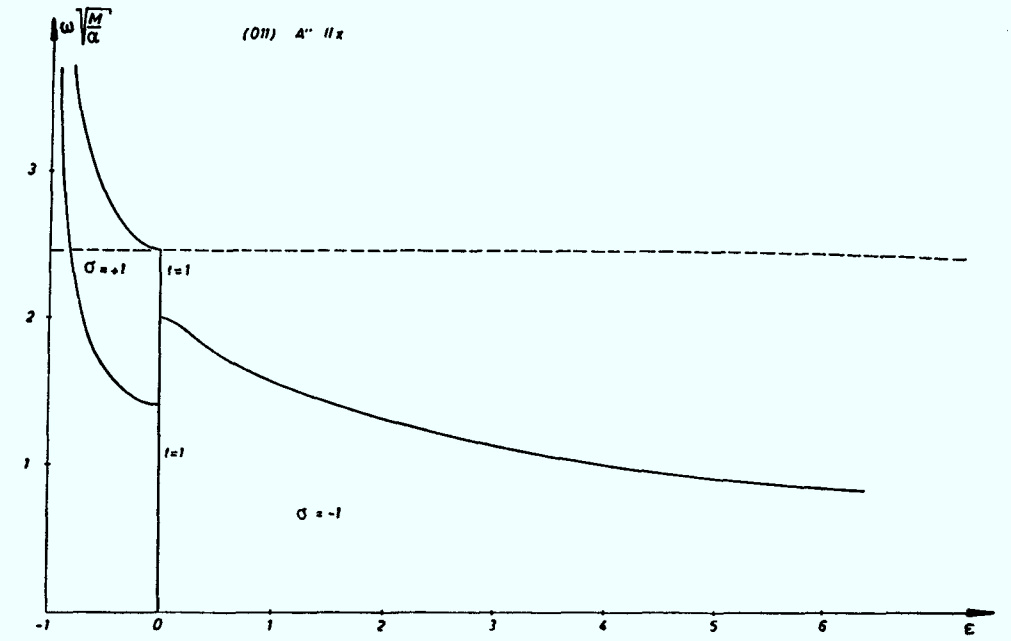

FIG. 3. See Fig. 2 (011)-plane, displacements $\|x$, A''-state.

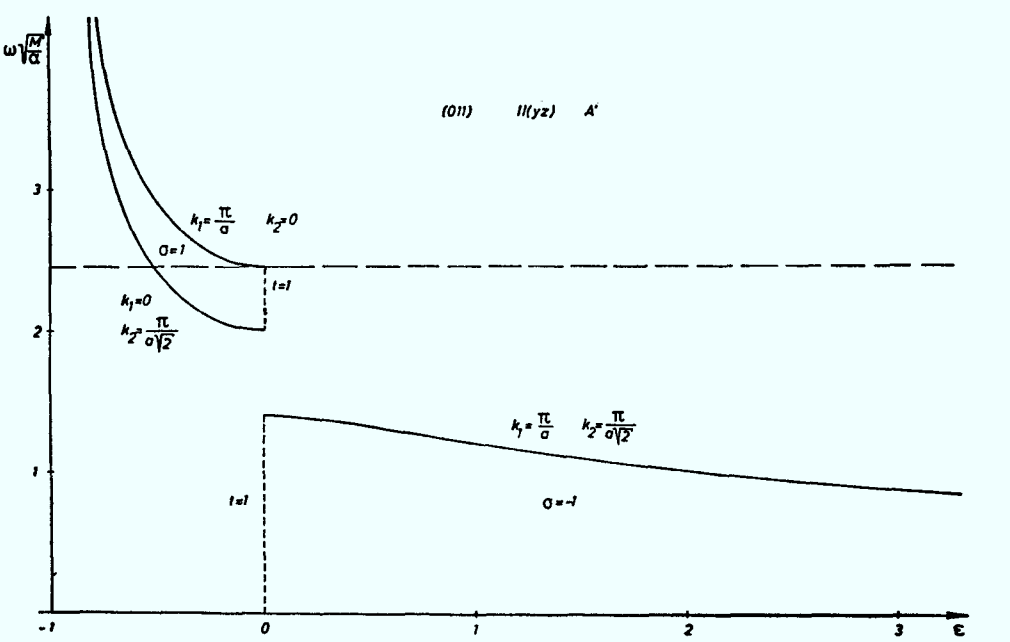

FIG. 4. See Fig. 2 (011)-plane, displacements $\|y$-z-plane, A'-state.

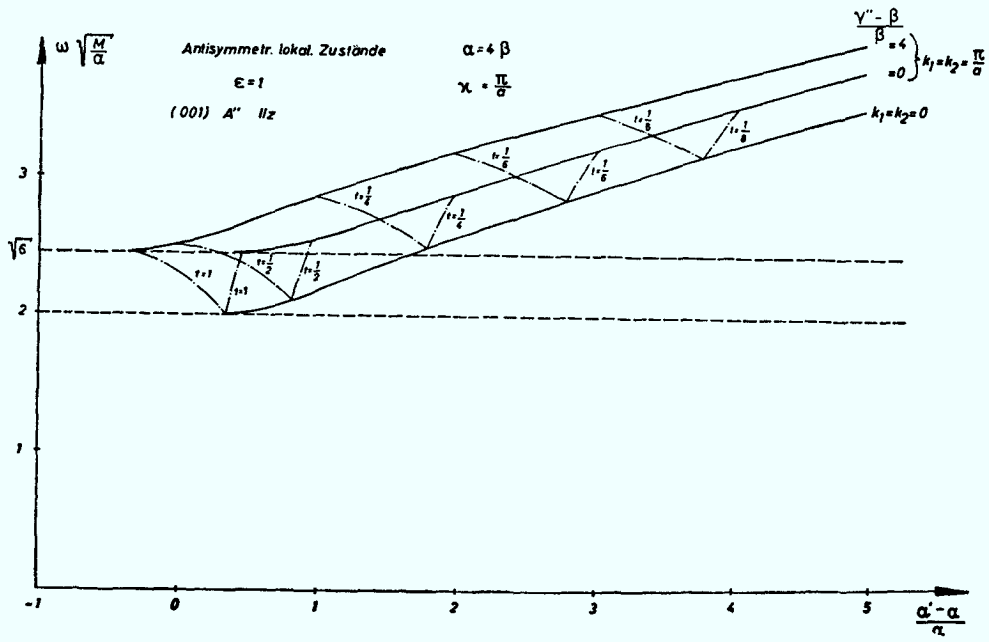

FIG. 5. Optical band as function of $(\alpha' - \alpha)/\alpha$ with $\varepsilon = 1$ and $(\gamma'' - \beta)/\beta = 0$ and 4 as parameters. (001)-plane, displacements $\parallel z$, A''-state.

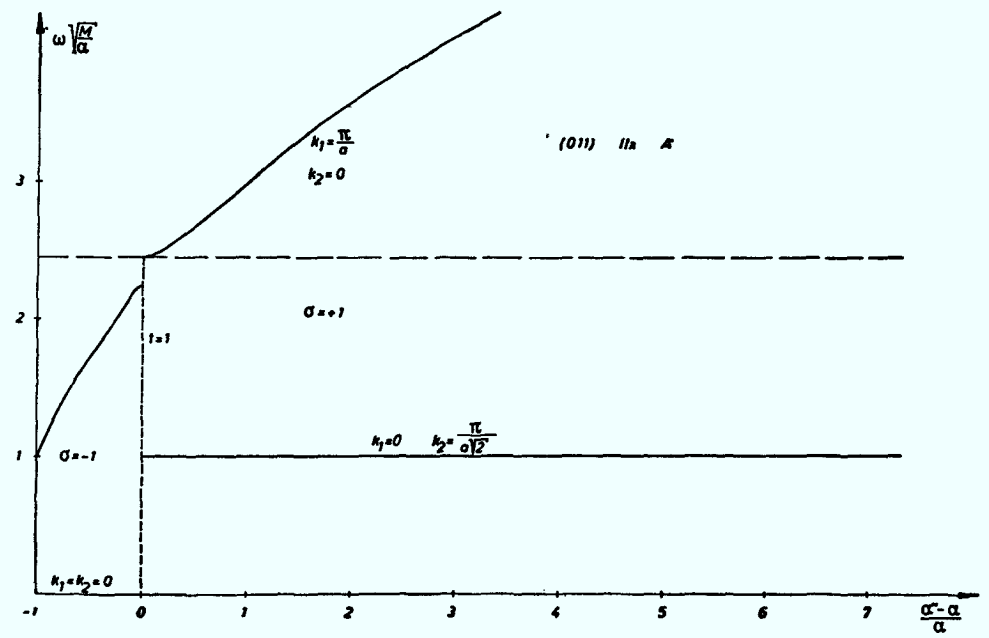

FIG. 6. Optical and acoustical band as function of $(\alpha'' - \alpha)/\alpha$. Other cp's unchanged. (011)-plane, displacements $\parallel x$, A'-state.

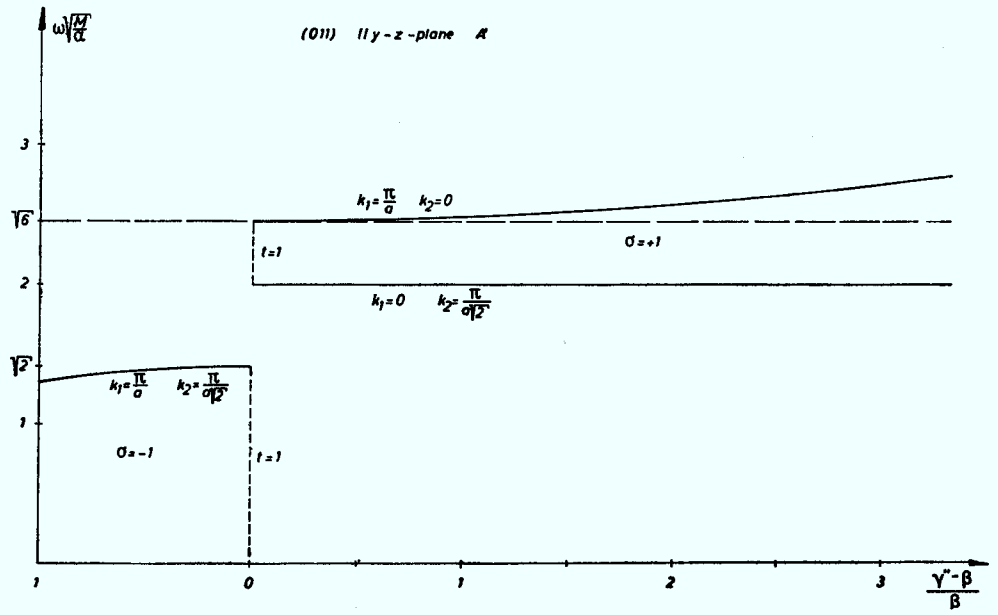

FIG. 7. Optical and acoustical band as function of $(\gamma'' - \beta)/\beta$. Other cp's unchanged. (011)-plane, displacements $\|y$-z-plane, A'-state.

agating wave. If there is a running wave in y-direction, for example, this wave has an attenuated standing-wave character in z-direction. The dependence $k_3(k_2)$ is shown in Fig. 8 for a special example. However, in more general cases k_3 will depend on k_1 as well as on k_2; e.g. this will be so for an (111)-impurity plane. In Fig. 10 there are given the dispersion curves of the localized modes for an (011)-impurity plane; the notation with respect to the Brillouin zone of the impurity plane is defined in Fig. 9. Optical and acoustical branches do not occur at the

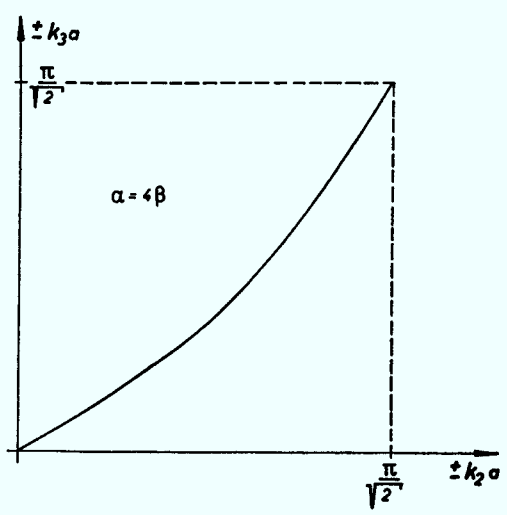

FIG. 8. Component of wave-vector perpendicular to impurity plane (k_3) as function of k_2. $\alpha = 4\beta$.

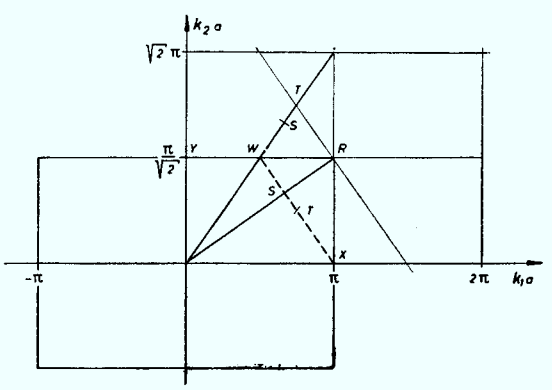

FIG. 9. Brillouin zone of (011)-impurity plane.

same time; the optical exist only for $(\gamma'' - \beta)/\beta = (\alpha'' - \alpha)/\alpha = +\frac{1}{2}$ and the acoustical only for $(\gamma'' - \beta)/\beta = (\alpha'' - \alpha)/\alpha = -\frac{1}{2}$. – Apart from

the fact that there are only two, these dispersion curves behave essentially as those of the ideal lattice modes.

Unfortunately, it is not possible to construct a free surface for this crystal model, for if one satisfies the rotational condition (1.9) in this case [all one-primed cp's equal to zero], the crystal would not be elastically stable, or if one makes the crystal stable, the condition (1.6) cannot be satisfied. Nevertheless, it is possible to make some qualitative statements concerning the wave-forms of surface waves in crystals. It can be said that in general the waves will have a non-zero real k_3-component of the wave vectors, depending on k_1 and k_2 (generalized Rayleigh-type waves in the long wave limit). There will be only an acoustical band. Qualitatively the dispersion-curves will behave as those given in Fig. 11 for a (011)-surface, which have been drawn disregarding the conditions (1.9). Quantitatively one must be cautious to make conclusions from this behaviour. A (001)-surface has no surface modes in this "wrong"-model, as has already been realized.[7,8] As discussed in simple cases of elastic surface waves,[8] in lattice theory too there might be surfaces with and without surface modes and special surfaces may have surface modes in special directions of the propagation vector, having none in other directions.

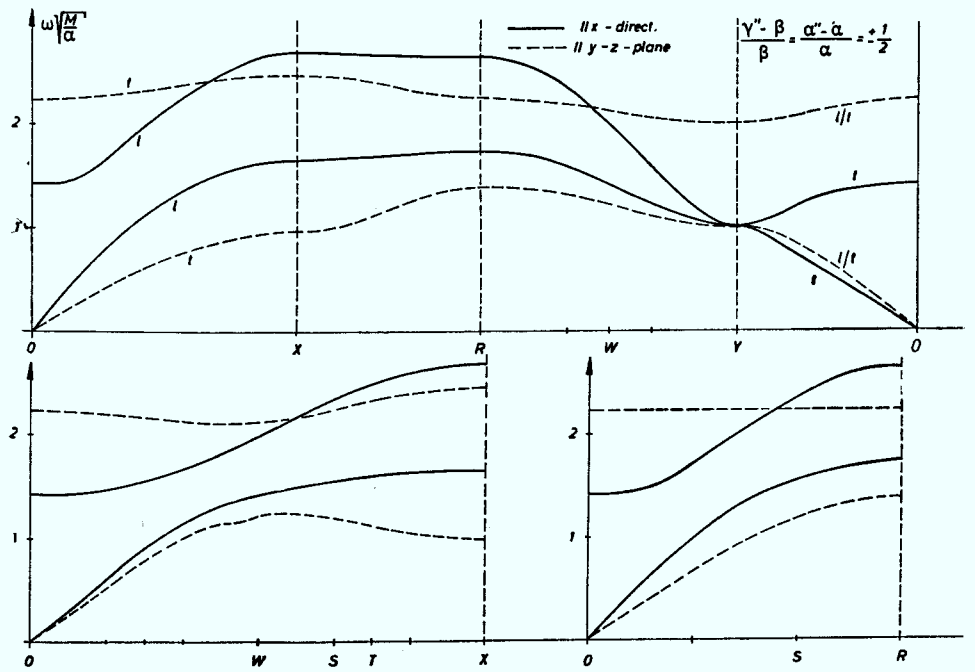

FIG. 10. Dispersion curves of localized states of (011)-impurity plane. In case of $(\beta'' - \beta)/\beta = (\alpha'' - \alpha)/\alpha = +\frac{1}{2}$ there is only the optical band, for $-\frac{1}{2}$ only the acoustical. Full line is for displacements in x-direction, broken line for displacements in y-z-plane.

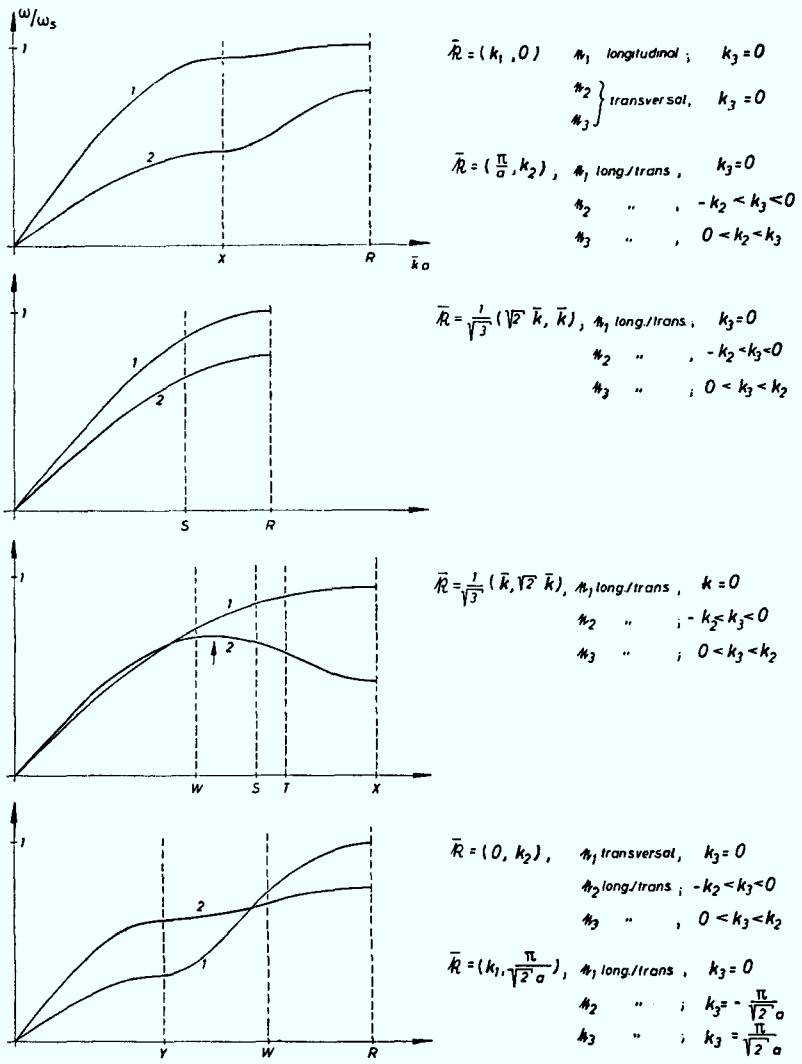

FIG. 11. Dispersion curves of free surface modes, but with rotational condition not satisfied!

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