NOVI SAD J. MATH.
VOL. 31, No. 1, 2001, 55-64

MICROTHEORETICAL AND NUMERICAL CALCULATION OF PHONON SPECTRA IN SUPERLATTICES

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Abstract. The Green's functions method, adjusted to bounded crystalline structures (*PriM 9-13*th), is applied to obtain the phonon dispersion law in superlattices. The system of difference equations defining Green's functions of displacement type for a superlattice motive is given. Poles of Green's functions define phonon spectra. They can be determined by solving the secular equation. In general case and for different boundary parameters, this problem is solved numerically (*Mathematica 4*) and presented graphically (*CorelDraw 9*). The correlation with spectra of phonons in the corresponding unbounded and film-structures is established in the work. The crystalline systems with the basic motive (made up from 2 different ultrathin films with specific interconnections) periodically repeating itself along one direction normal to the connected motive boundaries are the superlattices.

AMS Mathematics Subject Classification (1991): 82B24

Key words and phrases: superlattice, Green's functions, phonon spectra

1. Introduction

Precise structuring of solids at the nanometer-sized dimension is most important for modern science of solids nowadays [1,2], especially in the field of electronics, optoelectronics and high-temperature superconductivity. There are many reasons for interest in low-dimensional structures (thin films, superlattices, quantum wires and quantum dots) as more real structures than the infinite ones. Phenomena connected with such low dimensions cause the formation of new and different(changed) characteristics of solids and specific effects [3-5], which are interesting not only from the fundamental physical point of view but also as the structures of widespread practical significance.

Phonons are basic excitations in crystals and describe oscillatory movements of their components. The study of the contribution and influence of the phonon subsystem on physical characteristics of solids is of particular importance to the theory of solids, because phonons are always present in crystals, no matter

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whether as main carriers of the mechanisms which "produce" certain physical characteristics, phenomena and effects in crystalline structures appear electrons, excitons, ferroelectronic inducements, or some other forms of the elementary excitation.

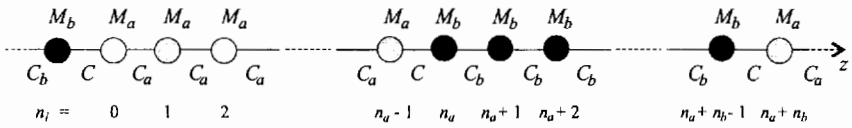

Figure 1: Arrangement of atoms in the basic motive of the superlattice

The phonon spectra in crystal superlattices were analyzed here using the method of two-time temperature dependent retarded Green's functions.

2. Phonons in superlattices

Superlattices are ultrathin layered crystal structures, periodical in one direction, with the period exceeding the constant of the lattice about twenty times [1,2]. The scope of our study in this paper is the superlattice, the basic motive of which are composed n_a layers of one and n_b layers of another type of atoms, alternately arranged along the z-direction, while it is unbounded along the x and y directions. To make connected layers consisting of different atoms possible, the lattice constants along the x and y directions must respectively be equal, i.e. $a_x^a = a_x^b \equiv a_x$ and $a_y^a = a_y^b \equiv a_y$, whereas along the z-direction they may be different $a_z^a \equiv a^a \neq a_z^b \equiv a^b$ and $a_z^{a-b} \equiv a$).

We introduce the following notation:

$$\vec{n} \equiv \{n_x, n_y, n_z\}\ , \quad n_{x/y/z} \in \left[-\frac{N_{x/y/z}}{2}, +\frac{N_{x/y/z}}{2}\right]\ ,$$

where: $n_{x/y}$ - is the atom site counter along the x (i.e. y) direction, n_z - is the position counter of the basic motive of the superlattice (z-direction), while: n_l - is the atom site counter in the basic motive.

Starting from the standard Hamiltonian of the phonon subsystem for bulk structures [6-9], the phonon subsystem Hamiltonian of superlattices

$$H = T + V_{eff}^P + V_{eff}^Z \equiv H_P + H_Z\ , \tag{1}$$

can be presented in the following separated form:

- operator of the kinetic energy

$$T = T_1 + T_2\ , \tag{2}$$

$$T_1 = \sum_{\vec{n},\alpha} \sum_{n_l=0}^{n_a-1} \frac{\left[p^{(a)}_{\vec{n},n_l;\alpha}\right]^2}{2M_a}\,; \quad T_2 = \sum_{\vec{n},\alpha} \sum_{n_l=n_a}^{n_a+n_b-1} \frac{\left[p^{(b)}_{\vec{n},n_l;\alpha}\right]^2}{2M_b}\,; \tag{3}$$

- interaction potential related to the interfaces between crystalline films

$$V^P_{eff} = V^P_1 + V^P_2 + V^P_3 + V^P_4\,, \tag{4}$$

where the corresponding components refer to the surfaces $n_l = 0$, $n_a - 1$, n_a i $n_a + n_b - 1$, i.e.

$$\begin{aligned}
V^P_1 &= \sum_{\vec{n}} \Big\{ \frac{C^x_a}{4} \left[(u_{n_x,n_y,n_z,0} - u_{n_x+1,n_y,n_z,0})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,0} - u_{n_x-1,n_y,n_z,0})^2 \right] + \\
&+ \frac{C^y_a}{4} \left[(u_{n_x,n_y,n_z,0} - u_{n_x,n_y+1,n_z,0})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,0} - u_{n_x,n_y-1,n_z,0})^2 \right] + \\
&+ \frac{C^z_a}{2} (u_{n_x,n_y,n_z,0} - u_{n_x,n_y,n_z,1})^2 + \\
&+ \frac{C}{2} (u_{n_x,n_y,n_z,0} - u_{n_x,n_y,n_z-1,n_a+n_b-1})^2 \Big\}\,;
\end{aligned} \tag{5}$$

$$\begin{aligned}
V^P_2 &= \sum_{\vec{n}} \Big\{ \frac{C^x_a}{4} \left[(u_{n_x,n_y,n_z,n_a-1} - u_{n_x+1,n_y,n_z,n_a-1})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,n_a-1} - u_{n_x-1,n_y,n_z,n_a-1})^2 \right] + \\
&+ \frac{C^y_a}{4} \left[(u_{n_x,n_y,n_z,n_a-1} - u_{n_x,n_y+1,n_z,n_a-1})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,n_a-1} - u_{n_x,n_y-1,n_z,n_a-1})^2 \right] + \\
&+ \frac{C^z_a}{2} (u_{n_x,n_y,n_z,n_a-1} - u_{n_x,n_y,n_z,n_a-2})^2 + \\
&+ \frac{C}{2} (u_{n_x,n_y,n_z,n_a-1} - u_{n_x,n_y,n_z-1,n_a})^2 \Big\}\,;
\end{aligned} \tag{6}$$

$$\begin{aligned}
V^P_3 &= \sum_{\vec{n}} \Big\{ \frac{C^x_b}{4} \left[(u_{n_x,n_y,n_z,n_a} - u_{n_x+1,n_y,n_z,n_a})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,n_a} - u_{n_x-1,n_y,n_z,n_a})^2 \right] + \\
&+ \frac{C^y_b}{4} \left[(u_{n_x,n_y,n_z,n_a} - u_{n_x,n_y+1,n_z,n_a})^2 + \right. \\
&+ \left. (u_{n_x,n_y,n_z,n_a} - u_{n_x,n_y-1,n_z,n_a})^2 \right] + \\
&+ \frac{C^z_b}{2} (u_{n_x,n_y,n_z,n_a} - u_{n_x,n_y,n_z,n_a+1})^2 + \\
&+ \frac{C}{2} (u_{n_x,n_y,n_z,n_a} - u_{n_x,n_y,n_z,n_a-1})^2 \Big\}\,;
\end{aligned} \tag{7}$$

$$
\begin{aligned}
V_4^P &= \sum_{\vec{n}} \Bigg\{ \frac{C_b^x}{4} \left[\left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x+1,n_y,n_z,n_a+n_b-1} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x-1,n_y,n_z,n_a+n_b-1} \right)^2 \right] + \\
&+ \frac{C_b^y}{4} \left[\left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x,n_y+1,n_z,n_a+n_b-1} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x,n_y-1,n_z,n_a+n_b-1} \right)^2 \right] + \\
&+ \frac{C_b^z}{2} \left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x,n_y,n_z,n_a+n_b-2} \right)^2 + \\
&+ \frac{C}{2} \left(u_{n_x,n_y,n_z,n_a+n_b-1} - u_{n_x,n_y,n_z+1,0} \right)^2 \Bigg\} .
\end{aligned} \tag{8}
$$

- interaction potential in relation with the inner region of each crystalline film

$$
V_{eff}^Z = V_1^Z + V_2^Z \ , \tag{9}
$$

$$
\begin{aligned}
V_1^Z &= \sum_{\vec{n}} \sum_{n_l=1}^{n_a-2} \Bigg\{ \frac{C_a^x}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x+1,n_y,n_z,n_l} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x-1,n_y,n_z,n_l} \right)^2 \right] + \\
&+ \frac{C_a^y}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y+1,n_z,n_l} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y-1,n_z,n_l} \right)^2 \right] + \\
&+ \frac{C_a^z}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y,n_z,n_l+1} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y,n_z,n_l-1} \right)^2 \right] \Bigg\} \ ;
\end{aligned} \tag{10}
$$

$$
\begin{aligned}
V_2^Z &= \sum_{\vec{n}} \sum_{n_l=n_a+1}^{n_a+n_b-2} \Bigg\{ \frac{C_b^x}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x+1,n_y,n_z,n_l} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x-1,n_y,n_z,n_l} \right)^2 \right] + \\
&+ \frac{C_b^y}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y+1,n_z,n_l} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y-1,n_z,n_l} \right)^2 \right] + \\
&+ \frac{C_b^z}{4} \left[\left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y,n_z,n_l+1} \right)^2 + \right. \\
&+ \left. \left(u_{n_x,n_y,n_z,n_l} - u_{n_x,n_y,n_z,n_l-1} \right)^2 \right] \Bigg\} \ .
\end{aligned} \tag{11}
$$

Taking into account that the superlattice represents the periodical crystal structure, for an arbitrary function of the position the cyclic conditions of x, y and z indexes are valid, by which the permitted validities of x, y and (particu-

larly) z-components of the wave vector can be obtained:

$$(12)\quad \begin{array}{ll} f_{m_x m_y m_z m_l + N_{x/y}} = f_{m_x m_y m_z m_l} & \Rightarrow \quad \mathrm{e}^{iN_{x/y}k_{x/y}a_{x/y}} = \mathrm{e}^{2\pi\nu_{x/y}i}\,, \\ f_{m_x m_y m_z m_l + (n_a+n_b)N_z} = f_{m_x m_y m_z m_l} & \Rightarrow \quad \mathrm{e}^{i(n_a+n_b)N_z k_z \tilde{a}} = \mathrm{e}^{2\pi\nu_z i}\,. \end{array}$$

For counting the allowed values of the z-component of the wave vector k_z, the counter $\nu_z \in \{0, \pm 1, \pm 2, \ \ldots \ \pm N_z/2\}$ is used, by which the boundaries of the first Brillouin zone along the z-direction are defined:

$$(13)\quad k_z \in \left[-\frac{\pi}{(n_a+n_b)\tilde{a}}, +\frac{\pi}{(n_a+n_b)\tilde{a}}\right]\,,$$

where the notation $\tilde{a}$ for the average validity of the lattice-constant along the z-direction is introduced as:

$$(14)\quad \tilde{a} = \frac{(n_a-1)a^a + (n_b-1)a^b + 2a}{n_a+n_b}\,.$$

We are looking for the phonon dispersion law with the aid of the phonon two-time commutator Green's function

$$(15)\quad \begin{array}{rcl} G_{\vec{n},n_l;\vec{m},m_l}(t-t') & \equiv & \langle\langle u_{\vec{n},n_l}(t) | u_{\vec{m},m_l}(t')\rangle\rangle = \\ & = & \Theta(t-t')\langle[u_{\vec{n},n_l}(t), u_{\vec{m},m_l}(t')]\rangle\,, \end{array}$$

which satisfies the equation of motion

$$(16)\quad \begin{array}{rcl} M_i \dfrac{d^2}{dt^2} G_{\vec{n},n_l;\vec{m},m_l}(t-t') & = & -i\hbar\delta_{\vec{n},\vec{m}}\delta_{n_l,m_l}\delta(t-t') + \\ & + & \dfrac{\Theta(t-t')}{i\hbar}\langle[[p_{\vec{n},n_l}(t), H(t)], u_{\vec{m},m_l}(t')]\rangle\,, \end{array}$$

where $M_i \in (M_a, M_b)$. Assuming that $t' = 0$ and after performing time Fourier transform, the last equation acquires the form

$$(17)\quad -M_i\omega^2 G_{\vec{n},n_l;\vec{m},m_l}(\omega) = -\frac{i\hbar}{2\pi}\delta_{\vec{n},\vec{m}}\delta_{n_l,m_l} + \frac{1}{i\hbar}\langle\langle[p_{\vec{n},n_l}, H] | u_{\vec{m},m_l}\rangle\rangle_\omega\,.$$

Next, we are going to calculate the commutators in Green's function which appears in the equation (17).

Since the translational invariance of the system we are studying is broken, we introduce the partial spatial Fourier-transform by indexes x, y and z (because by the index l, the translational symmetry has been disturbed)

$$(18)\quad G_{\vec{n},n_l;\vec{m},m_l}(\omega) = \frac{1}{N}\sum_{\vec{k}} G_{n_l;m_l}\,\mathrm{e}^{i[a_x k_x(n_x-m_x) + a_y k_y(n_y-m_y) + \tilde{a}(n_a+n_b)k_z(n_z-m_z)+J]}$$

where $N = N_x N_y N_z$, $\vec{k} \equiv \{k_x, k_y, k_z\}$ and:

$$J = \begin{cases} 1.\ a^a k_z (n_l - m_l) & , \ n_l - m_l < n_a \\ 2.\ a^a k_z (n_a - 1) + a k_z & , \ n_l - m_l = n_a \\ 3.\ a^a k_z (n_a - 1) + a k_z + a^b k_z (n_l - m_l - n_a) & , \ n_a < n_l - m_l < n_a + n_b \\ 4.\ a^a k_z (n_a - 1) + a^b k_z (n_b - 1) + 2 a k_z & , \ n_l - m_l = n_a + n_b \end{cases}$$

Applying this to the equations of motion of each layer inside the basic motive of the superlattice, we obtain the system of $n_a + n_b$ of nonhomogeneous algebraic-difference equations with the same number of undetermined Green's functions:

$$\begin{aligned}
\left(\omega^2 - \mathcal{F}^a_{xy} - \Omega^2_{a_z} - \Omega^2_A\right) G_{0;m_l} \ + \\
+ \Omega^2_{a_z} e^{i a^a k_z} G_{1;m_l} + \Omega^2_A e^{-i a k_z} G_{n_a+n_b-1;m_l} &= \frac{i\hbar}{2\pi M_a} \delta_{0,m_l} \\
\left(\omega^2 - \mathcal{F}^a_{xy} - 2\Omega^2_{a_z}\right) G_{1;m_l} \ + \\
+ \Omega^2_{a_z} e^{i a^a k_z} G_{2;m_l} + \Omega^2_{a_z} e^{-i a^a k_z} G_{0;m_l} &= \frac{i\hbar}{2\pi M_a} \delta_{1,m_l} \\
\qquad * \qquad\quad * \qquad\quad * \qquad\quad * \\
\left(\omega^2 - \mathcal{F}^a_{xy} - 2\Omega^2_{a_z}\right) G_{n_a-2;m_l} \ + \\
+ \Omega^2_{a_z} e^{i a^a k_z} G_{n_a-1;m_l} + \Omega^2_{a_z} e^{-i a^a k_z} G_{n_a-3;m_l} &= \frac{i\hbar}{2\pi M_a} \delta_{n_a-2,m_l} \\
\left(\omega^2 - \mathcal{F}^a_{xy} - \Omega^2_{a_z} - \Omega^2_A\right) G_{n_a-1;m_l} \ + \\
+ \Omega^2_A e^{i a k_z} G_{n_a;m_l} + \Omega^2_{a_z} e^{-i a^a k_z} G_{n_a-2;m_l} &= \frac{i\hbar}{2\pi M_a} \delta_{n_a-1,m_l} \\
\left(\omega^2 - \mathcal{F}^b_{xy} - \Omega^2_{b_z} - \Omega^2_B\right) G_{n_a;m_l} \ + \\
+ \Omega^2_{b_z} e^{i a^b k_z} G_{n_a+1;m_l} + \Omega^2_B e^{-i a k_z} G_{n_a-1;m_l} &= \frac{i\hbar}{2\pi M_b} \delta_{n_a,m_l} \\
\left(\omega^2 - \mathcal{F}^b_{xy} - 2\Omega^2_{b_z}\right) G_{n_a+1;m_l} \ + \\
+ \Omega^2_{b_z} e^{i a^b k_z} G_{n_a+2;m_l} + \Omega^2_{b_z} e^{-i a^b k_z} G_{n_a;m_l} &= \frac{i\hbar}{2\pi M_b} \delta_{n_a+1,m_l} \\
\qquad * \qquad\quad * \qquad\quad * \qquad\quad * \\
\left(\omega^2 - \mathcal{F}^b_{xy} - 2\Omega^2_{b_z}\right) G_{n_a+n_b-2;m_l} \ + \\
+ \Omega^2_{b_z} e^{i a^b k_z} G_{n_a+n_b-1;m_l} + \Omega^2_{b_z} e^{-i a^b k_z} G_{n_a+n_b-3;m_l} &= \frac{i\hbar}{2\pi M_b} \delta_{n_a+n_b-2,m_l} \\
\left(\omega^2 - \mathcal{F}^b_{xy} - \Omega^2_{b_z} - \Omega^2_B\right) G_{n_a+n_b-1;m_l} \ + \\
+ \Omega^2_B e^{i a k_z} G_{0;m_l} + \Omega^2_{b_z} e^{-i a^b k_z} G_{n_a+n_b-2;m_l} &= \frac{i\hbar}{2\pi M_b} \delta_{n_a+n_b-1,m_l} \,.
\end{aligned} \tag{19}$$

where the following notations are introduced:

$$\begin{aligned}
\mathcal{F}^{a/b}_{xy} &\equiv 4\left(\Omega^2_{a/b_x} \sin^2 \tfrac{a_x k_x}{2} + \Omega^2_{a/b_y} \sin^2 \tfrac{a_y k_y}{2}\right) ; \\
\tfrac{C^{x/y/z}_a}{M_a} = \Omega^2_{a_{x/y/z}} \,, \quad \tfrac{C}{M_a} = \Omega^2_A \,, \quad & \tfrac{C^{x/y/z}_b}{M_b} = \Omega^2_{b_{x/y/z}} \,, \quad \tfrac{C}{M_b} = \Omega^2_B \,.
\end{aligned} \tag{20}$$

In further calculation, the described model is reduced by the following substitutions:

$$a^a = a^b = \tilde{a} = a \equiv a_z\ ; \qquad \Omega^2_{a_x} = \Omega^2_{a_y} = \Omega^2_{a_z} \equiv \Omega^2_a = \frac{\Omega^2_A}{\alpha}\ ;$$
$$a_x^{a/b} = a_y^{a/b} = a_z \equiv a\ ; \qquad \Omega^2_{b_x} = \Omega^2_{b_y} = \Omega^2_{b_z} \equiv \Omega^2_b = \frac{\Omega^2_B}{\beta}\ ,$$

to the simple cubic lattice model. Introducing symbols:

$$\varrho_a = \frac{\omega^2}{\Omega^2_a} - 4\left(\sin^2\frac{ak_x}{2} + \sin^2\frac{ak_y}{2}\right) - 2\ ;$$
$$\varrho_b = \frac{\omega^2}{\Omega^2_b} - 4\left(\sin^2\frac{ak_x}{2} + \sin^2\frac{ak_y}{2}\right) - 2\ , \tag{21}$$

we obtain the system of equation, the determinant which can be written in the following form:

$$\left|\begin{array}{ccc|ccc|ccc}
A & e^+ & 0 & 0 & 0 & 0 & 0 & 0 & \alpha e^- \\
e^- & \varrho_a & e^+ & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & e^- & \varrho_a & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
- & - & - & - & - & - & - & - & - \\
\hline
0 & 0 & 0 & A & \alpha e^+ & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \beta e^- & B & e^+ & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & e^- & \varrho_b & 0 & 0 & 0 \\
\hline
- & - & - & - & - & - & - & - & - \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & \varrho_b & e^+ & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & e^- & \varrho_b & e^+ \\
\beta e^i & 0 & 0 & 0 & 0 & 0 & 0 & e^- & B
\end{array}\right|_{\mathcal{N}_{II}} \tag{22}$$

where $A = \varrho_a + 1 - \alpha$, $B = \varrho_b + 1 - \beta$, $\mathcal{N}_{II} = (n_a + n_b) \times (n_a + n_b)$, $e^+ = e^{iak_z}$, $e^- = e^{-iak_z}$. $n_a + n_b$ undetermined Green's functions can be expressed as follows: $G_{m_z} = \dfrac{D_{m_z}}{D}$, where D_{m_z} is the determinant of the variable, and D the determinant of the system. Poles of Green's functions by which the phonon dispersion law is determined, can be obtained on the condition that the determinant of the system (22) is equal to zero [10].

As the equation for D=0, is not in general solvable analytically, we applied here the numerical method as the approach to certain cases. Different combinations of atom numbers n_a and n_b have been examined, and also the changes of relations of Hooke's elastic constants between and inside the crystalline films. During further analysis, the superlattices made of films (with n_a and n_b layers) of the same atom types have been examined in two different cases:

1. When the connection between the atoms within the layers is weaker than the one between the atoms on the boundary surfaces of the films ($\alpha = \beta = 2.0$).

2. When the connection between the atoms within the layers is stronger than the connection between the atoms on the boundary surfaces of the films ($\alpha = \beta = 0.5$).

These two cases are graphically presented in Fig. 2, where one can see the reduced phonon frequencies (ω/Ω)[5] on the ordinate and reduced wave vectors along the z-direction $\tilde{a}k_z(n_a + n_b)/\pi$ on the abscissa. Only the centre of the first Brillouin zone was taken into consideration ($k_x = k_y = 0$). Numbers of atoms in the relative layers are shown in the brackets: (n_a, n_b).

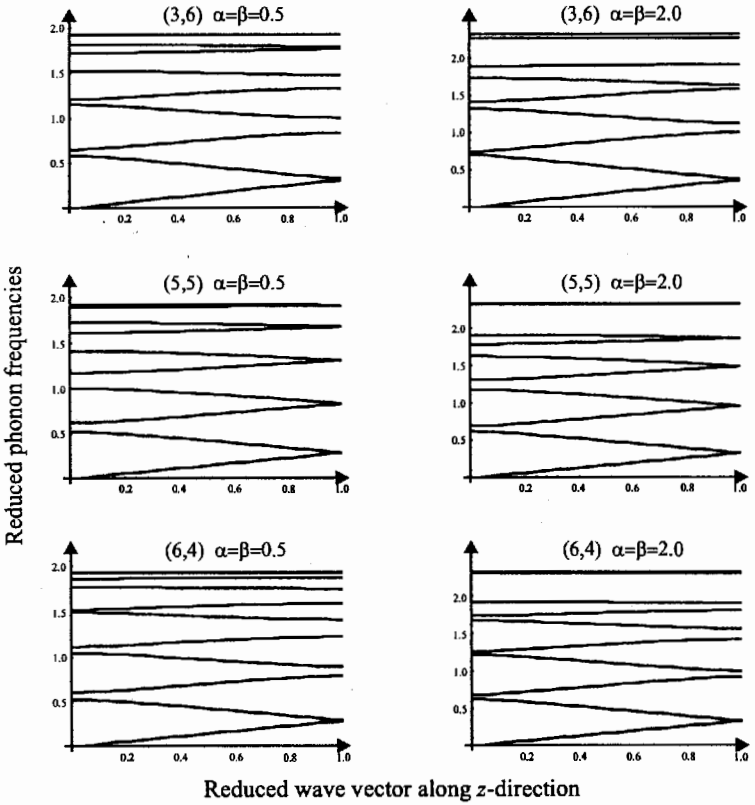

Figure 2: Energy spectra of phonons in superlattices with two layers

[5]Based on the expression (21), the frequencies Ω_A and Ω_B are connected with the equation: $\Omega_A^2 = \frac{M_b}{M_a}\Omega_B^2 \equiv m\Omega_B^2$. It is supposed in the analysis that $m = 1$, from what follows: $\Omega_A = \Omega_B \equiv \Omega$.

3. Conclusion

First of all, we formulated the Hamiltonian of the described model structure of the phonon subsystem of the superlattice and obtained the system of equations for calculation of phonon frequencies. After that we analyzed the energy phonon spectra in the superlattices, composed of alternately repeated ultrathin films of the same materials. The influences of superlattice parameters on phonon spectra were examined (the relation of elastic constants inside and between film layers and number of their atoms). On the basis of these analyzes we have come to the following conclusion:

1. As the result breaking of the translational invariance along the z-direction, the energy zone (which is continual as in unbounded crystals) passes into the subzones separated by the forbidden energy zones.
2. Since the length of the motive, repeating itself along the z-direction of the superlattice is greater than the distance between atoms, the z-component of the wave vector must be redefined.
3. With the increase of energy, the density of phonon states in all examined cases becomes higher.
4. In case of the symmetric superlattice ($n_a = n_b$) with the identical atoms, energy levels join at the boundary of the first Brillouin zone.
5. In case of a loose connection between the layers of the superlattice, shifting of energy levels takes place inside the bulk zone ($\omega/\Omega = 2$) irrespective of the total number of atoms inside the basic motive of the superlattice. If the connection between the layers of the superlattice is stronger, energy levels are being shifted above the bulk zone.

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