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FORCE CONSTANTS FOR A DISORDERED SYSTEM WITH A CRYSTAL TOPOLOGY

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Force constants for the harmonic theory of atomic vibrations have been derived for a disordered system having a crystal topology. The screening in the system has been described in terms of the dielectric matrix for an effective periodic crystal. The formulas for the force constants are expressed by actual ion-electron potentials and the dielectric matrix of the effective crystal. This result should be correct for some alloys of the constituents of the same valency.

The absence of permanent displacements of atoms (except for thermal vibrations) has been shown for the Bravais structure crystals.

1. Introduction

The energy of vibrations of any stable solid may be always, in the harmonic approximation, written as follows [1, 2]

$$E = \sum_i \frac{\vec{p}_i^2}{2M_i} + \tfrac{1}{2} \sum_{ij} \vec{u}_i \overleftrightarrow{\Phi}_{i,j} \vec{u}_j, \tag{1}$$

where the indices i, j label atoms of the system, $\vec{u}_i$, $\vec{p}_i$ stand for the atomic displacements and momenta, the force constants matrices $\overleftrightarrow{\Phi}_{i,j}$ describe the coupling between the atoms. For ideal periodic crystal we have $M_i = M$, $\overleftrightarrow{\Phi}_{i,j} = \overleftrightarrow{\Phi}_{i-j}$ and equations of motion, corresponding to (1), can be solved easily. For other systems it is usually a problem, although at the present time there exist some powerful methods of solving them, applicable to many important cases [1, 2].

The matrix $\overleftrightarrow{\Phi}_{i,j}$ long has been treated phenomenologically. Only for ideal periodic crystals the microscopic derivation of $\overleftrightarrow{\Phi}$ has been given some years ago, within the pseudopotential approach [3], or, more generally, within the dielectric matrix approach [6, 7]. On the other hand, no systematic quantum-mechanical treatment of the force constants for disordered systems have appeared so far, it seems.

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For some disordered alloys, the electron-ion interaction of constituents being "weak", the pseudopotential approach turned out to be successful [3–5]. In such cases the calculation of static and dynamic properties goes much the same as for ideal periodic crystals of simple metals. For most alloys however, the assumption of weak electron-ion interaction is not fulfilled.

In the present paper the microscopic derivation of the matrix $\overleftrightarrow{\Phi}_{i,j}$, for "slightly" disordered systems having a "crystal topology" (Sec. 3) has been given. A concept of an effective, periodic crystal has been introduced (Sec. 4) and the dielectric matrix of the system written in terms of the one-electron energy levels and Bloch functions for the effective crystal. In Sec. 5 the total electron energy of the system has been expressed as a quadratic form of atomic displacements, its coefficients being identified as the corresponding force constants. This allows one to consider the problem of occurence of small permanent displacements of atoms from their lattice sites in perfect crystals — Section 6. The applicability of the result obtained has been discussed in Sec. 7.

2. Total energy for a system of Bloch electrons in the Hartree approximation

In this section we remind ourselves of some results known for an ideal periodic crystal. Let H be the one-electron Hamiltonian involving the appropriate periodic potential, its eigenvalues and eigenfunctions being E_k, $\psi_k(\vec{r})$, where $k \equiv (n, \vec{k} \in BZ)$ and n is the band number. Let $V(\vec{r})$ be a perturbation. Total electron energy in the presence of the perturbation, in the Hartree approximation is [6, 7]

$$E^{e'} = E^e + \varrho(1)V(1) + S(1,2)V(1)V(2) + O(V^3), \tag{2}$$

where integration over doubled indices is understood (i.e. $A(1)B(1) \equiv \int d\vec{r}_1 A(\vec{r}_1)B(\vec{r}_1)$, etc.), higher order terms are collected in $O(V^3)$,

$$\varrho(\vec{r}) = \sum_k f(E_k - \mu)\psi_k^*(\vec{r})\psi_k(\vec{r}), \tag{3}$$

$$S(1,2) = \tfrac{1}{2}\varrho(1,3)\varepsilon^{-1}(3,2), \qquad \varepsilon(1,2) = \delta(1-2) - \frac{e^2}{|1-3|}\varrho(3,2), \tag{4}$$

$$\varrho(\vec{r},\vec{r}') = \sum_{k,m} \frac{f(E_k-\mu)-f(E_m-\mu)}{E_k-E_m}\psi_k^*(\vec{r})\psi_m(\vec{r})\psi_m^*(\vec{r}')\psi_k(\vec{r}'), \tag{5}$$

μ is the Fermi energy, and

$$E^e = \sum_k f(E_k-\mu)E_k - \frac{e^2}{2}\varrho(1)\frac{1}{|1-2|}\varrho(2) \tag{6}$$

is the electron energy of an unperturbed crystal in the Hartree approximation.

3. *Disordered systems of a crystal topology*

In the present work we are considering disordered systems having a crystal topology. By this we mean that it is possible to insert into the system a regular structure of points, $\vec{L} = \vec{l} + \vec{b}$ (where the lattice vectors are $\vec{l} = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$, l_1, l_2, l_3 are integers, $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are primitive translations and $\vec{b}$'s are the basis vectors) such that: a) there is a unique, one to one correspondence between the atoms of the system and the structure points $\vec{L}$, b) each atom is closer to "its" structure point than to any other structure point (Fig. 1).

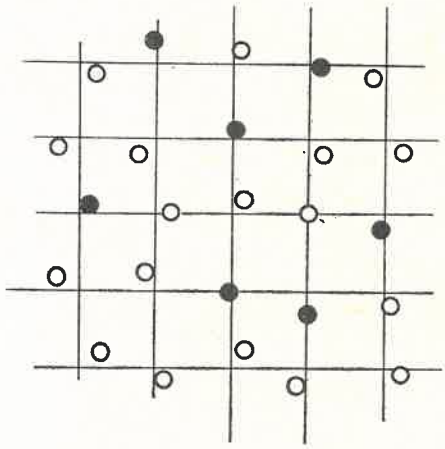

Fig. 1. The lattice inscribed into a disordered system

We note that this condition practically eliminates the systems containing macroscopic precipitations of the composition much different from the average one. It is also clear that for the disordered system of crystal topology we can define the reciprocal lattice vectors $\vec{\kappa}(\vec{l} \cdot \vec{\kappa} = 2\pi \cdot \text{integer number})$ and therefore the concept of the Brillouin zone is well defined.

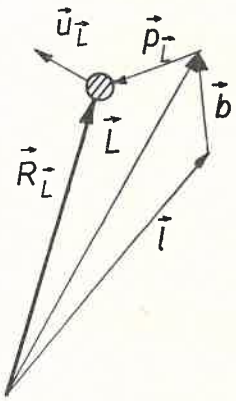

Fig. 2. Average position of an ion — $\vec{R}_L$, structure point — $\vec{L}$, "permanent displacement" — $\vec{p}_{\vec{L}}$, and instantenous displacement — $\vec{u}_{\vec{L}}$

Once we have the lattice, we can introduce the vector $\vec{p}_{\vec{L}}$ — the "permanent" displacement of the $\vec{L}$-th atom from "its" site (Fig. 2):

$$\vec{R}_{\vec{L}} = \vec{L} + \vec{p}_{\vec{L}}. \tag{7}$$

In the foregoing we assume for the sake of simplicity the Bravais structures (i.e. $\vec{b} = 0$), but the generalization of formulas derived is straighforward.

The system considered has a long-range order, but in general is without a short-range order. Indeed, the scattering function $S(\vec{k})$ for the elastic scattering of X-rays and neutrons exhibits Bragg peaks. To show it, let us write the atomic formfactors as

$$f_{\vec{K}}^{\vec{l}} = f_K + \delta_{\vec{K}}^{\vec{l}}.$$

Assuming that atomic positions at large distances are uncorelated, we have

$$S(\vec{K}) = |\langle \sum_{\vec{l}} f_{\vec{K}}^{\vec{l}} e^{i\vec{K}\cdot\vec{R}_{\vec{l}}} \rangle|^2 = |f_{\vec{K}}|^2 |\langle \sum_{\vec{l}} e^{i\vec{K}\cdot\vec{R}_{\vec{l}}} \rangle|^2$$

$$+ (f_{\vec{K}}^* \langle \sum_{\vec{l}} e^{-i\vec{K}\cdot\vec{R}_{\vec{l}}} \rangle \langle \sum_{\vec{l}} \delta_{\vec{K}}^{\vec{l}} e^{i\vec{K}\cdot\vec{R}_{\vec{l}}} \rangle + \text{c.c.}) + |\langle \sum_{\vec{l}} \delta_{\vec{K}}^{\vec{l}} e^{i\vec{K}\cdot\vec{R}_{\vec{l}}} \rangle|^2.$$

$\langle\rangle$ means the averaging over all possible configurations of atoms, and by definition $\langle f_{\vec{K}}^{\vec{l}} \rangle = f_{\vec{K}}$, i.e. $\langle \delta_{\vec{K}}^{\vec{l}} \rangle = 0$. $\delta_{\vec{K}}^{\vec{l}}$ is determined by properties of the $\vec{l}$-th atom, whereas its permanent displacement $\vec{p}_{\vec{l}}$ depends mainly on the positions of its neighbours. It means that in first approximation both quantities are uncorrelated i.e.

$$\langle \delta_{\vec{K}}^{\vec{l}} e^{i\vec{K}\cdot\vec{p}_{\vec{l}}} \rangle \cong \langle \delta_{\vec{K}}^{\vec{l}} \rangle \langle e^{i\vec{K}\cdot\vec{p}_{\vec{l}}} \rangle = 0 \tag{8}$$

and in the same approximation we have for $S(\vec{K})$ (using $\Sigma_{\vec{l}} e^{i\vec{K}\cdot\vec{l}} = N\Sigma_{\vec{\kappa}} \delta_{\vec{K},\vec{\kappa}}$, see also [10])

$$S(\vec{K}) \cong |f_{\vec{K}}|^2 e^{-2L_{\vec{K}}} N^2 \sum_{\vec{\kappa}} \delta_{\vec{K},\vec{\kappa}} + \text{a smooth contr.}, \tag{9}$$

where $\exp(-L_{\vec{K}}) \equiv \langle \exp(i\vec{K}\cdot\vec{p}_{\vec{l}}) \rangle$ for small displacements is analogous to the Debye–Waller factor for thermal vibrations, whereas for "large" $\vec{p}_{\vec{l}}$'s the Krivoglaz formulation is more appropriate [11].

4. Effective periodic potential and effective crystal

In the rigid ion approximation the bare electron potential is the sum of one-ion potentials $w^{\vec{L}}$, i.e. [8]:

$$W(\vec{r}) = \sum_{\vec{L}} w^{\vec{L}}(\vec{r} - \vec{R}_{\vec{L}}) \tag{10}$$

where the superscript $\vec{L}$ in $w^{\vec{L}}$ reminds us that, in general, our system is built up of different atoms. In general, therefore, $W(\vec{r})$ is not periodic.

As an essential step of the present we introduce an effective potential $P(\vec{r})$, which is by assumption periodic having the lattice period introduced in Sec. 3, and is in a certain

sense rather close to the true potential $W(\vec{r})$. It is understood, that the one-electron eigenproblem with the potential $P(\vec{r})$ can be solved, and the relevent quantities of the energy treatment (2 — 6) are marked by the subscript P: E_P — total electron energy (6), $\varrho_P(\vec{r})$ — electron density (3), etc.

Now the difference $(W-P)$ will be treated as a perturbation. According to Eq. (2), for the total electron energy of our disordered system we have

$$E^e \cong E_P^e + \varrho_P(1)\,[W(1)-P(1)] + S_P(1,2)\,[W(1)-P(1)]\,[W(2)-P(2)] \tag{11}$$

where the higher order terms have been assumed negligible.

Let us discuss the construction of the periodic potential $P(\vec{r})$. The most satisfactory would be the potential corresponding to a minimum of E_W. However, in E_P, P is involved also implicitely, so the calculations concerned would be extremely difficult.

But we known that P should be "close" to W so that $W-P$ be (roughly speaking) a small quantity and the perturbation series (11) — quickly convergent. Therefore, let us simply set the first order term of the series to be zero.

$$\varrho_P(1)P(1) = \varrho_P(1)W(1). \tag{12}$$

Formally, this is a self-consistant equation in P, because the electron density ϱ_P can be calculated only after solving the one-electron Schroedinger equation involving the P which we just want to construct. However, bearing in mind that the $\varrho_P(\vec{r})$ is periodic, we can take as a solution the periodic function given by its Fourier transforms

$$P_{\vec{\kappa}} = \frac{1}{\Omega}\int dW(\vec{r})e^{i\vec{\kappa}\cdot\vec{r}} = \sum_{\vec{L}} e^{i\vec{\kappa}\cdot(\vec{b}+\vec{p}_{\vec{L}})}w_{\vec{\kappa}}^{\vec{L}}. \tag{13}$$

This is a generalization of the virtual crystal approximation: $P_{\vec{\kappa}}^{\mathrm{VCA}} = \Sigma_{\vec{L}} w_{\vec{\kappa}}^{\vec{L}}$ [8, 2]. In (13) not only the compositional $(w^{\vec{L}})$ but also the positional $(\vec{p}_{\vec{L}})$ disorder is accounted for.

Let us calculate $\langle|P_\kappa|^2\rangle$, the quantity relevent for electronic structure calculations. With the same approximations as those assumed for $S(\vec{K})$ we obtain

$$\langle|P_{\vec{\kappa}}|^2\rangle \cong e^{-2L_{\vec{\kappa}}}|P_\kappa^{\mathrm{VCA}}|^2. \tag{14}$$

With the Gaussian shape of the $\exp(-2L_{\vec{\kappa}})$ factor we have, that the positional disorder diminishes the large $\vec{\kappa}$ energy gaps, which is not a trivial result.

With P given by Eq. (13) we have for the total electron energy, to the second order

$$E_W^e \cong E_P^e + S_P(1,2)\,[W(1)-P(1)]\,[W(2)-P(2)]. \tag{15}$$

The second order term shows a similarity to the expression for an alloying [5] (ordering [3]) energy of the pseudopotential approach.

Another choice of $P(\vec{r})$, more involved but perhaps closer to reality, could be the one

based on the coherent potential approximation [2]. Chosen in whatever way, this periodic effective potential determines a reference crystal which we shall call the effective crystal.

5. *Force constants*

In the previous section we have constructed an effective periodic potential for our disordered system at rest. Now let us allow the atoms of the system to vibrate about their average positions $\vec{R}_{\vec{L}}$. In the rigid ion approximation we have as the perturbation

$$V(\vec{r}) = \sum_{\vec{L}} w^{L}(\vec{r}-\vec{R}_{\vec{L}}-\vec{u}_{\vec{L}})-P(\vec{r})$$

$$= W(\vec{r})-P(\vec{r})+\sum_{\vec{L}}[\vec{u}_{\vec{L}}\cdot\nabla w^{\vec{L}}(\vec{r}-\vec{R}_{\vec{L}})+\tfrac{1}{2}\vec{u}_{\vec{L}}\vec{u}_{\vec{L}}\nabla\nabla w^{\vec{L}}(\vec{r}-\vec{R}_{\vec{L}})]. \tag{16}$$

By inserting it into Eq. (2) we obtain at once the following expression for the total electron energy in the presence of ionic vibrations

$$E^{e} = E^{e}_{W}+\sum_{\vec{L}}\vec{\Phi}^{e}(\vec{R}_{\vec{L}})\cdot\vec{u}_{L}+\tfrac{1}{2}\sum_{\vec{L}\vec{L}'}\vec{u}_{\vec{L}}\cdot\overleftrightarrow{\Phi}^{e}(\vec{R}_{\vec{L}},\vec{R}_{\vec{L}'})\cdot\vec{u}_{\vec{L}'} \tag{17}$$

where the first-order force constants are

$$\vec{\Phi}^{e}(\vec{R}_{\vec{L}}) = \varrho_{P}(1)\nabla w^{\vec{L}}(1-R_{\vec{L}})+2S_{P}(1,2)\,[W(1)-P(1)]\nabla w^{\vec{L}}(2-\vec{R}_{\vec{L}}). \tag{18}$$

For the second-order constants we have

$$\overleftrightarrow{\Phi}^{e}(\vec{R}_{\vec{L}},\vec{R}_{\vec{L}'}) = \delta_{\vec{L},\vec{L}'}\varrho_{P}(1)\nabla\nabla w^{\vec{L}}(1-\vec{R}_{\vec{L}})+2S_{P}(1,2)\nabla w^{\vec{L}}(1-\vec{R}_{\vec{L}})\nabla w^{\vec{L}'}(2-\vec{R}_{\vec{L}'}). \tag{19}$$

Note that $\overleftrightarrow{\Phi}^{e}(\vec{R}_{\vec{L}},\vec{R}_{\vec{L}'}) \neq \overleftrightarrow{\Phi}^{e}(\vec{R}_{\vec{L}}-\vec{R}_{\vec{L}'})$. Eq. (19) is the main result of the present paper. It says, that the coupling between two ions through the valence electrons is, roughly speaking, proportional to the product of the true ion-electron potentials, and to the susceptibility of the electron gas of the effective crystal to the density redistributions. The formula for an ideal periodic crystal is recovered from it by putting $w^{\vec{L}} \to w^{\vec{b}}$, $\vec{R}_{\vec{L}} \to \vec{L}$, $\varrho_{P} \to \varrho$, $S_{P} \to S$ [7].

The ions interact also directly, through the Coulombic forces. The total energy of this interaction is

$$E^{i} = \frac{e^{2}}{2}\sum_{\vec{L}\neq\vec{L}'}\frac{Z_{\vec{L}}Z_{\vec{L}'}}{|\vec{R}_{L}-\vec{R}_{L'}+\vec{u}_{\vec{L}}-\vec{u}_{\vec{L}'}|}$$

$$= \frac{e^{2}}{2}\sum_{\vec{L}\neq\vec{L}'}\frac{Z_{\vec{L}}Z_{\vec{L}'}}{|\vec{R}_{L}-\vec{R}_{L'}|}+\sum_{L}\vec{\Phi}^{i}(\vec{R}_{\vec{L}})\vec{u}_{\vec{L}}+\sum_{\vec{L},\vec{L}'}\vec{u}_{\vec{L}}\overleftrightarrow{\Phi}(\vec{R}_{\vec{L}},\vec{R}_{\vec{L}'})\vec{u}_{\vec{L}'} \tag{20}$$

where

$$\vec{\Phi}^i(\vec{R}_{\vec{L}}) = e^2 \sum_{\vec{L}' \neq \vec{L}} \nabla \frac{Z_{\vec{L}} Z_{\vec{L}'}}{|\vec{R}_{\vec{L}} - \vec{R}_{\vec{L}'}|}, \tag{21}$$

$$\overleftrightarrow{\Phi}^i(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}'}) = -e^2 \nabla\nabla \frac{Z_{\vec{L}} Z_{\vec{L}'}}{|\vec{R}_{\vec{L}} - \vec{R}_{\vec{L}'}|} \tag{22}$$

and

$$\overleftrightarrow{\Phi}^i(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}}) = -\sum_{\vec{L}' \neq \vec{L}} \overleftrightarrow{\Phi}^i(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}'}).$$

Total energy of our system is $E = E^i + E^e$. Equilibrium requires that the terms linear in $\vec{U}_{\vec{L}}$ must vanish:

$$\vec{\Phi}^i(\vec{R}_{\vec{L}}) + \vec{\Phi}^e(\vec{R}_{\vec{L}}) = 0. \tag{23}$$

As both $\vec{\Phi}^i$ and $\vec{\Phi}^e$ depend on $\vec{R}_{\vec{L}} = \vec{L} + \vec{p}_{\vec{L}}$, in principle we could treat Eq. (23) as the equations for permanent displacements $\vec{p}_{\vec{L}}$.

Finally we can write for the force constants

$$\overleftrightarrow{\Phi}(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}'}) = \overleftrightarrow{\Phi}^i(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}'}) + \overleftrightarrow{\Phi}^e(\vec{R}_{\vec{L}}, \vec{R}_{\vec{L}'}). \tag{24}$$

In general these force constants show no invariance with respect to lattice translation, as should be expected for a disordered system.

6. Do atoms in perfect crystals occupy their lattice sites?

For a perfect crystal one easily accepts that atoms vibrate about their average positions which form a regular lattice. The coherent elastic scattering of X-rays and neutrons confirm such a point of view. However, one should remember that diffraction patterns are always obscured by the presence of thermal vibrations. It is not easy to separate, in diffraction patterns, features due to thermal vibrations $\overleftarrow{u}_{\vec{L}}$ from those due to eventual permanent displacements $\vec{p}_{\vec{L}}$. In principle this can be done by extrapolating the measured Debye--Waller factor to 0 K. Only if the factor converges to a known value corresponding to zero--point vibrations, can one safely say that the permanent displacements are absent.

Let us consider the problem from the point of view of the theory developed above. The necessary condition for a system to be stable is that the first order force constants are zero and the phonon frequencies $\omega_q^2 > 0$. The equation $\vec{\Phi}(\vec{L}) = 0$ has been proven for the Bravais structure perfect crystals only, it seems. Namely, the less restrictive equation $\Sigma_{\vec{L}} \vec{\Phi}(\vec{L}) = 0$, expressing the translational invariance of the potential energy of ions in a perfect crystal has been shown to be fulfilled for monoatomic crystals with inversion symmetry [7]. For the Bravais crystals ($\vec{b} = 0$) both expressions are equivalent, because

$\vec{\Phi}(\vec{l}) = \vec{\Phi}(0)$, due to periodicity. It can be readily shown, by the Taylor expansion of the LHS of Eq. (23) with respect to $\vec{p}_{\vec{l}}$ that really $\vec{\Phi}(\vec{l}) = 0$ leads to $\vec{p}_{\vec{l}} = 0$.

We conclude that if a system structure is topologically equivalent to a Bravais structure and permanent displacements are small, then necessarily $\vec{p}_{\vec{l}} = 0$, i.e. simply the system has the Bravais structure. In the other words — there are no permanent displacements in the Bravais structure crystals and average atom positions coincide with lattice sites. For other crystals such a statement is not a priori obvious — perhaps there exist "perfect" monoatomic crystals with $\vec{p}_{\vec{L}} \neq 0$.

7. *Discussion*

The concept of the effective potential P requires that single ion-electron potentials $w^{\vec{L}}(\vec{r})$ be close to each other. It is possible only, when all ions of the system have equal valency, $Z_{\vec{L}} = Z$. It means that the present considerations should be applicable mainly to crystals with substitutional impurities and to the alloys of the elements of the same valency, eq. Na in K, Sb in Bi etc. Even then the concept of a crystal topology discriminates structural defects, like vacancies, interstitials etc.

The dielectric matrix formulation of the harmonic theory of lattice vibrations in an ideal, perfect crystal [6, 7] is complete in the sense, that terms of higher than second order in V (Eq. (2)) contribute to the crystal energy only the terms which are of the same order in ionic displacements $\vec{u}$. In the presence of permanent displacements $\vec{p}_{\vec{L}}$ these higher order terms are (roughly) $\sim(p+u)^n$, $n \geqslant 3$, and so produce the contributions $\sim u \cdot p^{n-1}$ and $u^2 \cdot p^{n-2}$. It seems that for the permanent displacements relatively small (e.g. $\langle p \rangle^2 \approx \langle u^2 \rangle$), these contributions are also small. Still, one should remember that the expressions for force constants (18, 19) are only approximate, being the first terms of an infinite expansions.

To carry out actual calculations one has to invert the "matrix" $\varepsilon_P(1,2)$. Let its Fourier transform be $\varepsilon_P(\vec{\kappa}+\vec{q}, \vec{\kappa}'+\vec{q})$. As it is defined for an effective crystal, we can calculate $\varepsilon_P^{-1}(\vec{\kappa}+\vec{q}, \vec{\kappa}'+\vec{q})$ using e.g. the localized function factorization method (see e.g. [9]), developed for ideal crystals, and then retransform it back to obtain $\varepsilon_P(1, 2)$.

The present theory is based on the Hartree approximation for the electron energy. It seems that the exchange effects can be accounted for in much the same way as for ideal crystals (see e.g. [6, 9]).

To conclude: The total static electron energy of our disordered system having the crystal topology has been expressed as the sum of the total electron energy of an effective periodic crystal and the perturbation contribution of the second order in an "ordering" potential. Second order force constants consist of the ion-ion interaction part and the electronic part, which describes the interaction between two real ions, caused by the electron redistribution of the fictitious effective crystal. The periodic electron potential of this crystal involves information on both positional and compositional disorder in the system.

It has been shown that in the Bravais structure crystals there is no the permanent displacements of atoms from their lattice sites.

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