ANHARMONICITY EFFECTS IN THE PHONON SPECTRUM OF ANISOTROPIC CRYSTALS

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Expressions for the renormalized force constants of anisotropic crystal due to the effects of anharmonicity have been obtained in the self-consistent harmonic approximation. The phonon spectra for metals with a hexagonal close-packed lattice have been calculated for various directions of the wave vector. The effects of anharmonicity and the contributions of non-central forces to the vibration spectrum of titanium have been studied. The frequencies of atomic vibrations and the heights of potential barriers for diffusion activation were found to diminish owing to anharmonicity effects. The anisotropy in the dependences of vibration frequencies on the wave vector has been demonstrated to increase, if the ratio between the lattice periods c/a decreases ($c/a < 1.633$). The frequencies of crystal lattice vibrations were shown to decrease with the temperature growth due to anharmonicity effects.

1. Introduction

Owing to a low relative density and a high thermal stability, titanium and Ti-based alloys are widely applied in aviation and space technique. However, their relatively high creep imposes considerable restrictions upon their application. There is no unequivocal explanation for this phenomenon. In this work, we made an attempt to explain this phenomenon by the effects of anharmonicity and anisotropy of a crystal. Anharmonicity effects in crystal lattice vibrations have been studied in a good many works (see, e.g., works [1–4]).

In the framework of approaches developed in works [1–3], we consider the influence of anharmonicity on the phonon spectrum and the diffusion coefficient of crystals with a hexagonal close-packed structure for different values of the anisotropy parameter c/a, where a and c are the crystal lattice constants in the basic plane and normally to it, respectively. The role of non-central forces in the atom-to-atom interaction has also been investigated. We have proposed an expression for the diffusion coefficient in a crystal, which takes both the anharmonicity of crystal lattice vibrations and the crystal anisotropy into account.

2. Hamiltonian and Force Constants for Strongly Anharmonic Crystals

To describe systems with a strong anharmonicity, the self-consistent harmonic approximation is used. To obtain relevant equations and to generalize this approximation, an approach based on the time Green's function method and expounded in works [1,2] is applied.

In the case of a strongly anharmonic solid, an instant position $\mathbf{r}(l)$ of the l-th atom can be presented in the form

$$\mathbf{r}(l) = \langle \mathbf{r}(l) \rangle + \mathbf{u}(l) \equiv \mathbf{r}_0(l) + \mathbf{u}(l), \tag{1}$$

where $\langle \dots \rangle$ denotes the temperature averaging, $\mathbf{r}_0(l)$ is the average or equilibrium position of the l-th atom, and $\mathbf{u}(l)$ is a displacement of the l-th atom from its equilibrium position. If the potential energy Φ is expanded in a power series of atomic displacements, the Hamiltonian of the anharmonic oscillatory system looks like [3]

$$H = \frac{1}{2} \sum_x \frac{p^2(x)}{M(x)} +$$

$$+ \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{x_1 x_2 \dots x_n} \Phi(x_1 x_2 \dots x_n) u(x_1) u(x_2) \dots u(x_n) + \text{const}. \tag{2}$$

Here, $u(x)$, $p(x)$, and $M(x)$ stand for the displacement $u_\alpha(l)$, momentum $p_\alpha(l)$, and mass $M(l)$ of the l-th atom, respectively, and

$$\Phi(x_1 x_2 \dots x_n) = \left[\nabla(x_1) \nabla(x_2) \dots \nabla(x_n) \right]_0 \tag{3}$$

is the force constant of the n-th order. The subscript 0 means that the expression in brackets is calculated at equilibrium atomic positions $\{\mathbf{r}(l)\}$.

To obtain the equation of motion for the time Green's functions, the following equations are used:

$$[u(x), H] = \frac{i\hbar p(x)}{M(x)},$$

$$[p(x), H] = -i\hbar \sum_{n=1}^{\infty} \sum_{x_1 x_2 \ldots x_n} \Phi(x_1 x_2 \ldots x_n) u(x_1) \ldots u(x_n),$$
(4)

as well as the Wick theorem and the Fourier transformation. As a result, the equation of motion for the crystal lattice in the self-consistent harmonic approximation looks like

$$M(x)\omega^2 G(xx', \omega) = \delta_{xx'} + \sum_{n=1}^{\infty} \frac{1}{n!} \times$$

$$\times \sum_{x_1 x_2 \ldots x_n} \tilde{\Phi}(xx_1 x_2 \ldots x_n) \langle\langle u(x_1) \ldots u(x_n); u(x') \rangle\rangle_\omega,$$
(5)

where $\tilde{\Phi}(x_1 x_2 \ldots x_n) = \nabla(x_1)\nabla(x_2) \ldots \nabla(x_n)\langle\Phi(r)\rangle$, $\langle\Phi(r)\rangle = \langle\exp\sum_x u(x)\nabla(x)\Phi(r_0)\rangle \Phi(r_0)$ is the "effective potential", and $\tilde{\Phi}(x_1 x_2 \ldots x_n)$ are the "effective force constants". If the terms with $n = 1$ are left in Eq. (5), the latter coincides with the equation that describes crystal lattice vibrations in the harmonic approximation.

The physical essence of the effective force constants and the effective potential is as follows [3]. In an anharmonic solid, every atom vibrates near its average position with a large amplitude, so that it is subjected to anharmonic forces from surrounding atoms. If those forces are to be calculated, it is impossible to consider atoms as rigidly fixed, because the forces depend on the character of motion of surrounding atoms. The vibrations of an arbitrary atom are therefore governed by a potential created by other atoms, the motion of which induces a chaotic thermal modulation of the potential for this atom. The motions of all the atoms should be equivalent and self-consistent, so that they are determined by effective potentials and force constants in anharmonic solids.

In the framework of the approximation of noninteracting renormalized harmonic phonons ($n = 1$), the equation of motion reads

$$M(x)\omega^2 G(xx', \omega) = \delta_{xx'} + \sum_{x_1} \tilde{\Phi}(xx_1) G(x_1 x', \omega),$$
(6)

where

$$\tilde{\Phi}(xx') = \Phi(xx') +$$

$$+ \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{x_1 x_2 \ldots x_n} \Phi(xx' x_1 x_2 \ldots x_n) \langle u(x_1) \ldots u(x_n) \rangle. \quad (7)$$

Hence, in contrast to the conventional harmonic approximation, the force constants in the renormalized harmonic one (6) are determined by the thermodynamic averaging of the second derivatives of the potential rather than their equilibrium values.

The correlation functions are approximated in accordance with the Wick theorem, so that

$$\langle u(x_1) \ldots u(x_n) \rangle \approx (n-1)\langle u(x_1)u(x_2) \rangle \langle u(x_3) \ldots u(x_n) \rangle \approx$$

$$\approx (n-1)(n-3) \ldots 1 \langle u(x_1)u(x_2) \rangle \ldots \langle u(x_{n-1})u(x_n) \rangle,$$
(8)

where the symmetry of force constants with respect to the subscript permutation has been taken into account.

By substituting Eq. (8) into Eq. (7), we obtain the following expression for renormalized force constants:

$$\tilde{\Phi}(xx') = \nabla(x)\nabla(x') \exp\left\{\frac{1}{2} \sum_{x_1 x_2} \langle u(x_1)u(x_2) \rangle \times\right.$$

$$\left.\times \nabla(x_1)\nabla(x_2)\right\} \Phi(r). \quad (9)$$

The essence of the self-consistent harmonic approximation is that the Green's functions G are determined by the force constants $\tilde{\Phi}$ (Eq. (9) which, in turn, depend on the Green's functions through the correlation functions $\langle u(x)u(x') \rangle$.

3. Dynamic Matrix of Crystals with Hexagonal Close-Packed Structure

The case where the potential energy of a crystal is described by a sum of pair potentials was examined in work [5]. However, the important role in the dynamics of a crystal lattice is also played by non-central forces of the atom-to-atom interaction. These forces were considered in works [6–8] for metals with a cubic structure and in works [9, 10] for metals with a hexagonal close-packed lattice. For the force constants to be described in more details, the non-central interaction forces between atoms of the crystal lattice are to be taken into consideration as well.

Let the potential energy $\Phi(\mathbf{r})$ of a crystal with a hexagonal close-packed lattice have the form

$$\Phi(\mathbf{r}) = \frac{1}{2} \sum_{\substack{ll' \\ \alpha\alpha'}} \tilde{\varphi}(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')). \quad (10)$$

Here,

$$\tilde{\varphi}(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')) = \varphi(\mathbf{r}(l) - \mathbf{r}(l')) + \varphi(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')), \tag{10a}$$

where the first term describes the pair interaction between crystal lattice atoms, and the second one the non-central interaction forces. The pair interaction forces are described by the Lennard-Jones potential [5]

$$\varphi(\mathbf{r}(l) - \mathbf{r}(l')) = \frac{b}{|\mathbf{r}(l) - \mathbf{r}(l')|^{12}} - \frac{a}{|\mathbf{r}(l) - \mathbf{r}(l')|^{6}}, \tag{11}$$

where $\mathbf{r}(l)$ and $\mathbf{r}(l')$ are the distances between atoms that are described by formula (1), and b and a are the Lennard-Jones constants. The non-central interaction forces are described by a model potential

$$\varphi(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')) = - \sum_{l'' \neq ll'} \beta_{l'l''} \varepsilon_{l'l''\alpha} \varepsilon_{l'l''\alpha'} u_\alpha(l) u_{\alpha'}(l'), \tag{12}$$

where $\beta_{l'l''}$ is the quasielastic coupling constant, $\varepsilon_{l'l''\alpha}$ is the unit vector that is perpendicular to the interval between atoms l' and l'' and lies in the equilibrium plane of the $ll'l''$-triangle, and $u_\alpha(l)$ and $u_{\alpha'}(l')$ are the displacement of atoms from their equilibrium positions.

Substituting Eq. 10) into formula (9) for renormalized force constants and taking into account that $x, x' \to \alpha, \alpha', l, l'$, we obtain the expression

$$\tilde{\Phi}^{ll'}_{\alpha\alpha'} = \nabla_\alpha(l) \nabla_{\alpha'}(l') \tilde{\Phi}(\mathbf{r}), \tag{13}$$

where

$$\tilde{\Phi}(\mathbf{r}) = \frac{1}{2} \sum_{\substack{l_2 l_2' \\ \alpha_2 \alpha_2'}} \exp\left\{ \frac{1}{2} \sum_{\substack{l_1 l_1' \\ \alpha_1 \alpha_1'}} C^{l_1 l_1'}_{\alpha_1 \alpha_1'} \nabla_{\alpha_1}(l_1) \nabla_{\alpha_1'}(l_1') \right\} \times$$

$$\times \tilde{\varphi}\big(\mathbf{r}(l_2), \mathbf{r}(l_2'), \mathbf{r}(l_2'')\big), \tag{14}$$

$\alpha, \alpha' = x, y, z, l, l'$ are the numbers of crystal lattice sites, and $C^{ll}_{\alpha\alpha'} = \langle u_\alpha(l) u_{\alpha'}(l') \rangle$ is the displacement correlation matrix (subscripts 1 and 2 are omitted).

Expanding the exponent in expression (14) in a series and confining the latter to terms linear in the displacement correlation matrix, we obtain the following expression for the potential energy:

$$\tilde{\Phi}(\mathbf{r}) = \frac{1}{2} \sum_{\substack{l_2 l_2' \\ \alpha_2 \alpha_2'}} \left[\left(1 + \frac{1}{2} \sum_{\substack{l_1 l_1' \\ \alpha_1 \alpha_1'}} C^{l_1 l_1'}_{\alpha_1 \alpha_1'} \nabla_{\alpha_1}(l_1) \nabla_{\alpha_1'}(l_1') \right) \times \right.$$

$$\times \big(\varphi(\mathbf{r}(l_2) - \mathbf{r}(l_2')) + \varphi(\mathbf{r}(l_2), \mathbf{r}(l_2'), \mathbf{r}(l_2'')) \big) \Big]. \tag{15}$$

Making use of formulas (10) to (15), the renormalized force constants are transformed to the form

$$\tilde{\Phi}^{ll'}_{\alpha\alpha'} = \nabla_\alpha(l) \nabla_{\alpha'}(l') \tilde{\varphi}(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')) +$$

$$+ \nabla_\alpha(l) \nabla_{\alpha'}(l') C^{ll'}_{\alpha\alpha'} \nabla_\alpha(l) \nabla_{\alpha'}(l') \tilde{\varphi}(\mathbf{r}(l), \mathbf{r}(l'), \mathbf{r}(l'')). \tag{16}$$

The dynamic matrix is known to be a Fourier transform of force constants, i.e.

$$\tilde{D}_{\alpha\alpha'}(\mathbf{k}) = \frac{1}{M} \sum_{l'} \tilde{\Phi}_{\alpha\alpha'}(l, l') \exp\left(i\mathbf{k}(\mathbf{r}(l) - \mathbf{r}(l')) \right), \tag{17}$$

where a new notation $\tilde{\Phi}^{ll'}_{\alpha\alpha'} \equiv \tilde{\Phi}_{\alpha\alpha'}(l, l')$ was introduced. Imposing the condition $\sum_{l'} \tilde{\Phi}_{\alpha\alpha'}(l, l') = 0$ on the force constants and putting $l = 0$, we obtain the expression for the dynamic matrix of the crystal in the form

$$\tilde{D}_{\alpha\alpha'}(\mathbf{k}) = \frac{1}{M} \sum_{l' \neq 0} \tilde{\Phi}_{\alpha\alpha'}(0, l') \big(\exp(i\mathbf{k}\mathbf{r}(l')) - 1 \big). \tag{18}$$

Provided that $\left. \frac{\partial \varphi(r)}{\partial r} \right|_0 = 0$, the renormalized force constants look like

$$\tilde{\Phi}_{\alpha\alpha'}(0, l') = -\alpha_{l'} \frac{r_\alpha r_{\alpha'}}{r^2(l')} - \sum_{l'' \neq ll'} \beta_{l'l''} \varepsilon_{l'l''\alpha} \varepsilon_{l'l''\alpha'} -$$

$$- C_{\alpha\alpha'}(0, l') \left[\gamma_{1l'} \left(\frac{r_\alpha r_{\alpha'}}{r^2(l')} \right)^2 + \gamma_{2l'} \frac{r_\alpha r_{\alpha'}}{r^2(l')} + \right.$$

$$\left. + \gamma_{3l'} \left(\frac{r_\alpha^2}{r^2(l')} + \frac{r_{\alpha'}^2}{r^2(l')} \right) + \gamma_{4l'} \right], \tag{19}$$

where the parameters $\alpha_{l'}$, $\gamma_{1l'}$, $\gamma_{2l'}$, $\gamma_{3l'}$, and $\gamma_{4l'}$ are expressed in terms of the derivatives of the pair interaction potential (the Lennard-Jones constants), because, for the chosen potential of non-central interaction forces, the derivatives of the orders higher than two are equal to zero. The force constants can be presented as two terms: the first term, $\Phi_{\alpha\alpha'}(0, l')$ corresponds to the harmonic approximation, whereas the second one, $\Delta\Phi_{\alpha\alpha'}(0, l')$, makes allowance for the anharmonicity of atomic vibrations in the crystal lattice (it is proportional to the displacement correlation matrix). Hence, the dynamic matrix looks like

$$\tilde{D}_{\alpha\alpha'}(\mathbf{k}) = D_{\alpha\alpha'}(\mathbf{k}) + \Delta D_{\alpha\alpha'}(\mathbf{k}). \tag{20}$$

The displacement correlation matrix reads

$$C_{\alpha\alpha'}(0,l') = \langle u_\alpha(0)u_{\alpha'}(l')\rangle = \frac{\hbar}{2NM}\sum_{kj}\frac{1}{\omega_j(\mathbf{k})}\times$$

$$\times e_\alpha\left(\begin{array}{c}\mathbf{k}\\j\end{array}\right)e_{\alpha'}^*\left(\begin{array}{c}\mathbf{k}\\j\end{array}\right)\left(2\bar{n}_{\mathbf{k}j}+1\right)\exp\left(-i\mathbf{kr}(l')\right), \quad (21)$$

where $e_\alpha\left(\begin{smallmatrix}k\\j\end{smallmatrix}\right)$ and $e_{\alpha'}^*\left(\begin{smallmatrix}k\\j\end{smallmatrix}\right)$ are the components of polarization vectors, $\bar{n}_{\mathbf{k}j}$ is the Bose distribution function, $\omega_j(\mathbf{k}) \cong v_jk$, v_j is the speed of sound propagation, $k = \frac{2\pi}{r_1}k'$ is the absolute value of the wave vector, r_1 is the radius of the first coordination sphere, and $k' = 0,1,2$.

In the general case, the displacement correlation matrix is determined by calculating the polarization vectors, and it is non-diagonal. Making the approximation $e_\alpha\left(\begin{smallmatrix}k\\j\end{smallmatrix}\right)e_{\alpha'}^*\left(\begin{smallmatrix}k\\j\end{smallmatrix}\right) = 0$ and supposing that the displacement correlation matrix depends only on the number of coordination sphere, we obtain that $C_{\alpha\alpha'}(0,l') = C_i\delta_{\alpha\alpha'}$. An increment to the dynamic matrix is diagonal, because the force constants $\Delta\Phi_{\alpha\alpha'}(0,l')$ responsible for the account of anharmonicity are proportional to the displacement correlation matrix $C_{\alpha\alpha'}(0,l')$. Therefore, the terms in expression (20) for the dynamic matrix are as follows:

$$D_{\alpha\alpha'}(\mathbf{k}) = \frac{1}{M}\sum_{l'\neq 0}\left(-\alpha_{l'}\frac{r_\alpha r_{\alpha'}}{r^2(l')} - \sum_{l'\neq ll'}\beta_{l'l''}\varepsilon_{l'l''\alpha}\varepsilon_{l'l''\alpha'}\right)\times$$

$$\times\left(\exp(i\mathbf{kr}(l'))-1\right), \quad (22)$$

$$\Delta D_{\alpha\alpha'}(\mathbf{k}) = \frac{1}{M}\sum_{l'\neq 0}\left(-C_i\left[\gamma_{1l'}\left(\frac{r_\alpha r_{\alpha'}}{r^2(l')}\right)^2 + \right.\right.$$

$$\left.\left.(\gamma_{2l'}+2\gamma_{3l'})\frac{r_\alpha r_{\alpha'}}{r^2(l')}+\gamma_{4l'}\right]\right)\left(\exp(i\mathbf{kr}(l'))-1\right)\delta_{\alpha\alpha'}. \quad (23)$$

The dependence of the frequency of atomic vibrations in the crystal lattice on the wave vector is determined from either the equation of motion (6) or the condition of existence of a nonzero solution

$$\det\left\|\tilde{D}_{\alpha\alpha'}(\mathbf{k}) - \omega^2(\mathbf{k})\delta_{\alpha\alpha'}\right\| = 0, \quad (24)$$

where the quantity ω^2 is composed of a harmonic-frequency component ω_0^2, which depends on the pair and non-central interaction forces and on an addition to the frequency $\Delta\omega^2$, which is associated with anharmonicity of atomic vibrations in the crystal lattice. Thus, the frequency looks like $\omega^2 = \omega_0^2 + \Delta\omega^2$, where $\omega_0^2 = \omega_p^2 + \omega_{up}^2$ and $\omega'^2 = \omega_p^2 + \Delta\omega^2$.

4. Phonon Spectrum of Crystals with Hexagonal Close-Packed Lattice

The approximation of three coordination spheres was used to calculate the influence of anharmonicity and non-central interaction forces between atoms on the phonon spectrum of Ti at various wave-vector directions. As a result, we obtained that the contributions of those factors manifest themselves in a reduction of the frequency of atomic vibrations in the crystal lattice, the influence of anharmonicity being substantial (Fig. 1). The results of phonon spectrum calculations, which make allowance for anharmonicity effects, are in agreement with the data on the dynamics of the hexagonal close-packed lattice of Ti obtained making use of inelastic neutron scattering [11].

Elastic and inelastic characteristics of metals with a hexagonal close-packed lattice depend considerably on the axis length ratio c/a. A special group of metals with a hexagonal structure includes metals with the ratio less than the ideal value ($c/a < 1.633$). An increase of the diffusion coefficient along the c-axis should be expected for them. The diffusion coefficient is related to longitudinal lattice vibrations. Therefore, for Ti, we calculated phonon spectra for various values of the ratio $s = c/a$ (Fig. 2). The closer the ratio s to the ideal value of 1.633, the higher is the frequency of longitudinal vibrations along the c-axis. This corresponds to a drastic growth of atomic diffusion in the crystal lattice.

We also studied the temperature-induced variation of the vibration frequency (Fig. 3). As the temperature grows, the frequency of atomic vibrations in the crystal lattice decreases. This can be explained by the fact that the temperature growth enhances anharmonicity; however, the frequency decreases due to anharmonicity. The ratio between the diffusion coefficients, which takes anharmonicity effects into account, looks like

$$\frac{D_\parallel}{D_\perp} = \left(\frac{1}{s}\right)^2\exp\left\{\frac{\Phi_\perp - \Phi_\parallel}{kT}\right\}\frac{\omega_{lx}}{\omega_{lz}}. \quad (25)$$

Due to anharmonicity effects, not only the frequency of atomic vibrations in the crystal lattice but also the potential barrier for the diffusion activation decrease.
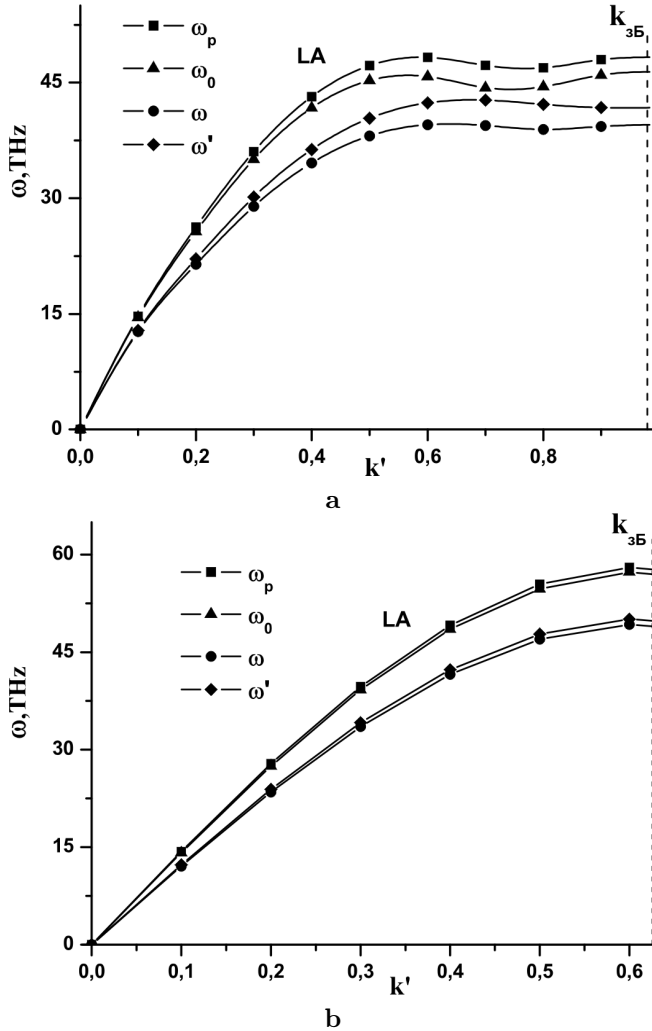
Fig. 1. Dependences of the frequency of longitudinal vibrations on the wave vector directed along (a) and perpendicularly (b) to the x-axis
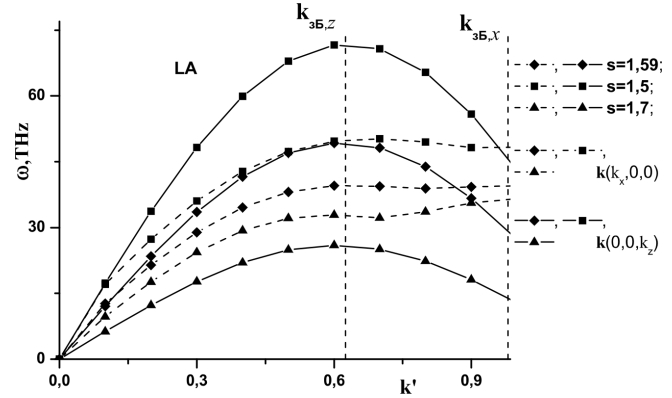

Fig. 2. Phonon spectra at various ratios between lattice constants
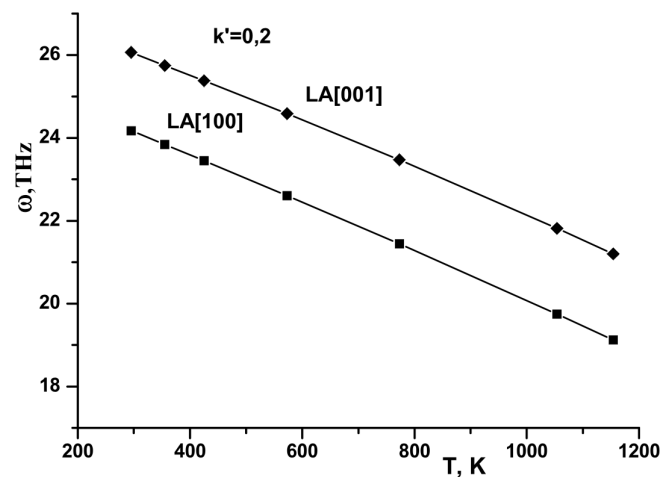
Fig. 3. Temperature dependences of the frequency of longitudinal vibrations along axes c and a

5. Conclusions

The effects of anharmonicity and the contribution of non-central interaction forces to the vibration spectrum of crystals have been studied. The anharmonicity effects were found to manifest themselves in a reduction of the force constants, the frequencies of crystal lattice vibrations, and the potential barriers for the diffusion activation. We have calculated the phonon spectra of metals with a hexagonal close-packed lattice for various directions of the wave vector. A reduction of the ratio c/a between lattice parameters was demonstrated to enhance the anisotropy in the dependences of the vibration frequencies on the wave vector.

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ЕФЕКТИ АНГАРМОНІЗМУ В ФОНОННОМУ СПЕКТРІ АНІЗОТРОПНИХ КРИСТАЛІВ

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Р е з ю м е

В самоузгодженому гармонічному наближенні одержано вирази для перенормованих силових сталих анізотропного кристала за рахунок ефектів ангармонізму. Виконано розрахунок фононного спектра для різних напрямків хвильового вектора для металів з гексагональною щільноупакованою ґраткою. Досліджено ефекти ангармонізму і внесок нецентральних сил взаємодії між атомами кристалічної ґратки в коливному спектрі титану. Встановлено, що за рахунок ангармонізму частоти коливання кристалічної ґратки та потенціальні бар'єри для активації дифузії зменшуються. Показано, що із зменшенням співвідношення між параметрами ґратки c/a ($c/a < 1,633$) збільшується анізотропія залежності частот коливання від хвильового вектора. Показано, що зі збільшенням температури частоти коливання кристалічної ґратки за рахунок ефектів ангармонізму зменшуються.