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SURFACE VIBRATIONS IN SEMI-INFINITE CHAINS WITH CONSIDERATION OF LONG-RANGE INTERACTION. SURFACE VIBRATIONS IN CUBIC CRYSTALS

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Vibrations within infinite and semi-infinite monoatomic and diatomic chains in approximation of nearest and next nearest neighbors have been considered. Phonon dispersion relations in an infinite and a semi-infinite cubic crystal have been studied. Calculations have been carried out using a unitary methodology based on solving the difference equations. The following methodology is of broad generality and can be used for studying of both continuous and discrete spectrum in crystal models close to real systems. For cubic crystals volume vibrations zones and localized states representing surface waves have been calculated.
KEY WORDS: phonons, localized state, surface waves, force constants matrix, adsorbed monolayer, long-range interaction.

ПОВЕРХНОСТНЫЕ КОЛЕБАНИЯ В ПОЛУОГРАНИЧЕННЫХ ЦЕПОЧКАХ С УЧЕТОМ ДАЛЬНОДЕЙСТВИЯ И В КУБИЧЕСКИХ КРИСТАЛЛАХ

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Изучены колебания в бесконечных и полуограниченных одно- и двухатомных цепочках в приближении первых и вторых соседей. Исследованы законы дисперсии фононов в кубическом бесконечном и полуограниченном кристалле. Вычисления проведены с помощью единой методики, основанной на решении разностных уравнений. Используемая методика обладает широкой общностью и может быть использована в моделях, близких к реальным системам, для изучения как непрерывного, так и дискретного спектра колебаний кристалла. Для кубических кристаллов найдены зоны объемных колебаний и вычислены локализованные состояния, соответствующие поверхностным волнам.
КЛЮЧЕВЫЕ СЛОВА: фононы, локализованное состояние, поверхностные волны, матрица силовых постоянных, адсорбированный монослой, дальнодействие.

ПОВЕРХНЕВІ КОЛИВАННЯ У НАПІВОБМЕЖЕНИХ ЛАНЦЮЖКАХ ІЗ УРАХУВАННЯМ ДАЛЬНОДІЇ ТА У КУБІЧНИХ КРИСТАЛАХ

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Розглянуто коливання, що виникають у безкінечних та напівбезкінечних одно- і двоатомних ланцюжках із урахуванням взаємодії між першими і другими сусідами, а також при урахуванні дальнодії. Досліджено закони дисперсії фононів у кубічному безкінечному та напівбезкінечному кристалі. Розрахунки було проведено за допомоги єдиної методики, що основана на розв'язанні різницевих рівнянь. Використана методика має широку спільність і може бути використана у моделях, близьких до реальних систем, для вивчення як безперервного, так і дискретного спектру коливань кристала. Для кубічних кристалів знайдено зони об'ємних коливань та вирахувано локалізовані стани, що відповідають поверхневим хвилям.
КЛЮЧОВІ СЛОВА: фонони, локалізований стан, поверхневі хвилі, матриця силових констант, адсорбований моношар, дальнодія.

The main purpose of the article is the use of one-dimensional models, as it is of definite interest, since they can be used to find out the basic properties of more complex physical objects close to reality. And, in addition, to provide a solution in closed form, which can be used to control the interpretation of the approximate and numerical solutions obtained in the expansion of real systems.

ATOMIC VIBRATIONS IN MONOATOMIC AND DIATOMIC CHAINS

A necessity of comparison the results with some reference physical models often rise in a process of studying the excitation spectra of different quasiparticles in real crystalline structures. In this connection the exactly solvable models can be used (for example, one-dimensional atomic or molecular chain) [1]. On one hand, these one-dimensional models are of academic interest, since they may be used for studying of the basic properties of more complex physical objects that are close to real systems. On the other hand, such model systems are also help to carry out the exact solutions used

for comparison and interpretation of the approximate and numerical solutions obtained for real systems.

In this section we consider vibrations which take place in monoatomic and diatomic chains when considering the nearest and the next nearest neighbours interaction. When taking into account an influence of the next nearest neighbours a situation may occur when α_2 constant corresponding the next neighbour interaction is of different sign with α_1 which is for interaction between nearest neighbours. This situation may be applied to so-called metamaterials simulation [2]. Presence of a negative constant α_2 leads to a problem of solutions stability which can be resolved by setting the restriction on the force constants. Consider now possibility of consideration a long-range interaction within such chains. In this connection we use a model representation of force interaction close to the real one. Account of the long-range interaction solves a problem of solution instability which arises when the long-range interaction is not considered.

Acoustic vibrations in a monatomic chain within approximation of first and second neighbours

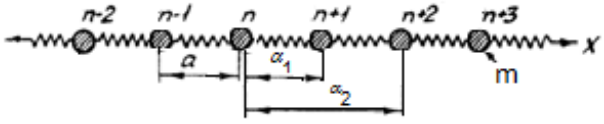

Fig. 1. The monoatomic chain model.

Consider an infinite one dimensional monatomic chain which consists of atoms connected with each other by means of force elastic interaction (Fig. 1). Consider a to be the interatomic distance, α_1 is a force constant corresponding for nearest neighbour interaction and α_2 is for the next nearest one.

The motion equation for the displacement of any n-th lattice-point atom within approximation of first and second neighbours is as follows:

$$m\ddot{u}_n = \alpha_1(u_{n-1} + u_{n+1} - 2u_n) + \alpha_2(u_{n-2} + u_{n+2} - 2u_n). \quad (1)$$

The equation (1) is sought in the form of plane waves

$$u_n(t) = u_0 \exp\{i(nka - \omega t)\}. \quad (2)$$

Here u_0 is a plane wave amplitude, ω and k are frequency and wave number correspondently.

After substituting (2) into (1) we receive

$$m\omega^2 = 2\alpha_1(1 - \cos ka) + 2\alpha_2(1 - \cos 2ka) \quad (3)$$

The dispersion equation (3) can be rewritten as:

$$\frac{m\omega^2}{\alpha_1} = 4\sin^2\frac{ka}{2} + 4\frac{\alpha_2}{\alpha_1}\sin^2 ka \quad (4)$$

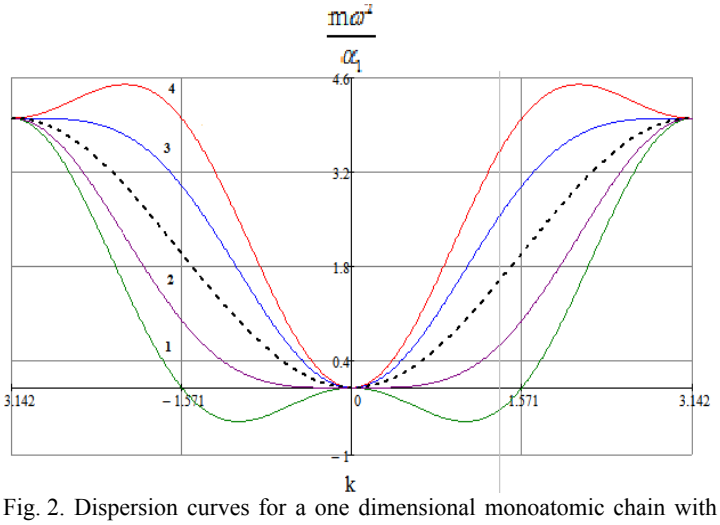

Fig. 2. Dispersion curves for a one dimensional monoatomic chain with accounting of nearest and next nearest neighbours (p = -1\2, -1\4, 0, 1\4, 1\2).

Introduce a designation $p=\alpha_2/\alpha_1$. Dispersion curves for a monatomic chain in approximation of nearest neighbours (p = 0, dashed curve) and second nearest ones (p = -1\2, curve 1; p = -1\4, curve 2; p = 1\4, curve 3; p = 1\2, curve 4) are shown in Fig. 2. An instability solution takes place at negative values of Here the condition of instability of negative values of, $\alpha_2/\alpha_1 \prec -1/4$ which is also represented at Fig. 2 (curve 1, p = -1\2). This situation can be applied in the simulation of metamaterials. The system considered is stable if $\alpha_2/\alpha_1 \prec -1/4$ (ω_2 is positive, (4)).

In case of an oscillating (alternating) interaction a restriction imposed on force constants comes out.

On considering interaction between the third neighbours, the dispersion equation transforms as following:

$$\frac{m\omega^2}{\alpha_1} = 4\sin^2\frac{ka}{2} + 4\frac{\alpha_2}{\alpha_1}\sin^2 ka + 4\frac{\alpha_3}{\alpha_1}\sin^2\frac{3ka}{2}. \quad (5)$$

Existence condition of a stable solution to implement in equation (5) is:

$$1 + 4\frac{\alpha_2}{\alpha_1} + 9\frac{\alpha_3}{\alpha_1} > 0. \tag{6}$$

Thus, when considering oscillatory (alternating) interactions a problem of system stability arises. It demands particular restriction on force constants connection.

Acoustic oscillations in the one-dimensional monatomic chain with long-range interaction

It is of high interest to take into account an interaction that exponentially decays with distance increasing (i.e., long-range interaction). This fact was shown in [3,4]. Therefore, consider interaction between all the atoms in an infinite chain. Motion equation is as follows

$$m\ddot{u}_n = \sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(u_{n+m'} - u_n\right) \tag{7}$$

The solution of equation (7) is sought in the form of plane waves (3). Thus,

$$m\omega^2 = \sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(1 - e^{im'k\alpha}\right). \tag{8}$$

From symmetrical reasoning $\alpha_{-m'} = \alpha_{m'}$, and we have

$$m\omega^2 = 2\sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(1 - \cos im'k\alpha\right). \tag{9}$$

Otherwise,

$$m\omega^2 = 4\sum_{m'=-\infty}^{+\infty} k_{m'} \sin^2 \frac{m'ka}{2}, \qquad k_{m'} = \alpha_{m'} / \alpha_1, \quad k_1 = 1. \tag{10}$$

The given equation cannot be solved without choosing of an appropriate model of force constants $\alpha_{m'}$ changing. The further the interacting atoms are situated the weaker the interaction is.

Consider the following model

$$\alpha_{m'} = \alpha_1 q^{m'-1}, \ |q| < 1, \tag{11}$$

which is an analog of RKKI exchange interaction which simplified obtaining of the magnetic materials excitation spectra [5]. It allows one to take into account when solving the problem of finding the excitation spectrum of the infinite-dimensional chain, the impact of long-range. Since in the model allows the existence of alternating force constants, it can be used to solve problems in physics metamaterials.

Substituting (11) into (10) and summing the expression, we get:

$$\frac{m\omega^2}{\alpha_1} = 2\frac{1+q}{1-q} \cdot \frac{1-\cos ka}{1-2q\cos ka+q^2}. \tag{12}$$

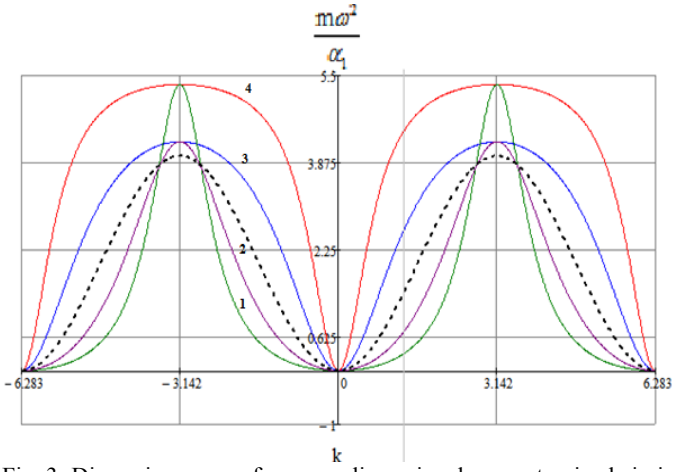

Fig. 3. Dispersion curves for a one dimensional monoatomic chain in approximation of nearest neighbours and when considering long-range interaction (q = -1\2, -1\4, 0, 1\4, 1\2).

Dispersion curves for a monatomic chain in approximation of nearest neighbours (q = 0, dashed curve) and for long-range interaction (q = -1\2, curve 1; q = -1\4, curve 2; q = 1\4, curve 3; q = 1\2, curve 4) are shown in Fig. 3. Account of the long-range interaction removes the problem of solution instability which appears when considering a finite number of neighbours.

Stability analysis of the equation (12) leads to the conclusion that solutions within the whole q range of definition are stable. When interaction between second and third neighbours is not considered a stability solution range narrows. As for only second neighbours consideration p should be p = [-1/4; 1]. Thus, consideration of the long-range interaction (when $|q| < 1$) allows removing the restrictions imposed upon the stability range of

dispersion equation solution.

Acoustic vibrations in an infinite monoatomic chain having a point defect

Consider an infinite chain consisting of atoms with m masses (Fig. 4) and a point defect with m' one within approximation of nearest neighbours interaction α. Maximum value of a square frequency for monoatomic ideal infinite chain is:

$$\omega_m^{\,2} = \frac{4\alpha}{m} \tag{13}$$

Let us study conditions of appearing and characteristics of so-called local vibrations.

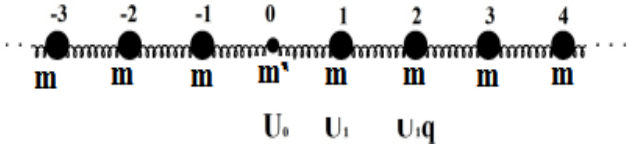

Fig. 4. An infinite atomic chain within which there is an impurity atom.

Without losing generality suppose that a defect atom is located in the grid origin. Solution is sought in the following form

$$\begin{cases} m'\ddot{u}_0 = -\alpha(u_1 + u_{-1} - 2u_0) \\ m\ddot{u}_1 = -\alpha(u_2 + u_0 - 2u_1) \\ m\ddot{u}_{-1} = -\alpha(u_0 + u_{-2} - 2u_{-1}) \end{cases}.$$

As for the other motion equations, they correspond those of the volume atoms (located far from the impurity one). We seek the solutions that coordinate the amplitudes decreasing on the sides of the defect atom, i.e.

$$\begin{cases} u_2 = u_1 q, \\ u_{-2} = u_{-1} q, \end{cases} \quad |q| < 1. \tag{14}$$

In (11) we had q for interaction decreasing parameter and in (14) it is an amplitude displacement parameter. Considering (14) we obtain a system below (we should take into account that $u \sim \exp(-i\omega t)$, see eq.(2))

$$\begin{cases} m'\omega^2/\alpha \cdot u_0 = \{2u_0 - u_1 - u_{-1}\}, \\ m\omega^2/\alpha \cdot u_1 = \{2u_1 - u_0 - u_1 q\}, \\ m\omega^2/\alpha \cdot u_{-1} = \{2u_{-1} - u_0 - u_{-1} q\}, \end{cases}$$

which has nontrivial solution if

$$\begin{pmatrix} (m'\omega^2/\alpha) - 2 & 1 & 1 \\ 1 & (m\omega^2/\alpha) - 2 + q & 0 \\ 1 & 0 & (m\omega^2/\alpha) - 2 + q \end{pmatrix} = 0. \tag{15}$$

Equation (15) is an equation for q expressed in terms of $m\omega^2$. Besides of it, we need the following equation to find q:

$$m\omega_л^2 = \alpha\left\{2 - \frac{1}{q} - q\right\}. \tag{16}$$

Hence,

$$q = \varepsilon/(\varepsilon - 2), \tag{17}$$

where $\varepsilon = m'/m$. From (17) it is obvious that $|q| < 1$ if $m'/m \prec 1$ which means that local vibrations appear without a threshold.

After substituting q into (16) we have:

$$\frac{m\omega_л^2}{\alpha} = \frac{4}{\varepsilon(2-\varepsilon)}. \tag{18}$$

Ratio of local and maximum frequencies (13) is:

$$\frac{\omega_л^2}{\omega_m^2} = \frac{1}{\varepsilon(2-\varepsilon)} \succ 1. \tag{19}$$

Dependences of $\omega_л^2/\omega_m^2$ on ε and q on ε are given in Fig. 5 (a and b respectively).

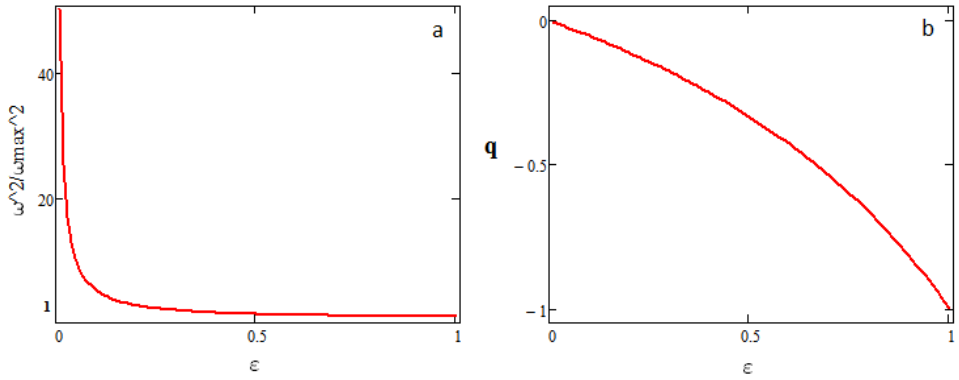

Fig. 5. Dependence of $\omega_л^2/\omega_m^2$ on ε (a) and of q on ε (b).

Local vibrations in one-dimensional semi-infinite chain having an impurity boundary atom

Consider a one-dimensional semi-infinite atomic chain consisting of atoms with m masses (Fig. 6) and one impurity m' boundary atom. Let us assume that $m' \prec m$. Similarly to the discussed above case of an infinite chain, local excitations will take place in the considered model. These local states are an analogue of the surface waves in one-dimensional system.

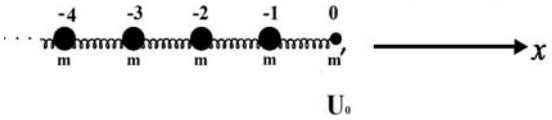

Fig. 6. A semi-infinite monoatomic chain having an impurity boundary atom.

We have obtained the following system in the given model

$$\begin{cases} m'\ddot{u}_0 = -\alpha\{u_{-1} - u_0\}, \\ m\ddot{u}_{-1} = -\alpha\{u_{-2} + u_0 - 2u_1\}, \\ m\ddot{u}_{-2} = -\alpha\{u_{-3} + u_{-1} - 2u_{-2}\}. \end{cases}$$

As we did in (14) let us rewrite this system in a following form

$$\begin{cases} m'\omega^2/\alpha \cdot u_0 = \{u_{-1} - u_0\}, \\ m\omega^2/\alpha \cdot u_{-1} = \{u_{-1}q + u_0 - 2u_{-1}\}, \end{cases} \tag{20}$$

which has a non-trivial solution on a condition that

$$\begin{pmatrix} (m'\omega^2/\alpha) - 1 & 1 \\ 1 & (m\omega^2/\alpha) - 2 + q \end{pmatrix} = 0. \tag{21}$$

For the second atom we have $m\ddot{u}_{-2} = \alpha\{u_{-3} + u_{-1} - 2u_{-2}\}$.

Hence,

$$m\omega^2 = \alpha\left\{2 - \frac{1}{q} - q\right\} \tag{22}$$

and

$$q = \frac{\varepsilon}{\varepsilon - 1}, \quad |q| \prec 1. \tag{23}$$

So, we can see that q is negative at $\varepsilon = m'/m \prec \frac{1}{2}$. It is also obvious that local vibrations arise if mass of an impurity boundary atom is twice lighter than the host one [6].

After substituting q into (22) we have:

$$\frac{m\omega_л^2}{\alpha} = \frac{1}{\varepsilon(1-\varepsilon)}. \tag{24}$$

Its maximum value is:

$$\omega_m^2/\alpha = 4/m. \tag{25}$$

Ratio of local and maximum frequencies is:

$$\frac{\omega_л^2}{\omega_m^2} = \frac{1}{4\varepsilon(1-\varepsilon)}. \tag{26}$$

Dependences of $\omega_л^2/\omega_m^2$ on ε (a) and q on ε are given in Fig. 7 (a and b respectively).

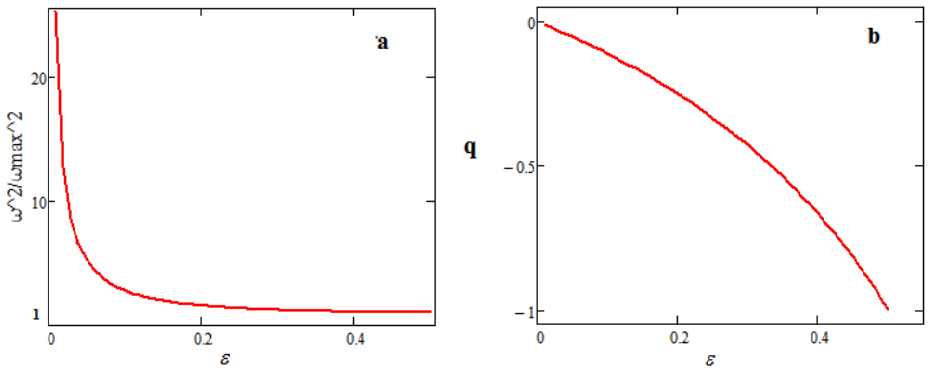

Fig. 7. Dependence of $\omega_л^2/\omega_m^2$ on ε (a) and of q on ε (b).

Diatomic infinite chain in model of the second-neighbour interaction

Consider a diatomic chain (Fig. 8). Assume the even numbers to be those of atoms with M masses and the odd numbers to be those with *m* ones.

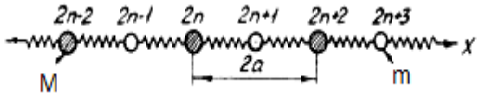

Fig.8. A diatomic chain.

$$\begin{cases} \text{m}\ddot{u}_{2n} = \alpha_1(u_{2n-1} + u_{2n+1} - 2u_{2n}) + \alpha_2(u_{2n-2} + u_{2n+2} - 2u_{2n}), \\ \text{M}\ddot{u}_{2n+1} = \alpha_1(u_{2n} + u_{2n+2} - 2u_{2n+1}) + \alpha_2'(u_{2n-1} + u_{2n+3} - 2u_{2n+1}). \end{cases} \tag{27}$$

The system equations are sought in the form of plane waves

$$\begin{aligned} u_{2n} &= u_1 \exp\{i(2nka - \omega t)\}, \\ u_{2n+1} &= u_2 \exp\{i([2n+1]ka - \omega t)\}. \end{aligned} \tag{28}$$

Substituting (28) into (27) we get

$$\begin{cases} \text{m}\omega^2 u_1 = 2\alpha_1(u_1 - \cos ka \cdot u_2) + 2\alpha_2(1 - \cos 2ka)u_1, \\ M\omega^2 u_2 = 2\alpha_1(u_2 - \cos ka \cdot u_2) + 2\alpha_2'(1 - \cos 2ka)u_2. \end{cases}$$

This system has non-trivial solutions for u_1 and u_2 if

$$\begin{vmatrix} 2\alpha_1 - \text{m}\omega^2 + 4\alpha_2 \sin^2 ka & -2\alpha_1 \cos ka \\ -2\alpha_1 \cos ka & 2\alpha_1 - M\omega^2 + 4\alpha_2' \sin^2 ka \end{vmatrix} = 0 \tag{29}$$

After evaluating a determinant obtained we get a dispersion relation for a diatomic chain.

$$\omega^4 - A(k)\omega^2 + B(k) = 0, \tag{30}$$

where

$$A(k) = \frac{2\alpha_1}{mM}(m+M) + 4\frac{m\alpha_2 + M\alpha_2'}{mM}\sin^2 ka,$$

$$B(k) = \frac{4\alpha_1^2}{mM}\sin^2 ka + 8\alpha_1\frac{\alpha_2 + \alpha_2'}{mM}\sin^2 ka + \frac{16\alpha_2\alpha_2'}{mM}\sin^4 ka.$$

Solutions of (29) are as follows

$$\omega_{\pm}^2(k) = \frac{1}{2}A(k) \pm \frac{1}{2}\sqrt{A^2(k) - 4B(k)}. \tag{31}$$

Dispersion curves for a diatomic chain in approximation of nearest neighbours (p = 0, dashed curve) and second nearest ones (p = -1\2, curve 1; p = 1\2, curve 2) are shown in Fig. 9. Here optical modes are marked with thin curves and acoustical ones are marked with thick curves.

Such plots demonstrate a condition of instability appearing for the acoustic vibrations within negative values of

$\frac{\alpha_2}{\alpha_1} \prec -\frac{1}{4}$ (p=-1\2). This result may be applied in simulation of metamaterials in acoustics.

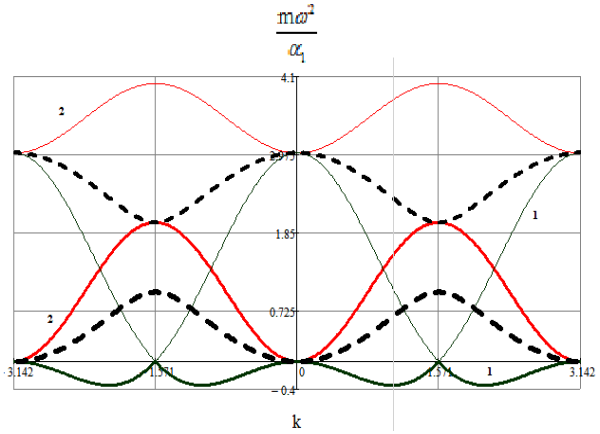

Fig. 9. Diatomic infinite chain with accounting of nearest and next nearest neighbours. (p=-1\2, 0, 1\2).

There are optical and acoustical vibrations in a diatomic chain (unlike a monoatomic one which doesn't have them). In our work we marked $\omega_+(k)$ as for optical modes and $\omega_-(k)$ as for acoustical ones. Solutions of (30) are stable if $A(k) > 0,\ \ 0 < B(k) < A^2(k)$.

Considering the form of *A(k)* and *B(k)*, these conditions bind both force constants and masses of various atoms. There is a gap between optical and acoustical excitations that appears in an infinite diatomic chain consisting of atoms of different type. The gap width can be estimated according to the dispersion curves form.

The lowest border is an optical mode which is $\omega^2_{+,\min} = \frac{m+M}{mM}$, and the upper one responds for acoustical vibrations $\omega^2_{-,\max} = \frac{1}{2}A(k) - \frac{1}{2}\sqrt{A^2_{\max} - 4B_{\max}}$.

Here $A_{\max} = \frac{2}{mM}(\alpha_1(m+M) + 2(m\alpha_2 + M\alpha_2'))$, $B_{\max} = \frac{4}{mM}(\alpha^2_1 + 2\alpha_1(\alpha_2 + \alpha_2') + 4\alpha_2\alpha_2')$ if accounting the next nearest neighbours.

Infinite diatomic chain with taking a long-range interaction into account

As for two types of atoms we have the following equations of motion:

$$\begin{cases} m\omega^2 u_1 = 2u_1 \sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska)) + 2\sum_{r=0}^{\infty} \alpha_{2r+1}(u_1 - u_2\cos[(2r+1)ka]), \\ M\omega^2 u_2 = 2u_2 \sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska)) + 2\sum_{r=0}^{\infty} \alpha_{2r+1}(u_2 - u_1\cos[(2r+1)ka]). \end{cases} \quad (32)$$

It is convenient to make a replacement

$$\begin{cases} m\omega^2 u_1 = F(ka)\cdot u_1 + G(ka)\cdot u_2, \\ M\omega^2 u_2 = G(ka)\cdot u_1 + F(ka)\cdot u_2, \end{cases} \quad (33)$$

where $F = 2\sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska))$, $G = 2\sum_{r=0}^{\infty} \alpha_{2r+1}(1-\cos[(2r+1)ka])$.

Equation system (33) has non-trivial solutions for u_1 and u_2 if

$$\begin{vmatrix} F(ka) - m\omega^2 & G(ka) \\ G(ka) & F(ka) - M\omega^2 \end{vmatrix} = 0. \quad (34)$$

Thus, we obtain

$$\omega^4 - A(ka)\omega^2 + B(ka) = 0, \quad (35)$$

where $A(ka) = \frac{m+M}{mM}F(ka)$, $B(ka) = \frac{F^2(ka) - G^2(ka)}{mM}$. We get $F(ka)$ and $G(ka)$.

Hence,

$$F(ka) = \frac{2\alpha_1}{1-q} - 2\alpha_1\frac{(\cos 2ka - q^2)\cdot q}{1+q^4-2q^2\cos 2ka}, \quad G(ka) = 2\alpha_1\frac{\cos ka(1-q^2)}{1+q^4-2q^2\cos 2ka}.$$

Solution of (35) is

$$\omega^2_{\pm}(ka) = \frac{1}{2}A(ka) \pm \frac{1}{2}\sqrt{A^2(ka) - 4B(ka)},$$

A and B are presented above.

Dispersion curves for a diatomic chain in approximation of nearest neighbours (q = 0, dashed curve) and second nearest ones (q = -1\2, green curve; q = 1\2, red curve) are shown in Fig. 10. Here optical modes are marked with thin curves and acoustical ones are marked with thick curves.

Account of the long-range interaction removes the problem of solution instability which appears when considering a finite number of neighbours. Long-range interaction takes away a restriction that $\alpha_2 < 0$.

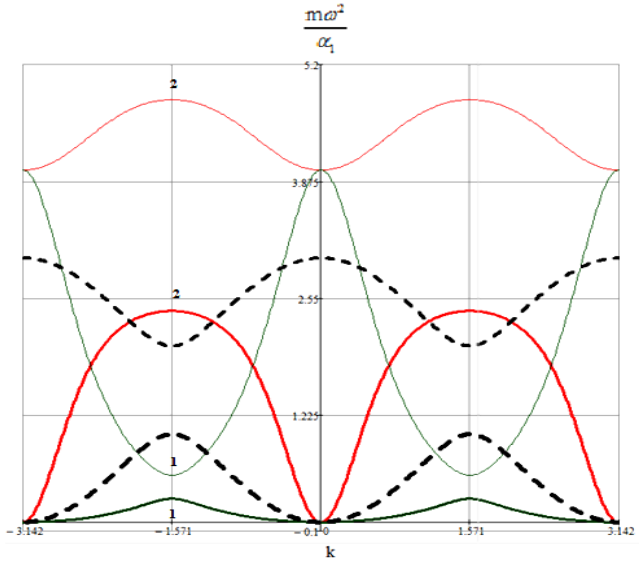

Fig.10. Diatomic infinite chain with accounting of nearest and next nearest neighbours. (q=-1\2, 0, 1\2).

INFLUENCE OF SURFACE PLANE ORIENTATION ON DYNAMICS OF VIBRATIONAL STATES IN A SEMI-INFINITE CUBIC CRYSTAL

Different theoretical and experimental studies of surface states of various nature (including elastic surface waves) cause deep interest both in the context of fundamental studies and technological applications. Pure shear surface waves having a horizontal polarization are of special interest. Such waves depend on surface characteristics much stronger than waves possessing Rayleigh polarization, for example [7, 8]. This comes from the fact that penetration depth of purely shear surface wave exceeds that of the Rayleigh wave within the long wavelength limit. If geometry of a studied crystal is of sufficiently high symmetry, pure shear surface waves split from the Rayleigh waves then.

Thus, without losing generality it is possible to study such surface waves using the so-called scalar models characterized by one displacement direction. For example, spin waves in magnetically ordered systems in the magnon approximation are described using this model.

In our paper we studied dispersion relations of phonons in a cubic crystal. For our calculations we used methodology stated in [9, 10]. The following methodology is of broad generality and can be used for studying of both continuous and discrete spectrum in crystal models close to real systems.

In a microscopic assumption we have studied zones of volume vibrations and properties of the single-component surface waves split off the volume zone, depending on surface orientation, direction of two-dimensional wave vector and its values in a two-dimensional Brillouin zone.

Volume vibrations

The equation of atomic motion for an ideal crystal in scalar model in harmonic approximation is as follows [11]:

$$m\ddot{u}(n,t) = -\sum_{n'} \hat{\Phi}(n,n')u(n',t). \tag{36}$$

Here $u(n,t)$ is a time-dependent displacement of the atom in the $n = (n_1, n_2, n_3)$ site from its equilibrium position, $\hat{\Phi}(n,n')$ is a force matrix and m is an atomic mass. Solution of (36) is sought in the form

$$u(n,t) = u(n_3) \cdot e^{i(k_\alpha n_\alpha - \omega t)}. \tag{37}$$

Here k_∞ are the components of a three-dimensional wave vector along a_1, a_2, a_3 (the unit vectors), $\alpha = 1,2,3$; ω is the wave frequency.

In order to study the surface waves, we examine first the situation where the chosen orientational plane is located deep in the crystal. Consider (001), (110) and (111) orientational planes. With (1) and (2), dispersion relations for each of the orientational planes in SC, FCC and BCC can be obtained.

- ***Simple cubic:***
  - *(001) plane*

$$\frac{m\omega_V^2}{\alpha} = 6 - 2\cos[k_1 a_0] - 2\cos[k_2 a_0] - 2\cos[k_3 a_0]. \tag{38}$$

Let us construct a diagram for volume vibration zone as a function of two-dimensional wave vector $\chi(k_1, k_2)$ at fixed k_3 (see Fig. 11, shaded area). For SC crystal lower and upper borders are as follows

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 2\cos[k_1] - 2\cos[k_2] - 2,$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 - 2\cos[k_1] - 2\cos[k_2] + 2. \tag{39}$$

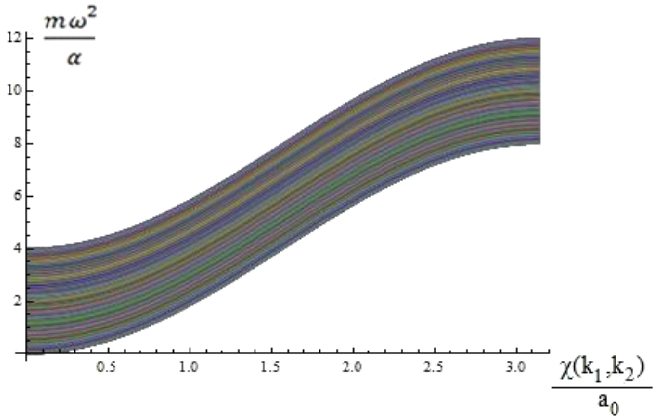

Fig. 11. A diagram of volume vibrations (shaded area) for (001) surface orientational plane in SC crystal.

Similarly, it is possible to find volume vibration zones for any other orientational plains.

- *(110) plane*

Equation for volume vibrations is

$$\frac{m\omega_V^2}{\alpha} = 6 - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_3\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0]. \tag{40}$$

And, hence, for lowest and highest boundaries we have (see Fig. 14, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 4\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 + 4\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0]. \tag{41}$$

- *(111) plane*

As for (111) orientational plane we have

$$\frac{m\omega_V^2}{\alpha} = 6 - 2\cos[K_3\frac{a_0}{\sqrt{3}} - K_2\frac{a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}} + K_3\frac{a_0}{\sqrt{3}}], \tag{42}$$

and (Fig. 12, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 2\cos[K_2\frac{a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}}],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 + 2\cos[K_2\frac{a_0}{\sqrt{6}}] + 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}}]. \tag{43}$$

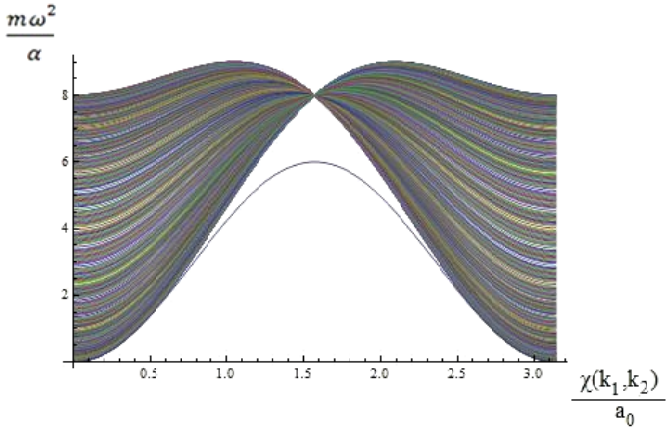

Fig. 12. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in BCC crystal.

- ***Face-centred cubic:***
  - *(001) plane*

Similarly to what was calculated for simple cubic crystal, for FCC with (001) orientational plane we have

$$\frac{m\omega_V^2}{\alpha} = 12 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] - 4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}] - 4\cos[k_2\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}]. \quad (44)$$

The lowest and the highest boundaries are as follows (Fig. 13, shaded area):

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 2 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] - 4\cos[k_1\frac{a_0}{\sqrt{2}}] - 4\cos[k_2\frac{a_0}{\sqrt{2}}],\\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 2 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] + 4\cos[k_1\frac{a_0}{\sqrt{2}}] + 4\cos[k_2\frac{a_0}{\sqrt{2}}].\end{aligned} \quad (45)$$

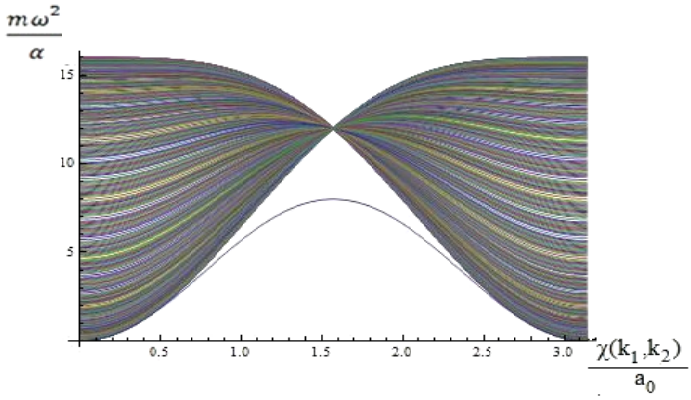

Fig. 13. A diagram of volume vibrations (shaded area) and surface wave for (001) surface orientational plane in FCC crystal.

  - *(110) plane*

$$\frac{m\omega_V^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] - 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}]\cos[K_3\frac{a_0}{2}], \quad (46)$$

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] - 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}],\\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] + 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}].\end{aligned} \quad (47)$$

The corresponding diagram is shown in Fig. 14, shaded area.

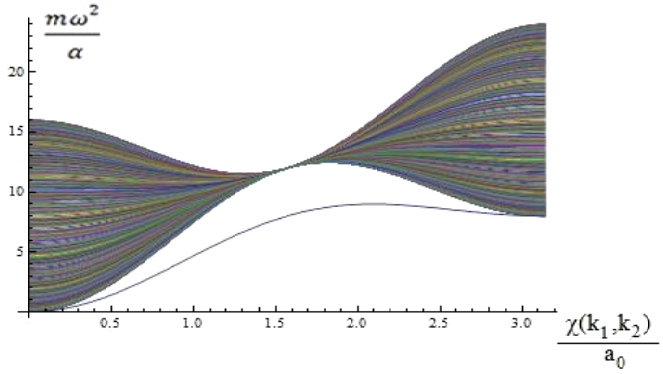

Fig. 14. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in FCC crystal.

  - *(111) plane*

In this case equations for volume vibrations are

$$\frac{m\omega_V^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[(\frac{K_2}{\sqrt{2}} + K_3)\frac{a_0}{\sqrt{3}}] - 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[(K_2\frac{a_0\sqrt{2}}{4} - K_3a_0)\frac{1}{\sqrt{3}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}] \quad (48)$$

and (see Fig. 15, shaded area):

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[\frac{K_2 a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[K_2\frac{a_0}{2\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[\frac{K_2 a_0}{\sqrt{6}}] + 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[K_2\frac{a_0}{2\sqrt{6}}] + 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}]. \quad (49)$$

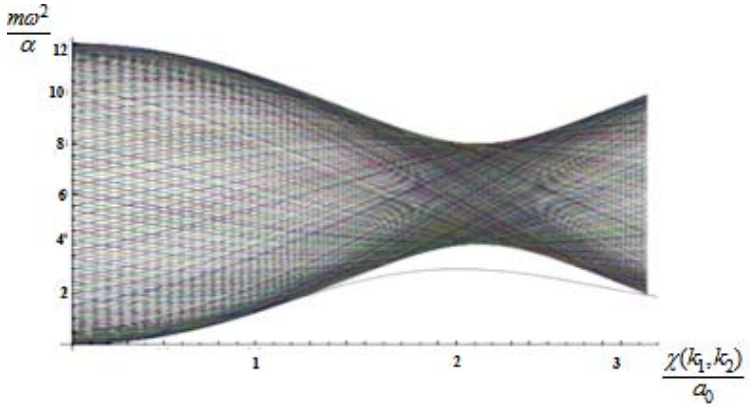

Fig. 15. A diagram of volume vibrations (shaded area) and surface wave for (111) surface orientational plane in SC crystal.

- ***Base-centred cubic:***
  - *(001) plane*

As for BCC, we have

$$\frac{m\omega_V^2}{\alpha} = 8 - 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}]. \quad (50)$$

Thus, dispersion equations for the lowest and the highest boundaries are as follows (see Fig. 16, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 8 - 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}]$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 8 + 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}] \quad (51)$$

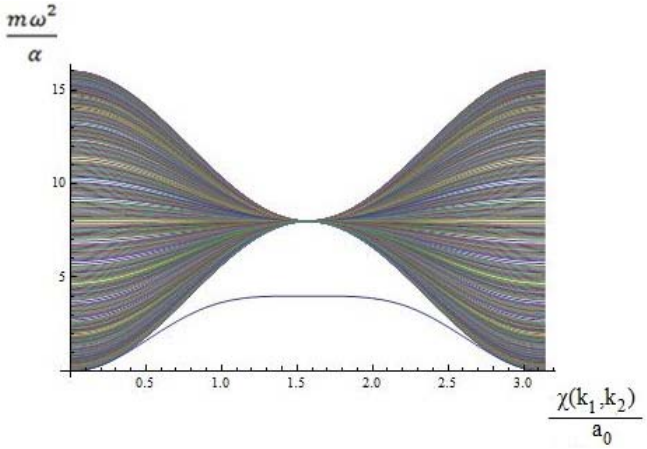

Fig. 16. A diagram of volume vibrations (shaded area) and surface wave for (001) surface orientational plane in BCC crystal.

  - *(110) plane*

Similarly,

$$\frac{m\omega_V^2}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2}]\cos[K_3\frac{a_0}{2\sqrt{2}}], \quad (52)$$

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2}]$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] + 4\cos[K_1\frac{a_0}{2}] \quad (53)$$

The following diagram is shown in Fig. 12, shaded area.

- *(111) plane*

In the following case, we have

$$\frac{m\omega_V^2}{\alpha} = 8 - 4\cos[\frac{2}{9}K_1a_0] - 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})]\cos[\frac{\sqrt{2}}{9}K_3a_0] \tag{54}$$

and (Fig. 17, shaded area)

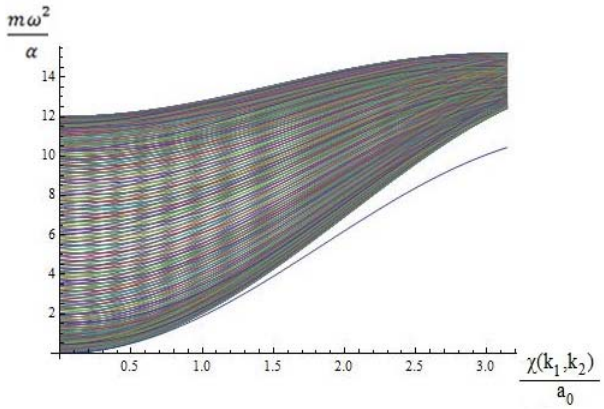

Fig. 17. A diagram of volume vibrations (shaded area) and surface wave for (111) surface orientational plane in FCC crystal.

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 8 - 4\cos[\frac{2}{9}K_1a_0] - 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})] \\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 8 - 4\cos[\frac{2}{9}K_1a_0] + 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})]\end{aligned} \tag{55}$$

Surface waves in cubic crystals

We use a Lifshitz Rosenzweig model [12] for describing a surface. In an infinite crystal we lay a plane that corresponds the needed orientation and then just "throw away" one of the halves of our crystal.

From (1) and (2) for surface plane we get

$$m\omega^2 u(n_3) = \sum_{n_3'} \hat{\Phi}(n, n_3'; n_1, n_2), \tag{56}$$

Here $\hat{\Phi}(n, n_3'; n_1, n_2)$ is a reduced dynamic matrix. Equation (56) are linear equations in finite differences of order $2s$ which set a sequence of $U(n)(n = 0,1,2,\ldots)$. It follows from the theory of finite difference equations [13] that, beginning from $n = N, U(n)$ can be presented as a sum of geometric progressions

$$u(n) = \sum_{j=1}^{2s} V_j q_j^n, \tag{57}$$

Here V_j are amplitudes of $2s$ partial waves, characterized by q_i parameters which determine degree of decrease (increase) of the partial wave with penetrating into crystal depth. q_i are solutions of the algebraic equation of $2s$ degree (in scalar model):

$$m\omega^2 - \sum_{n=-s}^{2s} \hat{\Phi}^0(n,k) q^n = 0 \tag{58}$$

As for $0 \prec n \prec N + s$ atomic motion equations for atoms situated in defect and intermediate layers (see (57)) play the role of boundary conditions and are used to determine relationship between the V_j and atomic vibrational amplitudes in defect layers. There are s summands left in (58) in case of SC, $|q| \prec 1$ for all of them. It was interesting for us to determine values of q and $m\omega^2/\alpha$ for different orientational surfaces.

Boundary conditions (motion equations for defect and intermediate layers) form a system of $N + s$ homogeneous linear equations for V_j and $u(n)(n = 0,1,\ldots N-1)$. The number of equations and unknowns are equal. Equating the determinant of this system to 0, we arrive to the equation for SC structure dispersion relation. Mathematically, the matter is to solve an algebraic equation and there is no need in integration over a continuous spectrum.

dispersion relations for phonons in cubic crystal with different orientational surface have been studied. So let us illustrate the technique used on some specific models.

(001) plane

- ***Simple cubic structure (SC).***

There are one defect $n=0(s=1)$ and one intermediate planes $n=1(N=1)$ for (001) surface plane in a SC crystal. Surface wave may be presented in the form of $u(n)=Vq^n$. For a $n=1$ intermediate layer and a $n=0$ surface defect layer equation system (58) transforms into:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6-2\cos[k_1a_0]-2\cos[k_2a_0]-(q+\frac{1}{q}),\ n\geq 1, \\ \frac{m\omega_s^2}{\alpha} = 5-2\cos[k_1a_0]-2\cos[k_2a_0]-q,\ n=0. \end{cases} \tag{59}$$

Here V is an atomic vibrational amplitude; s is a solution for a SC structure and ω_s is its frequency. From the expression for $n=0$ it's obvious that surface atoms have 5 neighbours, while those situated in any other layer inside the crystal have 6 neighbours.

An equation for $n=0$ in (59) plays the role of a boundary condition for surface waves. From (59) we obtain:

$$\begin{cases} q=1 \\ \frac{m\omega_s^2}{\alpha} = 4-2\{\cos[k_1a_0]-\cos[k_2a_0]\} \end{cases} \tag{60}$$

Thus, for the considered surface orientation equation $\omega_s(k)$, a surface wave corresponds the lowest boundary of volume vibration zone (see (38)). For such a situation we have $q=1$ which means that there are no surface vibrations for (001) orientational plane in SC. It is illustrated in Fig. 11.

A splitting value $\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}$ is a difference between dispersion relations for volume and surface vibrations. As for the considered situation it equals $\Delta=0$, as $\frac{m\omega_s^2}{\alpha}=\frac{m(\omega_V^2)_{\min}}{\alpha}=4-2\cos[k_1a_0]-2\cos[k_2a_0]$

- ***Face-centred cubic structure (FCC).***

Consider unit translation vectors and a two-dimensional vector o be as follows, respectively: $A_1=A_2=a_0/\sqrt{2}$, $k_1=k_2$. Then, we get:

$$\begin{aligned} &\frac{m\omega_s^2}{\alpha} = 12-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-2(q+\frac{1}{q})\{\cos[k_1\frac{a_0}{\sqrt{2}}]+4\cos[k_2\frac{a_0}{\sqrt{2}}]\},\ n\geq 1 \\ &\frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-2q\{\cos[k_1\frac{a_0}{\sqrt{2}}]+4\cos[k_2\frac{a_0}{\sqrt{2}}]\},\ n=0 \end{aligned} \tag{61}$$

Values for $m\omega_s^2/\alpha$ and q are obtained from (61):

$$\begin{cases} q=\frac{1}{2}(\cos[k_1\frac{a_0}{\sqrt{2}}]+\cos[k_2\frac{a_0}{\sqrt{2}}]) \\ \frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-\cos^2[k_1\frac{a_0}{\sqrt{2}}]+\cos^2[k_2\frac{a_0}{\sqrt{2}}] \end{cases} \tag{62}$$

In Fig. 16 the line beneath the shaded area corresponds to a surface wave. For (001) orientational plane in FCC crystal we have the following splitting value: $\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}=4(1-q)^2,$ which shows that a surface wave exists in such an orientation.

- ***Base-centred cubic structure (BCC).***

For defect $n=0$ and intermediate $n=1$ layers we have:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}](q+\frac{1}{q}),\ n\geq 1 \\ \frac{m\omega_s^2}{\alpha} = 8-4q\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}],\ n=0 \end{cases} \tag{63}$$

$$\begin{cases} q=\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}] \\ \frac{m\omega_s^2}{\alpha} = 4-4\cos^2[k_1\frac{a_0}{\sqrt{3}}]\cos^2[k_2\frac{a_0}{\sqrt{3}}] \end{cases} \tag{64}$$

In Fig. 13 a curve beneath the shaded reach corresponds to a surface wave. The splitting value is: $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 3(1-|q|)^2$.

(110) plane

- ***SC structure.***

As for (110) surface orientational plane in simple cubic crystal we choose unit transition vectors as follows: $A_1 = a_0/\sqrt{2}\,(1\bar{1}0), A_2 = a_0(001)$. The two-dimensional wave vector will have the following components then: $K_1 = k_0/\sqrt{2}\,(1\bar{1}0), K_2 = k_0(001)$. Number of defect and intermediate layers are $s = N = 1$. Equations for atoms in $n \geq 1$ and $n = 0$ are

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6 - 2\cos[K_1\frac{a_0}{\sqrt{2}}](q+\frac{1}{q}) - 2\cos[K_1 a_0],\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 4 - 2q\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_1 a_0],\ n = 0 \end{cases}. \quad (65)$$

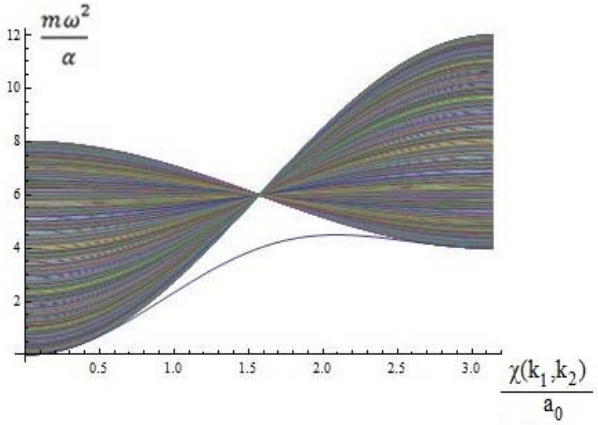

Fig. 18. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in SC crystal.

A solution for (65) is

$$\begin{cases} q = \cos[K_1\frac{a_0}{\sqrt{2}}] \\ \frac{m\omega_s^2}{\alpha} = 4 - 2\cos^2[K_1\frac{a_0}{\sqrt{3}}] - 2\cos[K_2 a_0] \end{cases}. \quad (66)$$

From (66) it follows that there is a surface wave for such a surface orientational plane. The penetration depth of the wave considered varies from a minimum value in $K_1 = k_0/\sqrt{2}\,\overline{(110)}$ direction up to infinity when spreading in $K_2 = k_0(001)$ direction. In Fig. 18 a curve beneath the shaded area corresponds to a surface wave. The splitting value is: $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 2(1-q)^2$.

- ***FCC structure.***

From the equations for $n \geq 1$ and $n = 0$:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}](q+\frac{1}{q}),\ n \geq 1, \\ \frac{m\omega_s^2}{\alpha} = 8 - 2\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4q\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}],\ n = 0 \end{cases}. \quad (67)$$

We get values of ω_s

$$\begin{cases} q = \cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{a_0}{2\sqrt{2}}], |q| \prec 1, \\ \frac{m\omega_s^2}{\alpha} = 8 - 2\cos[K_1 \frac{a_0}{\sqrt{2}}] - 2\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] \end{cases}. \quad (68)$$

Splitting of a surface wave from the continuous spectrum is shown in Fig. 14 and equals $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 4(1-q)^2$.

- ***BCC structure.***

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 8 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2\cos[K_1 \frac{a_0}{2}](q + \frac{1}{q}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 6 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2q\cos[K_1 \frac{a_0}{2}],\ n = 0 \end{cases} \quad (69)$$

For unit translation vectors $A_1 = a_0/2(001), A_2 = a_0/2\sqrt{2}(1\bar{1}0)$ we obtain the following equation system for defect $n=0$ and intermediate $n=1$ layers:

Hence,

$$\begin{cases} q = \cos[K_1 \frac{a_0}{2}], \\ \frac{m\omega_s^2}{\alpha} = 6 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2\cos^2[K_1 \frac{a_0}{2}] \end{cases} \quad (70)$$

In Fig. 12 a curve beneath the shaded area corresponds to a surface wave. The splitting value is:

$$\Delta = \frac{m(w_V^2)_{min}}{\alpha} - \frac{mw_s^2}{\alpha} = 2(1-q)^2$$

which shows that a surface wave exists in such an orientation.

(111) plane

- ***SC lattice.***

In case of SC crystal with (001) orientational surface we choose the following unit vectors in coordinate and impulse spaces: $A_1 = a_0/\sqrt{2}(1\bar{1}0), A_2 = a_0/\sqrt{6}(1\,1\bar{2})$; $K_1 = k_0/\sqrt{2}(1\bar{1}0), K_2 = k_0/\sqrt{2}(\bar{1}\bar{1}0)$. The dynamic equations for atoms located in defective ($n=0$) and intermediate ($n=1$) layers are as follows, respectively:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6 - 4qe^{iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{-3iK_2\frac{a_0}{\sqrt{2}}}) - \frac{1}{q}e^{-iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{3iK_2\frac{a_0}{\sqrt{2}}}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 3 - qe^{iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{-3iK_2\frac{a_0}{\sqrt{2}}}),\ n = 0 \end{cases} \quad (71)$$

Dispersion relation and q values are as follows then

$$\begin{cases} q = \frac{1}{3}e^{-iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{3iK_2\frac{a_0}{\sqrt{2}}}), \\ \frac{m\omega_s^2}{\alpha} = \frac{4}{3}(2 - \cos^2[K_1 \frac{a_0}{\sqrt{2}}] - \cos[K_1 \frac{a_0}{\sqrt{2}}]\cos[K_2 \frac{3a_0}{\sqrt{6}}]) \end{cases}. \quad (72)$$

The surface wave is shown in Fig. 15 as a curve splitting from continuous spectrum.

- ***FCC lattice.***

Having $A_1 = a_0/2\sqrt{2}(1\bar{1}0), A_2 = a_0/2\sqrt{6}(1\,1\bar{2})$ we get

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 12 - 2\cos[K_1 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{3a_0}{2\sqrt{6}}] - qe^{-iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{3iK_2\frac{a_0}{2\sqrt{6}}}) - \\ -\frac{1}{q}e^{-K_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{-3iK_2\frac{a_0}{2\sqrt{6}}}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 9 - 2\cos[K_1 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{3a_0}{2\sqrt{6}}] - qe^{-iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{3iK_2\frac{a_0}{2\sqrt{6}}}),\ n = 0. \end{cases} \quad (73)$$

From (73) we obtain

$$\begin{cases} q = e^{iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1\frac{a_0}{\sqrt{2}}]+e^{-3iK_2\frac{a_0}{2\sqrt{6}}}), \\ \frac{m\omega_s^2}{\alpha}=\frac{16}{3}(2-\cos^2[K_1\frac{a_0}{2\sqrt{2}}]-\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{3a_0}{2\sqrt{6}}]) \end{cases} \quad (74)$$

Splitting of a surface wave from the continuous spectrum (Fig. 17) equals $\Delta=\frac{m(w_V^2)_{min}}{\alpha}-\frac{mw_s^2}{\alpha}=2(1-q)^2$.

Cubic crystals having an adsorbed surface monolayer

Consider a cubic crystal that has a simple cubic lattice and (001) surface orientational plane of the (001). Consider now an adsorbed monolayer which consists of impurity atoms and is situated on the top of the surface layer. Equation (38) allows one to write the dispersion relations for the adsorbed surface monolayer ($n=0$) and a boundary layer located below it ($n=1$):

$$\begin{cases} \frac{m_0\omega_s^2}{\alpha}U_0=(5-2\cos[k_1a_0]-2\cos[k_2a_0])U_0-U_1 \\ \frac{m\omega_s^2}{\alpha}U_1=(6-2\cos[k_1a_0]-2\cos[k_2a_0])U_1-U_0-U_1q \end{cases}. \quad (75)$$

Here m_0 is a mass of an impurity atom and m is a mass of a host one. We had the dispersion relation for $n\succ 1$ layer given above (see (59)). From (75) we find the following determinant:

$$\begin{vmatrix} \frac{m_0\omega_s^2}{\alpha}-5+A & 1 \\ 1 & \frac{m\omega_s^2}{\alpha}-6+A+q \end{vmatrix}=0. \quad (76)$$

Hereinafter we introduce the following notation $A=2\cos[k_1a_0]+2\cos[k_2a_0]$. Equations (59), (76) are a system of two equations having two unknowns, q and $m\omega_s^2/\alpha$. For q in general case we have

$$q=\frac{-[m_0(6-A)-m(5-A)]\pm\sqrt{[m_0(6-A)-m(5-A)]^2+4m_0(m-m_0)}}{2(m-m_0)}. \quad (77)$$

A boundary transition should be hold: $q=1$ at $m_0=m$ (see (51), a (001) surface orientational plane in SC crystal). Denominator equals 0 then, so take a limit of (77). Let us set $X=[m_0(6-A)-m(5-A)]$, $Y=4m_0(m-m_0)$. Hence,

$2(m-m_0)=\frac{Y}{2m_0}$ and $q=\lim_{Y\to 0}2m_0\frac{-X\pm\sqrt{X^2+Y^2}}{Y}\approx -2m_0\frac{-X\pm(X+\frac{Y}{2X})}{Y}$. Since $|q|\prec 1$, only a positive root matches, and we get:

$$q=\frac{m_0}{X}=\frac{m}{X}=1. \quad (78)$$

Thus, the boundary condition is satisfied. It is easy to obtain $m\omega_s^2/\alpha$ knowing q.

Consider a situation when impurity atoms are lighter than the host ones $m_0\prec m$. Consider also a situation of heavy impurity atoms $m_0\succ m$.

For light impurity atoms $(m_0\prec m)$. In this connection $\frac{m_0}{m}=\frac{1}{2}$ and $\frac{m_0}{m}=\frac{1}{5}$ have been studied.

$$\frac{m_0}{m}=\frac{1}{2}: \quad \begin{cases} \frac{m\omega_s^2}{\alpha}=6+A+\sqrt{A^2-8A+20} \\ q=\frac{4-A-\sqrt{A^2-8A+20}}{2} \end{cases}. \quad (79)$$

At such ratio between masses of host and impurity atoms a surface wave splits off just from the highest boundary of the continuous spectrum (see Fig. 19).

$$\frac{m_0}{m}=\frac{1}{2}: \quad \begin{cases} \dfrac{m\omega_s^2}{\alpha}=\dfrac{105-20A+5\sqrt{16A^2-152A+377}}{8} \\ q=\dfrac{19-4A-\sqrt{16A^2-152A+377}}{8} \end{cases}. \tag{80}$$

Note that in both cases $q \prec 0$. Let us determine a splitting value now. From Fig. 19 it is obvious that a surface wave splits off the highest boundary of the continuous spectrum, so:

$$\Delta=\frac{m\omega_s^2}{\alpha}-\frac{m(\omega_V^2)_{\max}}{\alpha} \succ 0, \tag{81}$$

$$\frac{m_0}{m}=\frac{1}{2}: \Delta=8-A-2q \succ 0, \tag{82}$$

$$\frac{m_0}{m}=\frac{1}{5}: \Delta=17-4A-5q \succ 0. \tag{83}$$

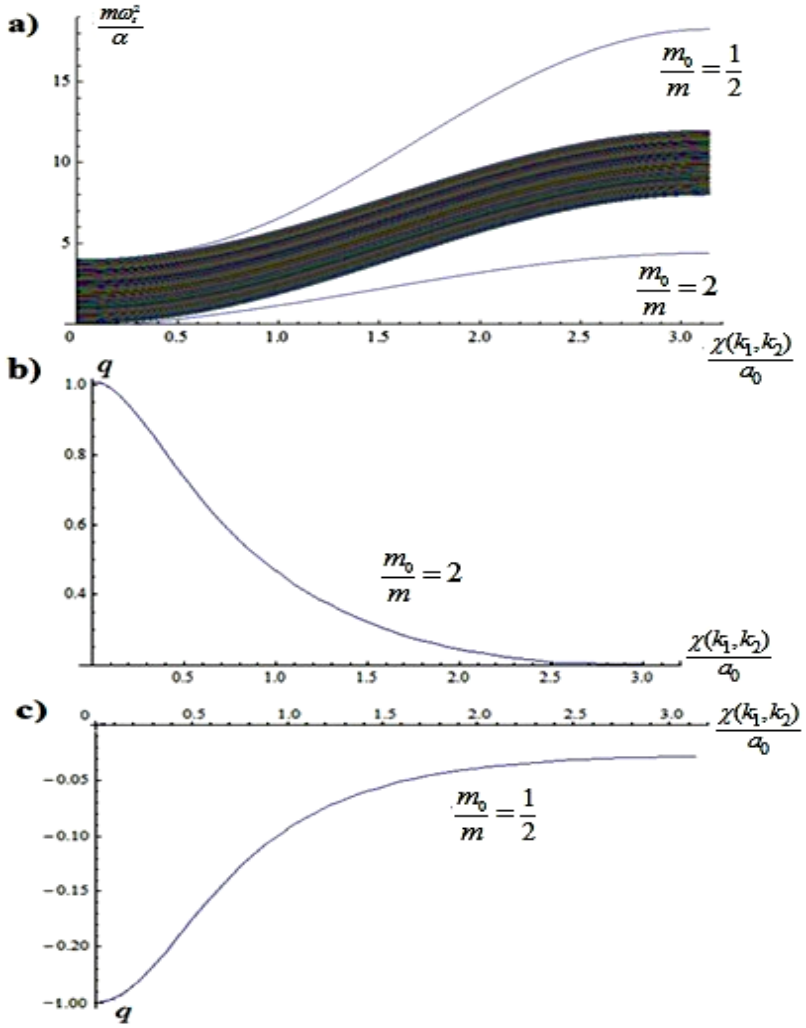

Fig. 19. A diagram of volume zone vibrations and surface waves for $m_0/m=1/2$ and $m_0/m=2$ (a); dependence of q on a two-dimensional wave vector if $m_0/m=2$ (b) and $m_0/m=1/2$ (c). All considered for a (001) adsorbed surface monolayer in a SC crystal.

Here q are the coefficients presented in (79) and (80) for each of the ratios. It's obvious that in both cases $\Delta \succ 0$ because . $q \prec 0, |q| \prec 1$ and A changes from -4 to 4 depending on the value of two-dimensional wave vector $\chi(k_1,k_2)=[0,\pi]$.

For heavy atoms ($m_0 \succ m$). Here $\frac{m_0}{m}=2$ and $\frac{m_0}{m}=5$ have been considered.

$$\frac{m_0}{m}=2:\begin{cases}\dfrac{m\omega_s^2}{\alpha}=\dfrac{3-A+\sqrt{A^2-14A+41}}{4}\\ q=\dfrac{7-A-\sqrt{A^2-14A+41}}{2}\end{cases}, \tag{84}$$

$$\frac{m_0}{m}=5:\begin{cases}\dfrac{m\omega_s^2}{\alpha}=\dfrac{15-4A+\sqrt{16A^2-200A+545}}{20}\\ q=\dfrac{25-4A-\sqrt{16A^2-200A+545}}{8}\end{cases}. \tag{85}$$

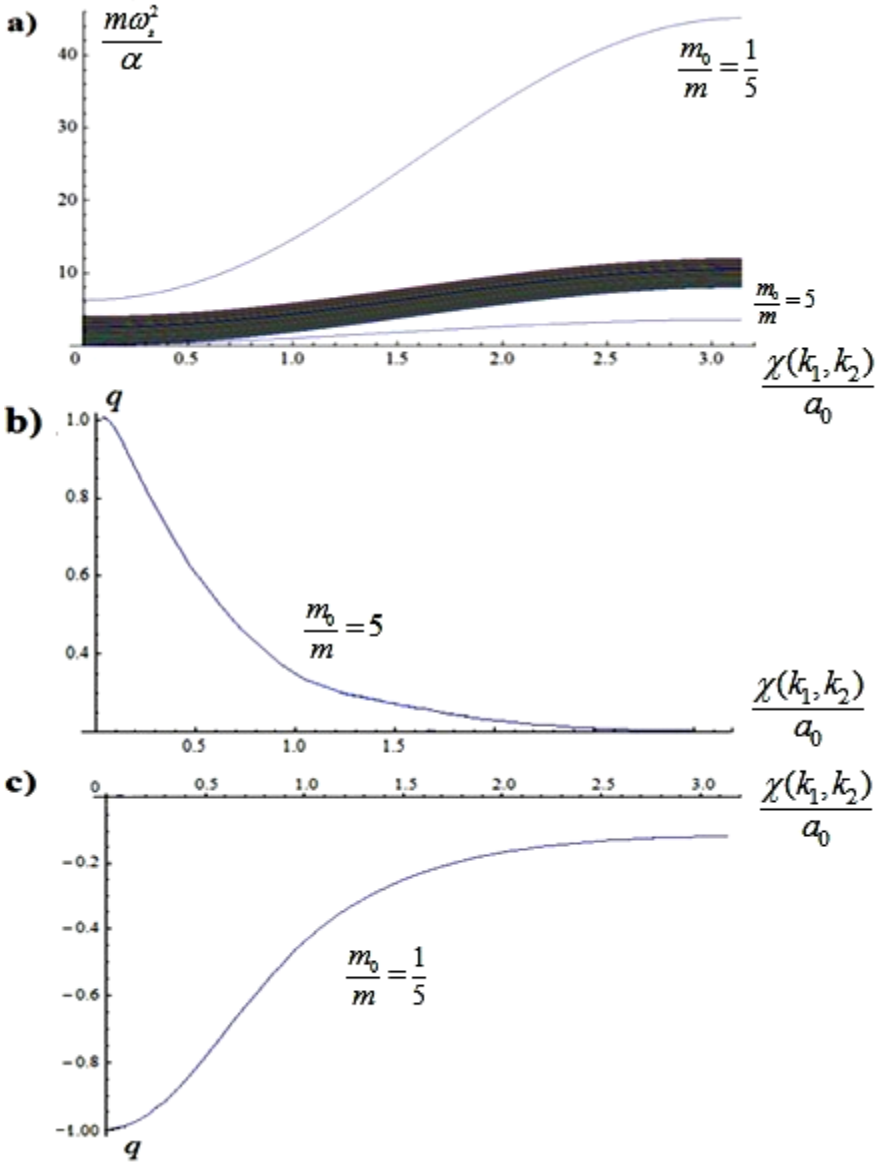

Fig. 20. A diagram of volume zone vibrations and surface waves for $m_0/m=1/5$ and $m_0/m=5$ (a); dependence of q on a two-dimensional wave vector if $m_0/m=5$ (b) and $m_0/m=1/5$ (c). All considered for a (001) adsorbed surface monolayer in a SC crystal.

A surface wave splits off the lowest boundary of the continuous spectrum (Fig. 20), so the splitting value is as follows:

$$\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}\succ 0. \tag{86}$$

For $m_0/m = 2$ we have $\Delta = \dfrac{3 - A + q}{2}$

From the form of (86) it isn't clear if $\Delta \succ 0$ as A varies from -4 to 4. However, in case of $\chi = 0$ and $A = -4$ we have $q = 1$ and $\Delta = 0$. With increasing of χ from 0 to $\pi/2$, q value decreases, and $\Delta \geq 0$ will always be true. Therefore,

$$\Delta = \frac{3 - A + q}{2} \geq 0. \tag{87}$$

As for $m_0/m = 5$ we get

$$\Delta = \frac{10 - 3A + 2q}{5} \geq 0. \tag{88}$$

q are given in (84) and (85). Similarly to $m_0/m = 2$ we find out that $\Delta \geq 0$ is realized for any χ. Based on the above stated, we conclude that, both in the cases of lights and heavy impurity atoms a surface wave splitting off the continuous spectrum exists. Diagrams for the continuous spectrum and surface waves splitted are shown in Fig. 20.

With decreasing of impurity atoms mass a splitting value increases. However, when averaged over all three values of wave vector $\vec{k}(k_1, k_2, k_3)$ the surface waves frequency gets into continuous spectrum. However, there is a sufficiently light impurity mass for a gap between volume zone and surface wave to appear. Let us find an appropriate ratio between impurity and host masses.

From Fig. 19 it's well seen that the lighter the impurity atoms are the greater the minimal surface wave frequency is. As for SC (001) $m(\omega_V^2)_{\max}/\alpha = 12$ (see Fig. 11). We need to find an appropriate m_0/m at which a gap exists, i.e. at which $m\omega_s^2/\alpha \succ m(\omega_V^2)_{\max}/\alpha$. We find q from:

$$m(\omega_V^2)_{\max}/\alpha = 12 = 2 - (q + 1/q) \tag{89}$$

$$q = -5 + \sqrt{24} \approx -1.101. \tag{90}$$

After substituting into (76) we get $m_0/m \approx 11$. Thus, a gap within spectrum appears if impurity atoms are lighter than the host ones in about 11 times.

CONCLUSIONS

The paper is dedicating to consideration of dispersion relations of an infinite and semi-infinite atomic chains consisting of similar and different types of atoms in approximation of the nearest neighbours. When taking to account the next nearest neighbours interaction it turns out that as for the model chosen both attractive ($\alpha_2 \succ 0$) and repulsive ($\alpha_2 \succ 0$) interactions take place. In the first case of problems with the stability of solutions arise. There are no stability problems for attraction, when there should be restriction imposed on α_2 in case of repulsion. In its turn, long-range interaction removes restriction at $\alpha_2 \prec 0$ .The same situation arises within diatomic chains. The features studied come up to the foreground when considering altering-sign chains within metamaterials (a sign before α_i alters)

Phonon and surface waves dispersion relations in cubic crystal are studied in the second section. Allowing for interactions between the nearest neighbors, dispersion relations of volume and surface vibrations for pure shear waves have been found in cases of (001), (110) and (111) surface orientations for simple cubic, face-centered cubic and body-centered cubic crystals. Method described in [14], has been used.

Furthermore, we have considered a monolayer adsorbed on crystal surface both having lighter atoms than those the crystal has, and having heavier ones. For the lighter atoms, consideration was given to $m_0/m = 1/2$ and $m_0/m = 1/5$; for heavier atoms we studied $m_0/m = 2$ and $m_0/m = 5$ (here m_0 is a mass of impurity atom in the adsorbed monolayer, m is a mass of one host atom). For light impurity atoms we have obtained splitting from the top edge of the continuous spectrum; for heavy atoms surface wave splits off from the lowest edge. Surface wave amplitude decreases monotonously in case of heavy atoms; in case of light ones amplitude decrease is oscillating (not monotonous). It has been shown that a gap within continuous spectrum and surface wave appears if $m_0/m \approx 11$.

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