7.75 — Mechanika sieci krystalicznej. Defekty. Dyslokacje.

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HAMILTONIAN FOR ANISOTROPIC BODIES WITH DEFECTS

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anharmonicity of crystal for various types of dislocations in a wide range of temperatures is given. But all considerations were restricted by using of Hamiltonian for isotropic bodies given by Bross [5], which appears to be a good example of the given above remarks. The great progress in experimental efforts to iluminate the fundamental facts in the dislocation dynamics which have been observed for the last fifteen years caused next demands on the theoretical studies and forced the more detailed calculations. These new requirements of experiments makes to leave the isotropic approximative description of anharmonicity and involve calculations with the more complete regarding the anisotropy of crystals.

The aim of the paper is the generalization of the Hamiltonian obtained by Bross [5] for the isotropic case, on the crystal with an arbitrary anisotropy. The immediate interest of a problem lyies among others on a fact that the most experiments made recently on the dynamics of dislocations were accomplished on crystals with the known third order elastic constants tensors while simultaneously there are no sufficient information on isotropic Murnaghan moduli [6 - 8]. In the construction of the Hamiltonian we follow all the approximations used by Bross [5], excluding isotropy. It means that we use continuous description of a body which is, strictly speaking, valid at low temperatures only, when in phonon spectrum predominate the long wave phonons. The obtained Hamiltonian describes the interaction of defects with the acoustic branch of phonons. As it was shown in [2] and [9], contribution of optical branch of phonons in interaction with defects can be macroscopically expressed in terms of electrostriction effect. The existing estimations exhibit however that the contribution of the optical phonons to dislocation dragging is usually non-esential as compared to the contribution of acoustical modes.

2. Hamiltonian

The interaction of lattice defects with thermal crystal vibrations /phonons/ exhibits in calculations if we include into considerations at least the first anharmonic terms of elastic energy. To be consequent in treatment we have to apply simultaneously the nonlinear theory of elasticity.

In frames of the continual approach the energy density of the deformed anisotropic medium described by the strain tensor γ_{ij} can be defined, with the accuracy to the third order terms, as follows

$$\Phi(\gamma) = \frac{1}{2} c_{ijkl} \gamma_{ij} \gamma_{kl} + \frac{1}{6} c_{ijklmn} \gamma_{ij} \gamma_{kl} \gamma_{mn} , \qquad /2.1/$$

where c_{ijkl} and c_{ijklmn} are the second and third order elastic constants tensors respectively. At the first glance it seems that to construct the Hamiltonian of the interaction of phonons with a lattice defect in the continual approximation it is enough to put into Eqn./2.1/ the sum of strain tensors of the defect field and thermal vibrations of a medium and the mixed terms appear the searched quantity. Unfortunately the above procedure, strictly speaking, is not correct, because in the nonlinear theory of elasticity the total strain tensor of the final deformation state is not the quantity that can be constructed as a simple sum of deformations caused by separate /here defects and thermal vibrations/ phenomena.

In our approach we use the notation /with certain modifications/ introduced by E.Kröner and A.Seeger [10] and E.Kröner [11] and developed by H.Bross [5].

We distinguish the three configurations of a body:

$C_{(1)}$ - ideal configuration, without defects of a crystal lattice, without any strains;

$C_{(2)}$ - configuration with defects of a lattice /point defects, dislocations etc./;

$C_{(3)}$ - configuration with defects of a lattice and strains caused e.q. by thermal vibrations.

We establish a certain Cartesian coordinate systems, called the common frame, in which we define distances between two neighbour mass points in all three configurations of a body:

$$d x^2_{(L)} = d x_i^{(L)} d x_i^{(L)} , \qquad i,L = 1,2,3. \qquad /2.2/$$

We denote by (L) the number of a configuration. Next we define the Green strain tensor $\gamma_{ij}^{(KL)}$ /in Lagrange coordinates/ and the Almansi - Cauchy strain tensor $\varepsilon_{ij}^{(KL)}$ /in Euler coordinates/ as follows

$$dx_{(L)}^2 - dx_{(K)}^2 = 2\gamma_{ij}^{(LK)}\, dx_i^{(K)}\, dx_j^{(K)} \;,$$

$$dx_{(L)}^2 - dx_{(K)}^2 = 2\varepsilon_{ij}^{(LK)}\, dx_i^{(L)}\, dx_j^{(L)} \;. \qquad L > K \qquad /2.3/$$

By $A_{ij}^{(KL)}$ we denote the operator which transforms the differentials in $C_{(L)}$ configuration into $C_{(K)}$ configuration /the bracket (KL) always means that we go from $C_{(L)}$ into $C_{(K)}$ cofiguration/, and for example

$$dx_k^{(2)} = A_{kj}^{(21)}\, dx_j^{(1)} \;, \quad dx_k^{(3)} = A_{kj}^{(32)}\, dx_j^{(2)} \;, \qquad /2.4/$$

and the Green and Almansi - Cauchy strain tensors are connected by the following transformation rules

$$\gamma_{ij}^{(21)} = A_{ki}^{(21)} A_{lj}^{(21)} \varepsilon_{kl}^{(21)} \;, \quad \varepsilon_{kl}^{(21)} = A_{ik}^{(12)} A_{jl}^{(12)} \gamma_{ij}^{(21)} \;. \qquad /2.5/$$

As it was shown by Bross [5] the total strain $\gamma_{ij}^{(31)}$ reads

$$\gamma_{ij}^{(31)} = \gamma_{ij}^{(21)} + \eta_{ij} \qquad /2.6/$$

where

$$\eta_{ij} = A_{ki}^{(21)} A_{lj}^{(21)} \gamma_{kl}^{(32)} \;, \qquad /2.7/$$

which is caused by an obvious fact that in a process of deformation the reference configuration is deformed and by the sequential deformation process the refrence configuration need to be changed. Below we give the set of formulae which we use through the paper. For more details see Bross [5].

We define the displacement vectors $\underline{s}$ and $\underline{u}$ as follows*

$$\underline{x}^{(2)} = \underline{x}^{(1)} + \underline{s} , \qquad \underline{x}^{(3)} = \underline{x}^{(2)} + \underline{u} . \qquad /2.8/$$

The operators $A_{ij}^{(21)}$ and $A_{ij}^{(32)}$ we can always represent in the following way

$$A_{ij}^{(21)} = \delta_{ij} + s_{i,j} , \quad A_{ij}^{(32)} = \delta_{ij} + u_{i,j} \qquad /2.9/$$

where $s_{i,j}$ is a distorsion field caused by lattice defects and $u_{i,j}$ is a distorsion caused by thermal vibrations.
If we put /2.9/ into the known expression for strain /see e.g. [12]/

$$\gamma_{ij}^{(21)} = \frac{1}{2}\left(A_{ki}^{(21)} A_{kj}^{(21)} - \delta_{ij}\right), \quad \gamma_{ij}^{(32)} = \frac{1}{2}\left(A_{ki}^{(32)} A_{kj}^{(32} - \delta_{ij}\right), \qquad /2.10/$$

we obtain that

$$\gamma_{ij}^{(21)} = s_{(ij)} + \frac{1}{2} s_{k,i} s_{k,j} , \quad \gamma_{ij}^{(32)} = u_{(ij)} + \frac{1}{2} u_{k,i} u_{k,j} , \qquad /2.11/$$

where

$$s_{(ij)} = \frac{1}{2}\left(s_{i,j} + s_{j,i}\right), \quad u_{(ij)} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right). \qquad /2.12/$$

The energy introduced into a body by no defect-type factors /e.g. thermal vibrations/

$$\Delta E = E_{(3)} - E_{(2)} , \qquad /2.13/$$

*In the case of a dislocation-type defect, we have to take into account the jump of the displacement field on the cut plane. This fact is with no importance in what follows, because we shall consider unique defined distorsions only.

where we define energies of the respective configurations as follows

$$E_{(2)} = \int dV_{(1)} \Phi(\gamma^{(21)}) \,, \quad E_{(3)} = \int dV_{(1)} \Phi(\gamma^{(31)}) \,, \qquad /2.14/$$

and the integration extends over the whole body. $V_{(K)}$ stands for the volume of the body in the configuration $C_{(K)}$.
We intend to provide all our calculations relative to the $C_{(2)}$ configuration, therefore we write

$$\Delta E = \int dV_{(2)} \left| \frac{\partial V_{(1)}}{\partial V_{(2)}} \right| \left[\Phi(\gamma^{(31)}) - \Phi(\gamma^{(21)}) \right] = \int dV_{(2)} \Psi \,, \qquad /2.15/$$

where $|\partial V_{(1)} / \partial V_{(2)}| = \varrho_{(2)} / \varrho_{(1)}$, $\varrho_{(K)}$ means the density of mass in a proper configuration, and

$$\Psi = \frac{\varrho_{(2)}}{\varrho_{(1)}} \left[\Phi(\gamma^{(31)}) - \Phi(\gamma^{(21)}) \right] = \Psi_{ph} + \Psi_{p-d} \qquad /2.16/$$

We denote by Ψ_{ph} the pure phonon terms, and by Ψ_{p-d} the terms describing the phonon-defect interactions. Taking into account Eqns /2.1/ and /2.6/ one obtains

$$\Phi(\gamma^{(31)}) = \Phi(\gamma^{(21)}) + \Phi(\eta) + \Phi_1 + S_{ij} \eta_{ij} \,, \qquad /2.17/$$

where

$$\Phi_1 = \frac{1}{2} c_{ijklmn} \eta_{ij} \eta_{kl} \gamma^{(21)}_{mn} . \qquad /2.18/$$

We deal in our approach with two stress tensors [12]:

S_{ij} - Kirchoff stress tensor, referred to the ideal configuration $C_{(1)}$;

σ_{ij} - Euler stress tensor, referred to the defected configuration $C_{(2)}$.

These two are connected by the following transformation rules

$$S_{ij} = \frac{\rho_{(1)}}{\rho_{(2)}} A^{(12)}_{il} A^{(12)}_{jm} \sigma_{lm} ,$$

$$\sigma_{lm} = \frac{\rho_{(2)}}{\rho_{(1)}} A^{(21)}_{li} A^{(21)}_{mj} S_{ij} , \qquad /2.19/$$

and read

$$S_{ij} = c_{ijkl} \gamma^{(21)}_{kl} + \frac{1}{2} c_{ijklmn} \gamma^{(21)}_{kl} \gamma^{(21)}_{mn} ,$$

$$\sigma_{ij} = c_{ijkl} \varepsilon^{(21)}_{kl} + \frac{1}{2} c_{ijklmn} \varepsilon^{(21)}_{kl} \varepsilon^{(21)}_{mn} . \qquad /2.20/$$

From /2.7/ and /2.19/ it follows that

$$S_{ij} \eta_{ij} = S_{ij} A^{(21)}_{ki} A^{(21)}_{lj} \gamma^{(32)}_{kl} = \frac{\rho_{(1)}}{\rho_{(2)}} \sigma_{kl} \gamma^{(32)}_{kl} \qquad /2.21/$$

Making use of /2.11/ one can write that /we shall write V for $V_{(2)}$/

$$I_{stress} = \int dV \frac{\rho_{(2)}}{\rho_{(1)}} S_{ij} \eta_{ij} = \int dV \sigma_{ij} \gamma^{(32)}_{ij} =$$

$$= \int dS^{(2)}_i \sigma_{ij} u_j - \int dV \sigma_{ij,j} u_i + \frac{1}{2} \int dV \sigma_{ij} u_{m,i} u_{m,j} . \qquad /2.22/$$

The first two terms in /2.22/ vanish because of the Born - von Karman periodic boundary conditions and due to equilibrium condition $\sigma_{ij,j} = 0$ respectively.

According to our approximation we take into account at most the third order terms, therefore

$$I_{stress} = \frac{1}{2} \int dV c_{ijkl}\, u_{m,i}\, u_{m,j}\, \varepsilon^{(21)}_{kl} \qquad /2.23/$$

If we apply Eqns /2.7/, /2.10/, /2.11/ and /2.5/ to the rest terms in /2.17/ we find that

$$\Phi_1 = \frac{1}{2} c_{ijklmn}\, u_{(ij)}\, u_{(kl)}\, s_{(mn)} \quad , \qquad /2.24/$$

and

$$\begin{aligned} \Phi(\eta) = {} & \frac{1}{2} c_{ijkl}\, u_{(ij)}\, u_{(kl)} + \frac{1}{6} c_{ijklmn}\, u_{(ij)}\, u_{(kl)}\, u_{(mn)} + \\ & \frac{1}{6} \left(c_{ijln} \delta_{km} + c_{kljn} \delta_{im} + c_{mnjl} \delta_{ik} \right) u_{i,j}\, u_{k,l}\, u_{m,n} + \\ & + \frac{1}{2} \left(c_{ijln} \delta_{km} + c_{ijkn} \delta_{lm} + e_{kljn} \delta_{im} + e_{klin} \delta_{jm} \right) u_{(ij)}\, u_{(kl)}\, s_{m,n} . \end{aligned} \qquad /2.25/$$

At this point we can built up the Hamiltonian of the problem under consideration

$$H = T + \Delta E , \qquad /2.26/$$

where the kinetic energy term T reads

$$T = \frac{1}{2} \int dV \varrho_{(2)}\, \dot{u}_i\, \dot{u}_i = \frac{1}{2} \int dV \varrho_{(1)}\, \dot{u}_i\, \dot{u}_i \left(1 - \varepsilon^{(21)}_{kk} \right) , \qquad /2.27/$$

and

$$\Psi_{ph} = \frac{1}{2} c_{ijkl} u_{(ij)} u_{(kl)} + \frac{1}{6} c_{ijklmn} u_{(ij)} u_{(kl)} u_{(mn)} + \\ + \frac{1}{6}\left(c_{ijln}\delta_{km} + c_{kljn}\delta_{im} + c_{mnjl}\delta_{ik}\right) u_{i,j} u_{k,l} u_{m,n} \, ,$$

$$\Psi_{p-d} = \frac{1}{2} c_{ijklmn} u_{(ij)} u_{(kl)} s_{(mn)} + \frac{1}{2} c_{ijkl} u_{s,i} u_{s,j} \varepsilon^{(21)}_{kl} + \\ + \frac{1}{2}\left(c_{ijln}\delta_{km} + c_{ijkn}\delta_{lm} + c_{kljn}\delta_{im} + c_{klin}\delta_{jm}\right) u_{(ij)} u_{(kl)} s_{mn} \\ - \frac{1}{2} c_{ijkl} u_{(ij)} u_{(kl)} \varepsilon^{(21)}_{ss} \, . \qquad /2.28/$$

It follows from Eqns $/2.12_1/$ and $/2.8_1/$ that

$$\varepsilon^{(21)}_{ij} \approx \gamma^{(21)}_{ij} \, , \qquad /2.29/$$

with the accuracy to the second order terms. On the other hand the similar situation takes place for $\gamma^{(21)}_{ij}$ and $s_{(ij)}$ /Eqn. /2.10//. Thus we do not make an error, beeing consistent with our approximation, if we, taking into account the symmetry of the expression, put into Eqn. /2.28/

$$\varepsilon^{(21)}_{ij} \approx s_{(ij)} \, , \qquad /2.30/$$

and we can write Eqn. /2.28/ in a more compact form

$$\Psi_{ph} = \frac{1}{2}\left(c_{ijkl} u_{i,j} u_{k,l} + \bar{c}_{ijklmn} u_{i,j} u_{k,l} u_{m,n}\right) ,$$

$$/2.31/$$

$$\Psi_{p-d} = \frac{1}{2} \tilde{c}_{ijklmn} u_{i,j} u_{k,l} s_{m,n} \, ,$$

where

$$\bar{c}_{ijklmn} = \frac{1}{3}\left(c_{ijklmn} + c_{ijln}\delta_{km} + c_{kljn}\delta_{im} + c_{mnjl}\delta_{ik}\right) \qquad /2.32/$$

$$\tilde{c}_{ijklmn} = c_{ijklmn} - c_{ijkl}\delta_{mn} + c_{mnjl}\delta_{ik}$$
$$+ c_{ijln}\delta_{km} + c_{ijkn}\delta_{lm} + c_{kljn}\delta_{im} + c_{klin}\delta_{jm} . \qquad /2.33/$$

Equations /2.32/ and /2.33/ show how the existence of a defect in a crystal lattice modifies elastic properties of a body.

3. First and second quatization

We follow the standard procedure /see e.g. Maradudin et al. [13]/, and introduce the following representation

$$u_i(\underline{x}) = \frac{1}{\sqrt{\varrho_{(1)} V_{(2)}}} \sum_{\alpha} e_{\alpha i} Q_\alpha(t) e^{i\underline{k}\,\underline{x}} ,$$

$$u_{i,j}(\underline{x}) = \frac{i}{\sqrt{\varrho_{(1)} V_{(2)}}} \sum_{\alpha} e_{\alpha i} Q_\alpha(t) k_j e^{i\underline{k}\,\underline{x}} , \qquad /3.1/$$

$$s_{i,j}(\underline{x}) = \sum_{\underline{q}} \hat{s}_{i,j}(\underline{q}) e^{i\underline{q}\,\underline{x}} ,$$

where $\alpha = (\underline{k}, \lambda)$, $\underline{k}$ is the wave vector and λ polarization mode of the wave with the wave vector $\underline{k}$. By $\underline{e}_\alpha$ we denote the polarization vector. The normalizing factor $1/\sqrt{\varrho_{(1)} V_{(2)}}$ allows to represent the kinetic energy term in the canonical form. From the reality of displacement it follows that

$$Q^*_\alpha(t) = Q_{\bar{\alpha}}(t) = Q_\lambda(-\underline{k}, t) . \qquad /3.2/$$

The polarization vectors $\underline{e}_\alpha$ fulfil the obvious orthonormality and clousure conditions [13]

$$\underline{e}_\lambda(\underline{k}) \cdot \underline{e}_{\lambda'}(\underline{k}) = \delta_{\lambda\lambda'} , \qquad /3.3/$$

$$\sum_{\lambda} e^{*}_{\lambda i}(\underline{k})\, e_{\lambda_j}(\underline{k}) = \delta_{ij} \,. \qquad /3.4/$$

Simple calculations give the following formula

$$\begin{aligned} H = {} & \frac{1}{2}\sum_{\alpha}\left[\dot{Q}_{\alpha}(t)\dot{Q}^{*}_{\alpha}(t) + \omega^{2}_{\alpha} Q_{\alpha}(t) Q^{*}_{\alpha}(t)\right] + \\ & + \frac{1}{2}\sum_{\alpha\beta}\Big[- e_{\alpha i} e^{*}_{\beta i}\, \dot{Q}_{\alpha}(t)\dot{Q}^{*}_{\beta}(t)\, \hat{s}_{j,j}(\underline{k}'-\underline{k}) + \\ & \quad + \frac{1}{\varrho_{(1)}} \tilde{c}_{ijrpmn}\, e_{\alpha i} e^{*}_{\beta r} k_j k'_p\, Q_{\alpha}(t) Q^{*}_{\beta}(t)\, \hat{s}_{m,n}(\underline{k}'-\underline{k})\Big] + \\ & - \frac{iV}{2(\varrho_{(1)}V)^{3/2}} \sum_{\alpha\beta\gamma} \bar{c}_{ijrpmn}\, e_{\alpha i} e_{\beta r} e_{\gamma m}\, k_j k'_p k''_n\, Q_{\alpha} Q_{\beta} Q_{\gamma}\, \delta_{\underline{k}'', -(\underline{k}+\underline{k}')} \,, \end{aligned} \qquad /3.5/$$

where we used the relation

$$c_{ijmn}\, e_{\alpha m} k_n k_j = \varrho_{(1)}\, \omega^{2}_{\alpha}\, e_{\alpha i} \,, \qquad /3.6/$$

and obtained, that for two - phonon interactions /here scattering of phonons on lattice defects/

$$\underline{k}' = \underline{k} + \underline{q} \qquad /3.7/$$

Alone the third term in /3.5/ is volume dependent because it describes the termal expansion of a body.
The second quantization takes place if we introduce the creation $a^{+}_{\alpha} = a^{+}_{\lambda}(\underline{k})$ and annihilation $a_{\alpha} = a_{\lambda}(\underline{k})$ operators [13] in the following way

$$\begin{aligned} Q_{\alpha} &= \sqrt{\frac{\hbar}{2\omega_{\alpha}}}\left(a^{+}_{\alpha} + a_{\alpha}\right) = \sqrt{\frac{\hbar}{2\omega_{\alpha}}}\, A_{\alpha} \,, \\ P_{\alpha} &= \dot{Q}_{\alpha}(t) = i\sqrt{\frac{\hbar\omega_{\alpha}}{2}}\left(a^{+}_{\alpha} - a_{\alpha}\right) = -i\sqrt{\frac{\hbar\omega_{\alpha}}{2}}\, B_{\alpha} \,. \end{aligned} \qquad /3.8/$$

The operators fulfil the following commutation rules

$$[Q_\alpha, P_\beta^*] = i\hbar\,\delta_{\alpha\beta}, \quad [a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}, \quad [a_\alpha, a_\beta] = [a_\alpha^\dagger, a_\beta^\dagger] = 0, \tag{3.9}$$

where

$$\delta_{\alpha\beta} = \delta_{\underline{k}\,\underline{k}'}\,\delta_{\lambda\lambda'}. \tag{3.10}$$

If we put /3.8/ into /3.5/ we obtained that

$$\begin{aligned} H = {} & \sum_\alpha \left(a_\alpha^\dagger a_\alpha + \tfrac{1}{2}\right)\hbar\omega_\alpha + \\ & + \frac{1}{2}\sum\Big(-e_{\alpha i}e_{\beta i}^*\,\hat{s}_{j,j}(\underline{k}'-\underline{k})\,\frac{\hbar\sqrt{\omega_\alpha\omega_\beta}}{2}\,B_\alpha B_\beta^\dagger + \\ & + \tilde{c}_{ijrpmn}\,e_{\alpha i}\,e_{\beta r}^*\,k_j k_p'\,\hat{s}_{m,n}(\underline{k}'-\underline{k})\,\frac{\hbar}{2\varrho_{(1)}\sqrt{\omega_\alpha\omega_\beta}}\,A_\alpha A_\beta^\dagger\Big) + \\ & - \frac{iV}{2}\left(\frac{\hbar}{\varrho_{(1)}V}\right)^{3/2}\sum_{\alpha\beta\gamma}\frac{\bar{c}_{ijrpmn}\,e_{\alpha i}\,e_{\beta r}\,e_{\gamma m}\,k_j k_p' k_n''\,A_\alpha A_\beta A_\gamma}{\sqrt{\omega_\alpha\omega_\beta\omega_\gamma}}\;\delta_{\underline{k}'',-(\underline{k}+\underline{k}')}, \end{aligned} \tag{3.11}$$

where we used the following properties of A_α and B_α operators

$$A_\lambda(\underline{k}) = A_\lambda^\dagger(-\underline{k}), \tag{3.12}$$

$$B_\lambda(\underline{k}) = -B_\lambda^\dagger(-\underline{k}), \tag{3.13}$$

and that

$$\frac{1}{4}\sum_\alpha \hbar\omega_\alpha\left(A_\alpha A_\alpha^\dagger + B_\alpha B_\alpha^\dagger\right) = \sum_\alpha \hbar\omega_\alpha\left(a_\alpha^\dagger a_\alpha + \tfrac{1}{2}\right). \tag{3.14}$$

The obtained Hamiltonian /3.11/ describes two- and three-phonon processes in a crystal lattice with defects.

4. Comparison with the isotropic case

For the crystals with the highest anisotropy, i.e. for those which belong to the triclinic system, we have 81 and 729 non vanishing components of the second and third order elastic constants tensors respectively. Symmetry conditions reduce them considerably and for the cubic crystals we have independent three and six components only, and moreover [14]

- for the second order

$$\begin{aligned} &c_{11} = c_{22} = c_{33}, \\ &c_{12} = c_{23} = c_{13}, \\ &c_{44} = c_{55} = c_{66}, \text{ and all others zero} \end{aligned} \qquad /4.1/$$

- for the third order

$$\begin{aligned} &c_{111} = c_{222} = c_{333}, \\ &c_{144} = c_{255} = c_{366}, \\ &c_{112} = c_{223} = c_{133} = c_{113} = c_{122} = c_{233}, \\ &c_{155} = c_{244} = c_{344} = c_{166} = c_{266} = c_{355}, \\ &c_{123}, \\ &c_{145}, \text{ and all others zero.} \end{aligned} \qquad /4.2/$$

We have used here the abbreviated Voigt notation

$$\begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \\ \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ 1 & 2 & 3 & 4 & 5 & 6 \end{array}$$

The isotropic bodies are described by two second order λ and μ and three third order ν_1, ν_2 and ν_3 Lamé constants, namely

$$\begin{aligned} &c_{11}^{iso} = \lambda + 2\mu, \quad c_{12}^{iso} = \lambda, \quad c_{44}^{iso} = \mu, \\ &c_{123}^{iso} = \nu_1, \quad c_{144}^{iso} = \nu_2, \quad c_{456}^{iso} = \nu_3, \\ &c_{112}^{iso} = \nu_1 + 2\nu_2, \quad c_{155}^{iso} = \nu_2 + 2\nu_3, \quad c_{111}^{iso} = \nu_1 + 6\nu_2 + 8\nu_3. \end{aligned} \qquad /4.3/$$

The energy density in this case has a form [15], [16]

$$\Phi = \frac{1}{6}[\nu_1 I_I^3(\gamma) + 6\nu_2 I_I(\gamma) I_I(\gamma^2) + 8\nu_3 I_I(\gamma^3)] =$$

$$= A_1 I_I^2(\gamma) + A_2 I_{II}(\gamma) + A_3 I_I^3(\gamma) + A_4 I_I(\gamma) I_{II}(\gamma) + A_5 I_{III}(\gamma), \qquad /4.4/$$

where

$$I_I(\gamma) = \gamma_{ii},$$

$$I_{II}(\gamma) = \frac{1}{2}[(\gamma_{ii})^2 - \gamma_{ij}\gamma_{ij}],$$

$$I_{III}(\gamma) = \frac{1}{6}[2\gamma_{ik}\gamma_{kj}\gamma_{ji} - 3\gamma_{kk}\gamma_{ij}\gamma_{ji} + (\gamma_{ii})^3], \qquad /4.5/$$

are strain invariants [17].

The constants A_i can be expressed by the Lamé constants and by the Murnaghan moduli l, m, n in the following way

$$A_1 = \frac{\lambda + 2\mu}{2}, \qquad A_3 = \frac{l + 2m}{3}$$

$$A_2 = -2\mu, \qquad A_4 = -2m, \qquad /4.6/$$

$$A_5 = n.$$

The third order Lamé constants and Murnaghan moduli are connected by the following relations [16]

$$\nu_1 = 6A_3 + 3A_4 + A_5 = 2l - 2m + n, \qquad l = \frac{1}{2}\nu_1 + \nu_2,$$

$$\nu_2 = -\frac{1}{2}A_4 + A_5 = m - \frac{1}{2}n, \qquad m = \nu_2 + 2\nu_3, \qquad /4.7/$$

$$\nu_3 = \frac{1}{4}A_5 = \frac{1}{4}n, \qquad n = 4\nu_3.$$

Now we introduce the shorthand notation which we shall use through this paragraph.

$$\Delta^{o}_{ijkl} = \delta_{ij}\,\delta_{kl} \,,$$

$$\Delta^{o}_{ijklmn} = \delta_{ij}\,\delta_{kl}\,\delta_{mn} \,,$$

$$\Delta_{ijkl} = \delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk} = \begin{cases} 2 & \\ 1 & \text{if} \\ 0 & \end{cases} \begin{array}{l} i=j=k=l \\ i=k \wedge j=l \vee i=l \wedge j=k, \\ \text{otherwise}, \end{array} \qquad /4.8/$$

$$\Delta_{ijklmn} = \delta_{ij}\,\Delta_{klmn} \,,$$

$$\nabla_{ijkl} = \delta_{ik}\,\delta_{jl} - \delta_{il}\,\delta_{jk} = \varepsilon_{sij}\,\varepsilon_{skl} \,,$$

$$\nabla_{ijklmn} = \delta_{ij}\left(\delta_{km}\,\delta_{ln} - \delta_{kn}\,\delta_{lm}\right) = \delta_{ij}\,\varepsilon_{skl}\,\varepsilon_{smn} \,.$$

The symbol Δ_{ijkl} has the following symmetry properties

$$\Delta_{ijkl} = \Delta_{klij} = \Delta_{jikl} = \Delta_{ijlk} \,. \qquad /4.9/$$

In this notation the isotropic elastic constants tensors [17], [18] have the form

$$c^{iso}_{ijkl} = \lambda\,\Delta^{o}_{ijkl} + \mu\,\Delta_{ijkl} \,,$$

$$\begin{aligned} c^{iso}_{ijklmn} &= \nu_1\,\Delta^{o}_{ijklmn} + \nu_2\left(\Delta_{ijklmn} + \Delta_{klijmn} + \Delta_{mnijkl}\right) + \\ &+ \nu_3\left(\Delta_{ikjlmn} + \Delta_{iljkmn} + \Delta_{jkilmn} + \Delta_{jlikmn}\right) = \qquad /4.10/ \\ &= 2l\,\Delta^{o}_{ijklmn} + m\,\bar{\Delta}_{ijklmn} + n\left(\tfrac{1}{4}\,\tilde{\Delta}_{ijklmn} - \tfrac{1}{2}\,\bar{\Delta}_{ijklmn}\right), \end{aligned}$$

where

$$\bar{\Delta}_{ijklmn} = \Delta_{ijklmn} + \Delta_{klijmn} + \Delta_{mnijkl} - 2\,\Delta^{o}_{ijklmn} \,,$$

$$\tilde{\Delta}_{ijklmn} = \Delta_{ikjlmn} + \Delta_{iljkmn} + \Delta_{jkilmn} + \Delta_{jlikmn} \,. \qquad /4.11/$$

It is easy to find that $\tilde{\Delta}_{ijklmn}$ has the following symmetries in indices

$$\tilde{\Delta}_{ijklmn} = \tilde{\Delta}_{klijmn} = \tilde{\Delta}_{ijmnkl} = \tilde{\Delta}_{jiklmn} = \tilde{\Delta}_{ijlkmn} = \tilde{\Delta}_{ijklnm} \qquad /4.12/$$

Our modified elastic constants tensors have, in the isotropic case, the form

$$\begin{aligned} \bar{c}^{\,iso}_{ijklmn} = \tfrac{1}{3}\big[&\lambda\,(\Delta^{\circ}_{kmlnij} + \Delta^{\circ}_{imjnkl} + \Delta^{\circ}_{ikjlmn}) + \\ &+\mu\,(\Delta_{kmlnij} + \Delta_{imjnkl} + \Delta_{ikjlmn}) + \qquad /4.13/ \\ &+ 2l\,\Delta^{\circ}_{kmlnij} + m\,\bar{\Delta}_{ijklmn} + n\,(\tfrac{1}{4}\tilde{\Delta}_{ijklmn} - \tfrac{1}{2}\bar{\Delta}_{ijklmn})\big], \end{aligned}$$

$$\begin{aligned} \tilde{c}^{\,iso}_{ijklmn} = &\lambda\,(\Delta^{\circ}_{kmlnij} + \Delta^{\circ}_{lmknij} + \Delta^{\circ}_{imjnkl} + \Delta^{\circ}_{jminkl} + \Delta^{\circ}_{ikjlmn} - \Delta^{\circ}_{mnijkl}) + \\ &+\mu\,(\Delta_{kmlnij} + \Delta_{lmknij} + \Delta_{imjnkl} + \Delta_{jminkl} + \Delta_{ikjlmn} - \Delta_{mnijkl}) + \qquad /4.14/ \\ &+ 2l\,\Delta^{\circ}_{ijklmn} + m\,\bar{\Delta}_{ijklmn} + n\,(\tfrac{1}{4}\tilde{\Delta}_{ijklmn} - \tfrac{1}{2}\bar{\Delta}_{ijklmn}). \end{aligned}$$

The compare our results with those of Bross [5], we have to bring his Eqn. /4.18/ to our form. In Bross Eqn. /4.18/ appear three kinds of expressions, which are proportional to: $\gamma^{(32)}_{ij}\,\gamma^{(32)}_{kl}\,\gamma^{(32)}_{mn}$, $\gamma^{(32)}_{ij}\,\gamma^{(32)}_{kl}\,\varepsilon^{(21)}_{mn}$ and $\gamma^{(32)}_{ij}\,\varepsilon^{(21)}_{kl}\,\varepsilon^{(21)}_{mn}$.
The third kind of terms is present if one does not make use of the gradient theorem /2.22/. If we put our Eqn. /4.5/ into Bross /4.18/, we find easily that results of Bross for modyfied elastic constants tensors coincide exactly with ours.

5. An example: dislocation dragging

In this paragraph we give an example of application of the obtained Hamiltonian to calculation the dragging coefficient of dislocation. It is known [1] that in a certain region of not very low temperatures we can neglect phonon - phonon processes and the thermal vibrations /flutter - effect/ of the dislocation line. In this temperature region phonon wind is the most important mechanism of dislocation dragging. If the dislocation moves uniformly with the velocity v, small as compared to the velocity of sound c, then the quasi - static description of the elastic field of the moving dislocation is applicable,

$$s_{ij}(\underline{x},t) \approx s_{ij}(\underline{x}-\underline{v}t) = \sum_{\underline{q}} \hat{s}_{ij}(\underline{q})\, e^{i\Omega_q t}\, e^{i\underline{q}\underline{x}} , \qquad /5.1/$$

where

$$\Omega_q = \underline{q}\cdot\underline{v} . \qquad /5.2/$$

The effect of interaction of phonons with a moving dislocation through the regular crystall lattice describes the second term of the Hamiltonian /3.11/ i.e.

$$H_{p-d} = \sum_{\alpha\beta} (\cdot)\, e^{i\Omega_q t} \qquad /5.3/$$

This term is small as compared to the rest of the Hamiltonian and the time - dependent perturbation theory can be used [19]. In the first order approximation the probability of the scattering of the phonon from the starting state α_s to the final state α_f is given by the so called "Fermi second gold rule" [20].

$$P(\alpha_s \to \alpha_f) = 2|\langle\alpha_f|H_{p-d}|\alpha_s\rangle|^2 \frac{1-\cos(\omega_{fs}-\Omega_q)t}{\hbar^2(\omega_{fs}-\Omega_q)^2} =$$

$$= 4|\langle\alpha_f|H_{p-d}|\alpha_s\rangle|^2 \frac{\sin^2[(\omega_{fs}-\Omega_q)t/2]}{\hbar^2(\omega_{fs}-\Omega_q)^2} , \qquad /5.4/$$

where $\omega_{fs} = \omega_{\alpha_f} - \omega_{\alpha_s}$ and Ω_q is the frequency of the harmonic perturbation. It can be shown [21] that the factor

$$\frac{4 \sin^2[(\omega_{fs} - \Omega_q)t/2]}{\pi(\omega_{fs} - \Omega_q)^2 t} , \qquad /5.5/$$

behaves like the Dirac delta - function. If we avail of the property of the $\delta(\underline{x})$ that

$$\delta(ax) = \frac{1}{a}\delta(x) , \qquad /5.6/$$

we obtain that for the unit of time

$$P(\alpha_s \to \alpha_f) = \frac{2\pi}{\hbar^2} |\langle \alpha_f | H_{p-d} | \alpha_s \rangle|^2 \, \delta(\omega_{\alpha_f} - \omega_{\alpha_s} - \Omega_q) . \qquad /5.7/$$

Ket $|\alpha\rangle$ describes the state in which there are n_α phonons with the wave vector $\underline{k}$ and polarization λ . In what follows we shall use the occupation - number representation. In this representation creation and annihilation operators act as follows

$$a^\dagger_\alpha |n_\alpha\rangle = \sqrt{n_\alpha + 1}\, |n_\alpha + 1\rangle ,$$

$$a_\alpha |n_\alpha\rangle = \sqrt{n_\alpha}\, |n_\alpha - 1\rangle , \qquad /5.8/$$

where we write $|n_\alpha\rangle$ for $|\alpha\rangle$. The state vectors $|n_\alpha\rangle$ are orthonormalized

$$\langle n_\alpha | n_\beta \rangle = \delta_{\alpha\beta} , \qquad /5.9/$$

because they are the eigenfunctions of the Hamiltonian H [22]. To calculate the probability $P(\alpha_s \to \alpha_f)$ we have to find at first the value of the matrix element

$$\Xi(\alpha_s, \alpha_f) = \langle \alpha_f | H_{p-d} | \alpha_s \rangle . \qquad /5.10/$$

Because [13]

$$A_\lambda(\underline{k}) = a_\lambda(\underline{k}) + a^\dagger_\lambda(-\underline{k}) = A^\dagger_\lambda(-\underline{k}) ,$$
$$B_\lambda(\underline{k}) = a_\lambda(\underline{k}) - a^\dagger_\lambda(-\underline{k}) = -B^\dagger_\lambda(-\underline{k}) , \qquad /5.11/$$

we have

$$A_\alpha A^\dagger_\beta = (a_\lambda(\underline{k}) + a^\dagger_\lambda(-\underline{k}))(a^\dagger_{\lambda'}(\underline{k}') + a_{\lambda'}(-\underline{k}')) =$$
$$= (a^\dagger_{\bar{\alpha}} a^\dagger_\beta + a_\alpha a_{\bar{\beta}}) + a^\dagger_{\bar{\alpha}} a_{\bar{\beta}} + a_\alpha a^\dagger_\beta ,$$
$$\qquad /5.12/$$
$$B_\alpha B^\dagger_\beta = (a_\lambda(\underline{k}) - a^\dagger_\lambda(-\underline{k}))(a^\dagger_{\lambda'}(\underline{k}') - a_{\lambda'}(-\underline{k}')) =$$
$$= -(a^\dagger_{\bar{\alpha}} a^\dagger_\beta + a_\alpha a_{\bar{\beta}}) + a^\dagger_{\bar{\alpha}} a_{\bar{\beta}} + a_\alpha a^\dagger_\beta .$$

It is obvious that

$$\langle n_\alpha - 1, n_\beta + 1 | a^\dagger_{\bar{\alpha}} a^\dagger_\beta | n_\alpha, n_\beta \rangle = 0 ,$$
$$\qquad /5.13/$$
$$\langle n_\alpha - 1, n_\beta + 1 | a_\alpha a_{\bar{\beta}} | n_\alpha, n_\beta \rangle = 0 .$$

Let there are n_γ and n_δ phonons with defined $\underline{k}''$ and $\underline{k}'''$ wave vectors, and let there are $n_\gamma - 1$ and $n_\delta + 1$ phonons after the scattering process on the dislocation line.
Our matrix element reads now

$$\Xi(\alpha_s, \alpha_f) = \sum_{\alpha\beta} \Gamma_{\alpha\beta} \langle n_\gamma - 1, n_\delta + 1 | a^\dagger_{\bar{\alpha}} a_\beta + a_\alpha a^\dagger_\beta | n_\gamma, n_\delta \rangle , \qquad /5.14/$$

where

$$\Gamma_{\alpha\beta} = \frac{\hbar}{4} e_{\alpha i} e^{*}_{\beta r} \hat{s}_{m,n}(\underline{k}'-\underline{k})\left(\frac{\tilde{c}_{ijrpmn} k_j k'_p}{\varrho(1)\sqrt{\omega_\alpha \omega_\beta}} - \sqrt{\omega_\alpha \omega_\beta}\, \delta_{ir} \delta_{mn}\right). \qquad /5.15/$$

The summation extends over all available wave vectors $\underline{k}$ and $\underline{k}'$, what causes that appear nonvanishing terms for which e.g. $\underline{k} = \underline{k}''$ and $\underline{k}' = \underline{k}'''$. It allows to renumerate the proper terms. Finally we have

$$\begin{aligned}\Xi(\alpha_s, \alpha_f) &= \Gamma_{\alpha\beta} \langle n_\alpha - 1, n_\beta + 1 | a^{\dagger}_\beta a_\alpha + a_\alpha a^{\dagger}_\beta | n_\alpha, n_\beta \rangle = \\ &= 2\Gamma_{\alpha\beta} \sqrt{n_\alpha} \sqrt{n_\beta + 1}\,,\end{aligned} \qquad /5.16/$$

$$P(\alpha_s \to \alpha_f) = \frac{8\pi}{\hbar^2} |\Gamma_{\alpha\beta}|^2 n_\alpha (n_\beta + 1)\, \delta(\omega_\alpha - \omega_\beta - \Omega_q). \qquad /5.17/$$

The factor n_α says, that the intensity of scattering from the state with the wave vector $\underline{k}$ is proportional to the number of excitations already existed in that state. On the other hand factor $(n_\beta + 1)$ shows, that the discussed probability depends on the occupation level of a state with the wave vector $\underline{k}'$ as well. This effect it is the so called induced emission, which is typical to the Bose - Einstein particles [22].
The density number of phononsin the state α is given by an expression

$$n_\alpha = \left[\exp\left(\frac{\hbar\omega_\alpha}{k_B T}\right) - 1\right]^{-1}, \qquad /5.18/$$

where k_B is the Boltzmann constant and T is the absolute temperature. In every event of scattering the energy $\hbar\Omega_q = \hbar(\omega_\beta - \omega_\alpha)$ is transferred thus the dissipation of energy D per unit time and per unit length of a dislocation line is given by the formula

$$D = -\frac{8\pi}{L\hbar^2}\sum_{\alpha\beta}\Omega_q|\Gamma_{\alpha\beta}|^2 n_\alpha(n_\beta+1)\,\delta(\omega_\beta-\omega_\alpha-\Omega_q). \qquad /5.19/$$

This formula can be rewritten in another form which shows the action of the phonon wind. In order to do it we change the sequence of the indices α and β and make a sum

$$D = \frac{1}{2}\left\{-\frac{8\pi}{L\hbar^2}\sum_{\alpha\beta}|\Gamma_{\alpha\beta}|^2\delta(\omega_\beta-\omega_\alpha-\Omega_q)\Omega_q\left[n_\alpha(n_\beta+1)-n_\beta(n_\alpha+1)\right]\right\} =$$

$$= -\frac{4\pi}{L\hbar^2}\sum_{\alpha\beta}\Omega_q|\Gamma_{\alpha\beta}|^2(n_\alpha-n_\beta)\,\delta(\omega_\beta-\omega_\alpha-\Omega_q) \qquad /5.20/$$

The sign minus appears because Ω_q is the only odd function in respect of $\alpha-\beta$ permutation /see /3.7//

$$\Omega_q = \underline{q}\cdot\underline{v} = (\underline{k}'-\underline{k})\cdot\underline{v}\ . \qquad /5.21/$$

The dragging coefficient of the moving dislocation B is defined as a quotient of the dissipation of energy D and the square of velocity of the dislocation v , i.e.

$$B = \frac{D}{v^2} \qquad /5.22/$$

Having the formulae /5.15/ and /5.18/ and knowing the dispersion of the body $\omega = \omega_\lambda(\underline{k})$ we can find the temperature dependence of B , what is important to many practical reasons.

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