

## Pseudocontinuum approach to the theory of interactions between impurity defects and crystal lattice(\*)

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THE PAPER presents a method allowing for an analytical description of interactions between the impurity electrons and crystal lattice. The method is based on the quasi-continuum approach to lattice dynamics and makes it possible to take into account both the finite range of interaction forces and the discreteness of the crystal structure. As a result, a general description of the phenomenon is obtained. The results derived by the two methods known so far (effective mass approximation and the quasi-molecule approach) constitute two limiting cases of the method presented here.

Przedstawiono metodę pozwalającą na opis analityczny oddziaływań między elektronami domieszek a siecią krystaliczną. Metoda oparta jest na podejściu quasi-kontynuualnym do dynamiki sieci i umożliwia uwzględnienie zarówno skończonego zasięgu sił oddziaływania jak i dyskretności struktury kryształu. Wyniki otrzymany za pomocą dwóch znanych dotąd metod (przybliżenie mas efektywnych i podejście quasi-molekularne) stanowią dwa przypadki graniczne uzyskanego tutaj rozwiązania.

Представлен метод позволяющий аналитически описать взаимодействия между электронами примесей и кристаллической решеткой. Метод основан на квази-континуальном подходе к динамике решетки и позволяет учесть как конечный радиус силового взаимодействия, так и дискретность кристаллической структуры. Результаты полученные с помощью двух ранее известных методов (приближение эффективных масс и квази-молекулярный подход) являются двумя предельными случаями предлагаемого решения.

### 1. Introduction

TWO different ways to calculate the interaction of impurity electrons with crystal are known at present. The first one is the effective mass approximation which corresponds to long range interaction and takes place, first of all, in the case of impurities in semiconductors. The other one, the quasi-molecule approach, is applied in the case of localized interaction and is made use of for some materials utilized in quantum electronics.

In this paper we present a method allowing for an analytical description of these interactions, which is based on the quasi-continuum approach to lattice dynamics. It allows us to take into account both the finite range of interaction forces and the discreteness of the crystal from the very beginning. As a result, we obtain a more general description that involves the above mentioned cases as limiting approximations.

The case of substitutional impurity in the bulk of a crystal is considered in detail. Sect. 2 comprises the pseudocontinuum analysis of interaction between the electron of the impurity and lattice deformation, and in Sect. 3 we consider the stresses and the static deformations due to the impurity defect.

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## 2. Perturbation of elastic energy of lattice due to substitutional impurity

The interaction between impurity electrons and lattice deformation can be described (in the linear approximation) by the expression [1]

$$(2.1) \quad \delta V(\bar{\tau}) = \sum V_{,\alpha}^s [\bar{\tau} - \bar{R}(\bar{l}_{\kappa_s})] u_{\alpha}(\bar{l}_{\kappa_s}),$$

where  $V$  is the potential energy of interaction between the valence electron of the impurity and the atom (or ion) belonging to the sublattice  $s$  (site  $\kappa_s$ ) of the unit cell  $\bar{l}$ ,  $\bar{u}$ —displacement vector, the dash denotes exclusion of the impurity site itself in the above summation,  $\alpha$ —Cartesian components.

For the sake of simplicity, we shall restrict our discussion to the case of crystals whose space groups of symmetry contain neither the screw axes nor the glide planes. The last assumption enables us to identify the symmetry group of the impurity centre and the point group of the crystal. We also assume that the extremum point of the nearest energy band (with respect to the localized level of impurity to be considered) is the point  $\Gamma$  of the Brillouin zone.

The above specification, in view of the well-known fact that the symmetry of a shallow impurity centre (that means of a large radius) is the same as the symmetry of a band at the extremum point allows for a generalized description with group—theoretical consideration of the both limiting cases.

The expression [1], in terms of symmetrical displacement (with respect to the point groups), can be written as

$$(2.2) \quad \delta V(\bar{\tau}) = \sum V_{\tilde{\Gamma}\tilde{\gamma}}^{s\bar{l}}(\bar{\tau}) u_{\tilde{\Gamma}\tilde{\gamma}}(\bar{l}_s),$$

where  $\tilde{\Gamma}$  and  $\tilde{\gamma}$  denote the irreducible representation and its row, respectively. The electron state of impurity can be expressed in the form of superposition of the generalized (symmetrized) Wannier functions (instead of a Bloch function) since they are specially fitted to this aim. Given the above assumptions, the subset of these functions, connected with a single unit cell yields a set of basic functions of irreducible representations of the point group.

According to the above remarks, the wave function of impurity belonging to the representation  $(\Gamma, \gamma)$  (in a general case, its projection into subspace  $(\Gamma, \gamma)$ ) may be expressed in the form

$$(2.3) \quad |\gamma\rangle = \sum_{\bar{l}} B_{\gamma}(\bar{l}) a_{\gamma}(\bar{\tau} - \bar{R}_{\bar{l}}),$$

as far as the  $B_{\gamma}(\bar{l})$  is a totally symmetrical function of  $\bar{l}$  (see below).

Hence we get for the matrix elements of the operator (2.1)

$$(2.4) \quad \langle \gamma' | \delta V | \gamma \rangle \equiv \delta V_{\gamma'\gamma} = \sum \langle \gamma' | V_{\tilde{\Gamma}\tilde{\gamma}}^{s\bar{l}} | \gamma \rangle u_{\tilde{\Gamma}\tilde{\gamma}}(\bar{l}_s),$$

where

$$(2.5) \quad \begin{aligned} \langle \gamma' | V_{\tilde{\Gamma}\tilde{\gamma}}^{s\bar{l}} | \gamma \rangle &= \sum_{\bar{n}, \bar{n}'} B_{\gamma'}^*(\bar{n}') B_{\gamma}(\bar{n}) \int a_{\gamma'}^*(\bar{\tau} - \bar{R}_{\bar{n}'}) V_{\tilde{\Gamma}\tilde{\gamma}}^{s\bar{l}}(\bar{\tau}) a_{\gamma}(\bar{\tau} - \bar{R}_{\bar{n}}) d\bar{\tau} \\ &\equiv \sum_{\bar{n}, \bar{n}'} B_{\gamma'}^*(\bar{n}') B_{\gamma}(\bar{n}) [V_{\tilde{\Gamma}\tilde{\gamma}}^s(\bar{n}, \bar{n}'; \bar{l})]_{\gamma'\gamma}. \end{aligned}$$

The eigenvalues of the matrix (2.4) determine the shift and the possible splitting of the impurity level caused by interaction between its electrons and lattice deformation.

Here we assume that the coefficients  $B_\gamma(\bar{l})$  are known. They are determined from the solution of non-perturbed impurity electron problem (the perturbation is given by Eq. (2.1)). In the pseudopotential model these coefficients have the meaning of the eigenfunctions of the impurity electron energy problem (as the pseudowave functions). As we see from Eq. (2.3)  $B_\gamma(\bar{l})$  plays the role of a "slowly varying" envelope of the cell functions  $a_\gamma(\bar{\tau} - \bar{R}_\tau)$ .

Neglecting the dependence of the "periodical" factor  $u_k^z(\bar{\tau})$  of the Bloch function on the wave vector  $\bar{k}$  (this corresponds to the commonly used Kohn-Luttinger approximation, in our case with respect to point  $\Gamma$ ), we have from the definition

$$(2.6) \quad a_\gamma(\bar{\tau} - \bar{R}_\tau) \approx \frac{\Omega_0^{1/2}}{(2\pi)^{3/2}} u_0^z(\bar{\tau}) \int_B e^{i\bar{k}(\bar{\tau} - \bar{R}_\tau)} d\bar{k} = (2\pi)^{3/2} \Omega_0^{1/2} u_0^z(\bar{\tau}) \delta_B(\bar{\tau} - \bar{R}_\tau),$$

where  $B$  denotes the first Brillouin zone and  $\delta_B(\bar{\tau})$  is the pseudocontinuum  $\delta$  function.

For slowly varying  $V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{\tau})$  as a function of  $\bar{l}$ , we get from orthogonality of the Wannier functions

$$(2.7) \quad V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n}, \bar{n}'; \bar{l}) \approx V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n}, \bar{n}'; \bar{l}) \delta_{\bar{n}, \bar{n}'} \equiv V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n}, \bar{l}) \delta_{\bar{n}, \bar{n}'}.$$

From the general relation

$$(2.8) \quad u_0^{z*}(\bar{\tau}) u_0^z(\bar{\tau}) = \delta_{\gamma', \gamma} + \sum_{\bar{K} \neq 0} C_{\gamma', \gamma}^{\bar{K}} e^{i\bar{K}\bar{\tau}},$$

where  $\bar{K}$  is a vector of reciprocal lattice (taking into account Eq. (2.6)), it follows that if we neglect the oscillations of the Wannier functions, the non-diagonal matrix elements of arbitrary potential will vanish.

The approximation which corresponds to pseudocontinuum approach is equivalent to neglecting the second term in Eq. (2.8). It is reasonable to apply that conclusion to the matrix elements (2.7) which combine the different cells  $\bar{n} \neq \bar{l}$ , provided the potential is varying slowly enough.

Finally, we obtain

$$(2.9) \quad [V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n}, \bar{l})]_{\gamma', \gamma} = [V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n} - \bar{l})]_{\gamma', \gamma} = (2\pi)^3 \delta_{\gamma', \gamma} \int \delta_B(\bar{\tau} - \bar{n}) V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{\tau}) d\bar{\tau} \\ = (2\pi)^3 \delta_{\gamma', \gamma} V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{n} - \bar{l}), \quad (\bar{R}_\tau \equiv \bar{n}).$$

This result gives an explicit form of the dependence on  $\bar{n} - \bar{l}$  if the potential of interaction between the impurity electrons and lattice ions (or atoms) is known.

When  $\bar{l} = \bar{n}$  the relation (2.9) is invalid; the matrix elements are then determined by the shape of the wave function within the unit cell according to the definition

$$(2.10) \quad [V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{l}, \bar{l})]_{\gamma', \gamma} = [W_{\bar{r}\bar{\gamma}}^{\bar{l}}]_{\gamma', \gamma} = \int a_{\gamma', (\bar{\tau} - \bar{l})}^* V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{\tau}) a_{\gamma, (\bar{\tau} - \bar{l})} d\bar{\tau}$$

and

$$(2.11) \quad [V_{\bar{r}\bar{\gamma}}^{\bar{l}}(0, 0)]_{\gamma', \gamma} \equiv [W_{\bar{r}\bar{\gamma}}^{00}]_{\gamma', \gamma} = \int a_{\gamma', \bar{\tau}}^* V_{\bar{r}\bar{\gamma}}^{\bar{l}}(\bar{\tau}) a_{\gamma, \bar{\tau}} d\bar{\tau}.$$

The matrix elements (2.10)–(2.11) do not vanish only under the condition

$$(2.12) \quad \tilde{\Gamma} \in [\Gamma^2]_s,$$

where  $([\Gamma^2]_s)$  denotes a symmetrical part of the direct product of the representations  $\Gamma$ .

As it follows from group theory considerations in the case of non-degenerate states the contribution given by Eqs. (2.10)–(2.11) is determined by the totally symmetrical (with respect to the point group) distortion only.

Having applied the Wigner-Eckart formula to the right parts of the relations (2.9)–(2.11) we finally get, after some calculations,

$$(2.13) \quad [V_{\tilde{\Gamma}\tilde{\gamma}}(\bar{n}, \bar{l})]_{\gamma,\gamma'} = C_{\tilde{\gamma}\gamma'}^{\tilde{\Gamma}\tilde{\gamma}} [W_{\tilde{\Gamma}}^{\text{os}} \delta_{\bar{n}\bar{o}}^{\text{os}} \delta_{\bar{l}\bar{o}} + W_{\tilde{\Gamma}}^{\text{s}} \delta_{\bar{n}\bar{l}}] + (2\pi)^3 \delta_{\gamma,\gamma'} V_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{n} - \bar{l}),$$

where  $\hat{C}$  denotes the matrix of the Clebsh-Gordan coefficients and  $W_{\tilde{\Gamma}}$ —can be thought to the phenomenological parameters.

It is essential, however, to emphasize that the above considerations are concerned with the case of sufficiently slowly varying potential.

Generally, its explicit analytic form is unknown and, for instance in the investigations of the localized impurity states, the model potential is often used. The last one is in fact a local approximation (in the sense of a multiplying operator) of the nonlocal (as the integral operator) pseudopotential which is determined by subtracting from the real potential its projection into a subspace of the core (i.e. inner) states. Owing to this the shape of that one is usually smooth (in general much smoother than the real potential). As it is known, the above fact is connected with the almost general applicability of the free electron approximation in investigations of the band structure.

This circumstance is the main reason for which we can enlarge the range of validity of Eq. (2.13), provided  $V(\bar{r})$  denotes a concrete model potential.

Basing on Eq. (2.13), we can write the matrix (2.5) in the form

$$(2.14) \quad \delta V_{\gamma,\gamma'} = \sum_{\tilde{\Gamma}\tilde{\gamma}\tilde{\delta}} \{ C_{\tilde{\gamma}\gamma'}^{\tilde{\Gamma}\tilde{\gamma}} [B_{\gamma'}^*(0) B_{\gamma}(0) W_{\tilde{\Gamma}}^{\text{os}} u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{os}}(\tilde{\delta}) + \sum_{\bar{l}} B_{\gamma'}^*(\bar{l}) B_{\gamma}(\bar{l}) W_{\tilde{\Gamma}}^{\text{s}} u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{l})] + (2\pi)^3 \delta_{\gamma,\gamma'} \sum_{\bar{l}, \bar{n} \neq \bar{l}} |B_{\gamma}(\bar{n})|^2 V_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{n} - \bar{l}) u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{\delta}) \}.$$

Introducing the notations

$$(2.15) \quad \begin{aligned} B_{\gamma'}^*(\bar{l}) B_{\gamma}(\bar{l}) W_{\tilde{\Gamma}}^{\text{s}} C_{\tilde{\gamma}\gamma'}^{\tilde{\Gamma}\tilde{\gamma}} - (2\pi)^3 V_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(0) \delta_{\gamma,\gamma'} |B_{\gamma}(\bar{l})|^2 &= w_{\tilde{\Gamma}}^{\text{s}} [v_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{l})]_{\gamma,\gamma'}, \\ B_{\gamma'}^*(0) B_{\gamma}(0) C_{\tilde{\gamma}\gamma'}^{\tilde{\Gamma}\tilde{\gamma}} &= [v_{\tilde{\Gamma}\tilde{\gamma}}^{\text{os}}]_{\gamma,\gamma'}, \\ (2\pi)^3 |B_{\gamma}(\bar{l})|^2 \delta_{\gamma,\gamma'} &= [b(\bar{l})]_{\gamma,\gamma'}. \end{aligned}$$

We shall write Eq. (2.14) in the (convenient for further considerations) operator form:

$$(2.16) \quad \delta \hat{V} = \sum_{\bar{l}} \delta \hat{V}(\bar{l}),$$

where

$$(2.17) \quad \delta \hat{V}(\bar{l}) = \sum_{\tilde{\Gamma}\tilde{\gamma}\tilde{\delta}} \{ \hat{v}_{\tilde{\Gamma}\tilde{\gamma}}^{\text{os}} w_{\tilde{\Gamma}}^{\text{os}} u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{os}}(\tilde{\delta}) \delta_{\bar{l},0} + \hat{v}_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{l}) w_{\tilde{\Gamma}}^{\text{s}} u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{\delta}) + \sum_{\bar{n}} \hat{b}(\bar{n}) V_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{n} - \bar{l}) u_{\tilde{\Gamma}\tilde{\gamma}}^{\text{s}}(\bar{\delta}) \}.$$

The diagonalization of the last matrix gives the interaction energy between impurity and deformation of the  $\bar{l}$ -th cell.

In the particular case of non-degenerate impurity level, it immediately gives the expression for the interaction energy

$$(2.18) \quad \Delta E(\bar{l}) = \sum \left\{ v_{\lambda_1}^{0s} w_{\lambda_1}^{0s} u_{\lambda_1}(\bar{l}) \delta_{l,0} + v_{\lambda_1}^s(\bar{l}) w_{\lambda_1}^s u_{\lambda_1}(\bar{l}) + \sum_{\bar{n}} b(\bar{n}) V_{\lambda_1}^s(\bar{n}-\bar{l}) u_{\lambda_1}(\bar{l}) \right\},$$

which is due to totally symmetrical displacements only.

### 3. Pseudocontinuum model of static deformations

The above mentioned properties of both the model potential  $V$  and the envelope function  $B_\nu(\bar{l})$  indicate the applicability of the pseudocontinuum model to a description of the interaction determined by the relations (2.16) and (2.17).

The relation (2.16) can then be written in the integral form

$$(3.1) \quad \delta \hat{V} = \int \delta \hat{V}(\bar{r}) d\bar{r},$$

where

$$(3.2) \quad \delta V(\bar{r}) = \sum_{\bar{r}'s} \left\{ v_{\bar{r}'s}^{0s} w_{\bar{r}'s}^{0s} u_{\bar{r}'s}(\bar{l}) \delta_B(\bar{r}) + \hat{v}_{\bar{r}'s}^s(\bar{r}) w_{\bar{r}'s}^s u_{\bar{r}'s}(\bar{l}) + \int \hat{b}(\bar{r}') V_{\bar{r}'s}^s(\bar{r}'-\bar{r}) d\bar{r}' u_{\bar{r}'s}(\bar{l}) \right\}.$$

Since the last matrix is of the scalar type in the point group, one can express it immediately in the initial (Cartesian) frame of coordinates and obtain the result in the form

$$(3.3) \quad \delta \hat{V}(\bar{r}) = \sum_{\alpha,s} \left\{ \Phi_{\alpha s}^0 u_{\alpha}(\bar{l}) \delta_B(\bar{r}) + \Phi_{\alpha s}(\bar{r}) u_{\alpha}(\bar{l}) + \int \hat{b}(\bar{r}') V_{\alpha}^s(\bar{r}'-\bar{r}) d\bar{r}' u_{\alpha}(\bar{l}) \right\},$$

where

$$[\Phi_{\alpha s}]_{\gamma\gamma'} = U^s(\alpha, \bar{l}) [v_{\bar{r}'s}^s]_{\gamma\gamma'},$$

$\hat{U}^s$ —the unitary transformation matrix.

The identification of  $\kappa_s$  with  $s$  in Eq. (3.3) is a consequence of the assumptions presented in Sect. 2.

It is important to note that if the last (diagonal) term does not vanish, then the non-totally symmetrical lattice deformations due to the interaction determined by Eq. (3.2) and (3.3) can be obtained only when the matrices  $\hat{\Phi}$  (or  $\hat{v}$ ) also have a diagonal form.

In the case of one-dimensional representations  $\Gamma$ , as can be seen from the conditions (2.13), the displacement has to be totally symmetric.

Further, we shall restrict ourselves to the above cases. Then for the matrix (3.3) we get

$$(3.4) \quad [\delta V(\bar{r})]_{\gamma\gamma'} = \Delta E_\gamma(\bar{r}) \delta_{\gamma\gamma'}.$$

From the above we obtain the following relations for the components of force density, which induce the static deformation of the crystal neighbourhood of the impurity:

$$(3.5) \quad f_{\bar{r}'s}^{\gamma s}(\bar{r}) = - \frac{\partial \Delta E_\gamma(\bar{r})}{\partial u_{\bar{r}'s}(\bar{r})} = - \left\{ v_{\bar{r}'s}^{0s} w_{\bar{r}'s}^{0s} \delta_B(\bar{r}) + v_{\bar{r}'s}^s(\bar{r}) w_{\bar{r}'s}^s + \int b_\gamma(\bar{r}') V_{\bar{r}'s}^s(\bar{r}'-\bar{r}) d\bar{r}' \right\}$$

and

$$(3.6) \quad f_{\alpha}^{ys}(\bar{r}) = -\left\{ \Phi_{\alpha s}^{0y} \delta_B(\bar{r}) + \Phi_{\alpha s}^y(\bar{r}) + \int b_y(\bar{r}') V_{\alpha}^s(\bar{r}' - \bar{r}) d\bar{r}' \right\}$$

for the symmetrized and Cartesian coordinates, respectively.

In the case of a one-dimensional electronic representation ( $\gamma = 1$ , then  $(\vec{I}, \vec{\gamma}) = A_1$ ), we get from Eq. (3.5) and (3.6),

$$(3.7) \quad f_{A_1}^s(\bar{r}) = -\left\{ v_{A_1}^{0s} w_{A_1}^{0s} \delta_B(\bar{r}) + v_{A_1}^s(\bar{r}) w_{A_1}^s + \int b(\bar{r}') V_{A_1}^s(\bar{r}' - \bar{r}) d\bar{r}' \right\}$$

and

$$(3.8) \quad f_{\alpha}^s(\bar{r}) = -\left\{ \Phi_{\alpha s}^0 \delta_B(\bar{r}) + \Phi_{\alpha s}(\bar{r}) + \int b(\bar{r}') V_{\alpha}^s(\bar{r}' - \bar{r}) d\bar{r}' \right\}.$$

The limiting case of a small radius corresponds to neglecting the two last terms in the relations (3.5)–(3.8) while the case of a large radius can be obtained by omitting the first term and neglecting the dependence of  $\hat{\Phi}$  and  $V$  on the position vector  $\bar{r}$  in the remaining ones.

We can determine the static displacements by making use of the equilibrium condition (for general nonlocal elastic interactions)

$$(3.9) \quad \sum_{s'\beta} \int C_{\alpha\beta}^{ss'}(\bar{r} - \bar{r}') u_{\beta}^{s'}(\bar{r}') d\bar{r}' = f_{\alpha}^{ys}(\bar{r}).$$

Taking into account the properties of convolution in the pseudocontinuum description we get for the Fourier transforms

$$(3.10) \quad \sum_{s'\beta} \tilde{C}_{\alpha\beta}^{ss'}(\bar{q}) \tilde{u}_{\beta}^{s'}(\bar{q}) = \tilde{f}_{\alpha}^{ys}(\bar{q}) = -\left\{ \Phi_{\alpha s}^{0y} + \tilde{\Phi}_{\alpha s}^y(\bar{q}) - iq_{\alpha} \tilde{b}(\bar{q}) \tilde{V}^s(\bar{q}) \right\}.$$

The solution of this equation is

$$(3.11) \quad \tilde{u}_{\alpha}^y(\bar{q}) = \sum_{\beta, s'} \mathcal{G}_{\alpha\beta}^{ss'}(\bar{q}) \tilde{f}_{\beta}^{ys'}(\bar{q}),$$

where the Green's function  $\mathcal{G}$  is the inverse matrix of  $(m_s m_{s'})^{-1/2} \tilde{C}_{\alpha\beta}^{ss'}(\bar{q})$ .

The analyticity of the transform  $\tilde{V}^s(\bar{q})$  is due to the limited range of the potential  $V(\bar{r})$ . In such a case the last term in Eq. (3.10) vanishes in the limit  $\bar{q} \rightarrow 0$ . This situation takes place if the valencies of both the impurity and replaced ion are the same and in the case of impurities with an uncompensated charge, provided the crystal manifests perceptible metallic properties. In each of these cases the typical form of the model potential is the Yukawa type (for the high symmetries).

The transform of the Green's function, in statical approximation, can be written as

$$(3.12) \quad \mathcal{G}_{\alpha\beta}^{ss'}(\bar{q}) = -\Omega_0 \sum_j \frac{\tilde{u}_{\alpha}^j(\bar{q}) \tilde{u}_{\beta}^j(\bar{q})}{\omega_j^2(\bar{q})},$$

where  $\Omega_0$  is the volume of the unit cell,  $\tilde{u}^j$  the polarization vector of the  $j$ -th mode.

It follows from the above relation that the main contribution to the statical tensor  $\hat{\mathcal{G}}_{\alpha\beta}^j$  are provided by the acoustical modes only.

This circumstance enables us to apply the pseudocontinuum model. The inversion of the transform  $\bar{u}(\bar{q})$  with the aid of the basic pseudocontinuum relation

$$(3.13) \quad \bar{u}(\bar{r}) = (2\pi)^{-3} \int_B e^{i\bar{q}\bar{r}} \bar{u}(\bar{q}) d\bar{q},$$

(where  $B$  denotes integration over the first Brillouin zone), gives immediately the statical displacements of the perturbed medium. In order to obtain the expression for the contribution to the stress tensor due to impurity, we shall express the relations (3.1)–(3.3) in terms of the continuum theory. For simplicity we shall restrict ourselves to the case of a monoatomic lattice. It is convenient to introduce the local strain tensor with the help of the relation

$$u_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}) = a \varepsilon_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}),$$

where  $\varepsilon_{\tilde{\Gamma}\tilde{\gamma}}$  denotes its symmetrized component (belonging to the irreducible representation of the point group) and  $a$  is, in our case, the lattice constant. Taking into account the main property of the groups scalar, we obtain

$$(3.14) \quad \sum_{\tilde{\Gamma}\tilde{\gamma}} \hat{v}_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}) w_{\tilde{\Gamma}} u_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}) = \sum_{\tilde{\Gamma}\tilde{\gamma}} \tilde{u}_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}) \hat{\varepsilon}_{\tilde{\Gamma}\tilde{\gamma}}(\bar{r}) = \sum_{\alpha\beta} \hat{\mu}_{\alpha\beta}(\bar{r}) \varepsilon_{\alpha\beta}(\bar{r}),$$

where  $\hat{\mu}_{\tilde{\Gamma}\tilde{\gamma}} = a \hat{v}_{\tilde{\Gamma}\tilde{\gamma}} w_{\tilde{\Gamma}}$ , and, as in the above relations, the sign  $\wedge$  denotes a matrix operator determined in the given electronic irreducible representation. Integrating by parts the contribution to the right part of Eq. (3.1) due to the last term of Eq. (3.3) and taking into account the limited range of the potential  $V$ , we get

$$\iint \hat{b}(\bar{r}') V_{,\alpha}(\bar{r}' - \bar{r}) u_{\alpha}(\bar{r}) d\bar{r}' d\bar{r} = - \iint \hat{b}(\bar{r}') V(\bar{r}' - \bar{r}) \varepsilon_{\alpha\alpha}(\bar{r}) d\bar{r}' d\bar{r}.$$

Therefore, Eq. (3.3) can finally be written in the form

$$(3.15) \quad \delta \hat{V}(\bar{r}) = \sum_{\alpha\beta} \left\{ \hat{\mu}_{\alpha\beta}^0 \varepsilon_{\alpha\beta}(\bar{r}) \delta_B(\bar{r}) + \hat{\mu}_{\alpha\beta}(\bar{r}) \varepsilon_{\alpha\beta}(\bar{r}) - \delta_{\alpha\beta} \int \hat{b}(\bar{r}') V(\bar{r}' - \bar{r}) d\bar{r}' \varepsilon_{\alpha\alpha}(\bar{r}) \right\}.$$

Equation (3.15) determines the dependence of the interaction energy on the local strain tensor and constitutes the generalization of the well-known deformation potential method.

Thus, for instance, in the case of non-degenerate impurity electron state, the contribution to the stress tensor is given by

$$(3.16) \quad \sigma_{\alpha\beta}^{(e)}(\bar{r}) = \frac{\partial \Delta E(\bar{r})}{\partial \varepsilon_{\alpha\beta}(\bar{r})} = \mu_{\alpha\beta}^0 \delta_B(\bar{r}) + \mu_{\alpha\beta}(\bar{r}) - \delta_{\alpha\beta} \int b(\bar{r}') V(\bar{r}' - \bar{r}) d\bar{r}'.$$

For the degenerate electron state it is necessary to carry out diagonalization of the matrix (3.15).

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