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Effects of the Mixture of One- and Three-Dimensional Inhomogeneities on the Wave Spectrum of Superlattices¶

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Dependences of the dispersion laws and damping of waves in an initially sinusoidal superlattice on the dimensionality of inhomogeneities modulating the period of the superlattice are studied. The cases of one- and three-dimensional modulations, as well as modulation by a mixture of inhomogeneities of both of these dimensionalities, are considered. The correlation function of the superlattice $K(\mathbf{r})$ has the form of a product of the same periodic function and a decreasing function that is significantly different for these different cases. The decreasing part of the correlation function for the mixture of inhomogeneities of different dimensionalities has the form of a product of the decreasing parts of the correlation functions of the components of the mixture. This leads to the nonadditivity of the contributions of the components of different dimensionalities to the resulting modification of the parameters of the wave spectrum that are due to the inhomogeneities (the damping of waves for the mixture of these components is smaller than the sum of the dampings of the components, the maximum gap in the spectrum corresponds to the simultaneous presence of both components of the mixture, not only of the three-dimensional inhomogeneities). *© 2003 MAIK "Nauka/Interperiodica".*

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1. Investigations of the spectrum of waves in partially randomized superlattices (SLs) have been carried out very intensively in recent years. This is due to the wide use of these materials in various high-technology devices, as well as to the fact that they are convenient models for developing new methods of theoretical physics for studying media without translation symmetry. Several methods now exist for developing a theory of such SLs: the modeling of the randomization by altering the order of successive layers of two different materials [1–7]; the numerical modeling of the random derivations of the interfaces between layers from their initial periodic arrangement [8–10]; the postulation of the form of the correlation function of a SL with inhomogeneities [11, 12]; the application of the geometrical optics approximation [13]; and the development of the dynamic composite elastic medium theory [14].

One more method for the investigation of the influence of inhomogeneities on the wave spectrum of a SL was suggested in [15]: the method of the random spatial modulation (RSM) of the period of the SL. This method is an extension of the well-known theory of the random frequency (phase) modulation of a radio signal [16, 17] to the case of spatial inhomogeneities in the SL. The advantage of this method is that the form of the correlation function (CF) of the SL is not postulated but is developed from the most general assumptions about the nature of a random spatial modulation of the SL period. It appeared that in the general case this function had quite a complicated form that depended on the dimensionality of the inhomogeneities. Knowledge of the CF corresponding to a particular type and dimensionality of the inhomogeneities permitted us to apply methods of investigation of averaged Green's functions to find the energy spectrum and other characteristics of the waves [15, 18–23]. The RSM method permitted us to consider inhomogeneities of different dimensionalities in the framework of the same model. Effects of one-dimensional (1D) and three-dimensional (3D) inhomogeneities on the wave spectrum were studied for sinusoidal SLs, SLs with sharp interfaces, and SLs with arbitrary thicknesses of interfaces. The influence of inhomogeneities of each dimensionality was studied separately. So, a significant aspect of the problem that was not considered up to now is the situation when inhomogeneities of different dimensionalities are present simultaneously in a superlattice. The study of this aspect is the objective of the present work.

2. Model and correlation function. A SL is characterized by the dependence of some material parameter A on the coordinates $\mathbf{x} = \{x, y, z\}$. The physical nature of the parameter $A(\mathbf{x})$ can be different. This parameter can be a density of matter or a force constant for the elastic system of a medium, the magnetization, anisotropy, or exchange for a magnetic system, and so on. We represent $A(\mathbf{x})$ in the form

$$A(\mathbf{x}) = A[1 + \gamma\rho(\mathbf{x})], \quad (1)$$

¶ This article was submitted by the authors in English.

where A is the average value of the parameter, γ is its relative rms variation, and $\rho(\mathbf{x})$ is a centered ($\langle\rho(\mathbf{x})\rangle = 0$) and normalized ($\langle\rho^2(\mathbf{x})\rangle = 1$) function. The function $\rho(\mathbf{x})$ describes the periodic dependence of the parameter along the SL axis z, as well as the random spatial modulation of this parameter, which, in the general case, can be a function of all three coordinates $\mathbf{x} = \{x, y, z\}$.

We will consider in this paper a SL that has a sinusoidal dependence of the material parameter on the coordinate z in the initial state when inhomogeneities are absent. According to the RSM method, we represent the function $\rho(\mathbf{x})$ in the form

$$\rho(\mathbf{x}) = \sqrt{2}\cos[q(z - u_1(z) - u_3(\mathbf{x})) + \psi], \qquad (2)$$

where $q = 2\pi/l$ is the SL wave number.

The function $u_1(z)$ describes 1D inhomogeneities of the phase of the function $\rho(\mathbf{x})$. The sensitivity of the profile of the function $\rho(\mathbf{x})$ to the action of the modulation $u_1(z)$ is different for different points of the function $\rho(\mathbf{x})$. The smallest changes of the profile occur in the vicinities of the minima and maxima of the function $\cos(qz)$. In contrast to this, the displacements of the zero points of $\cos(qz)$ by the values of $u_1(z)$ lead to the strongest changes in the profile. The zero points of the function $\rho(\mathbf{x})$ correspond to the interfaces of the SL. Because of this, we assume in the RSM method that the function $u_1(z)$ models 1D displacements of the interfaces from their initial periodic arrangement.

The function $u_3(\mathbf{x})$ is introduced in Eq. (2) to model a random deformation of the surfaces of the interfaces. At first glance, it would seem that this function must depend only on the two coordinates, x and y. But the function $u(x, y)$ describes in the RSM method a 2D deformation that is uniform for all interfaces of the SL, i.e., that has an infinite value of the correlation radius along the z coordinate. The directly opposed cases are of interest in reality, namely, the cases where the deformations of the two nearest interfaces are uncorrelated (the correlation radius along z is much smaller than $l/2$) or only several interfaces are correlated. That is why $u_3(\mathbf{x})$ must be a random function of all three coordinates x, y, and z.

In the general case, this function has an anisotropy of correlation properties, because the values of the correlation radii in the xy plane and along the z axis are determined by different physical reasons. But we restrict ourselves here to the simplest case and assume that $u_3(\mathbf{x})$ is a 3D random function with isotropic correlation properties. A coordinate-independent random phase ψ is introduced into Eq. (2) to ensure the fulfillment of the condition of ergodicity for the function $\rho(\mathbf{x})$ (see [15]); it is characterized by a uniform distribution in the interval $(-\pi, \pi)$. After averaging the product of the functions $\rho(\mathbf{x})$ and $\rho(\mathbf{x} + \mathbf{r})$ over the phase ψ, we obtain

$$\langle\rho(\mathbf{x})\rho(\mathbf{x}+\mathbf{r})\rangle_\psi = \cos(qr_z - \chi_1 - \chi_3), \qquad (3)$$

where

$$\begin{aligned}\chi_1 &= q[u_1(z + r_z) - u_1(z)],\\ \chi_3 &= q[u_3(\mathbf{x}+\mathbf{r}) - u_3(\mathbf{x})].\end{aligned} \qquad (4)$$

We assume that the random functions χ_1 and χ_3 are mutually uncorrelated and that each of them is a Gaussian random process. After averaging Eq. (3) over χ_1 and χ_3, we obtain a general expression for the CF of the SL in the form

$$K(\mathbf{r}) = \cos(qr_z)K_1(r_z)K_3(r), \qquad (5)$$

where

$$K_1(r_z) = \exp\left[-\frac{1}{2}Q_1(r_z)\right], \qquad (6)$$

$$K_3(r) = \exp\left[-\frac{1}{2}Q_3(r)\right], \qquad (7)$$

and the structure functions $Q_i(\mathbf{r})$ are defined by the equations

$$Q_1(r_z) = \langle\chi_1^2\rangle, \quad Q_3(r) = \langle\chi_3^2\rangle. \qquad (8)$$

One can see from Eqs. (6)–(8) that $K_1(r_z)$ and $K_3(\mathbf{r})$ are the decreasing parts of the CFs of the SLs with 1D or 3D inhomogeneities (recall that the complete CFs for these cases have the form of the product of $\cos(qr_z)$ and $K_1(r_z)$ or $K_3(\mathbf{r})$, respectively [15]. So, the decreasing part of the CF of a SL with a mixture of the mutually uncorrelated phase inhomogeneities of different dimensionalities has the form of the product of the decreasing parts of the CFs of the components of this mixture.

To find the structure functions $Q_1(r_z)$ and $Q_3(r)$, we must model the correlation properties of the modulating functions $u_1(z)$ and $u_3(\mathbf{x})$ or, more precisely, the correlation properties of their gradients. Both $Q_1(r_z)$ and $Q_3(r)$ were found in [15] (see also some refinements of the coefficients in these expressions in [21]) by the use of different forms of the model CFs for the random modulation. It was shown that the forms of the functions Q_i do not depend asymptotically (for both small and large values of r) on the form of the model CF but strictly depend on the dimensionalities of the inhomogeneities. For the exponential model CFs for $u_1(z)$ and $u_3(\mathbf{x})$, the structure functions were obtained in the forms

$$Q_1(r_z) = 2\gamma_1^2[\exp(-k_\parallel r_z) + k_\parallel r_z - 1], \qquad (9)$$

$$Q_3(r) = 6\gamma_3^2\left[1 - \frac{2}{k_0 r} + \left(1 + \frac{2}{k_0 r}\right)\exp(-k_0 r)\right], \qquad (10)$$

where γ_1 and $k_\parallel$ are the relative rms fluctuation and correlation wave number of the random modulation $u_1(z)$,

γ_3 and k_0 are the corresponding characteristics of the random modulation $u_3(\mathbf{x})$.

After the substitution of Eqs. (9) and (10) into them, Eqs. (6) and (7) become quite complicated. That is why approximate expressions for $K_1(r_z)$ and $K_3(r)$ were suggested for the 1D and 3D inhomogeneities (see [15, 23], respectively):

$$K_1(r_z) = \exp(-\gamma_1^2 k_\parallel r_z), \quad (11)$$

$$K_3(r) = (1-L)\exp(-\gamma_3^2 k_0 r) + L, \quad (12)$$

where $L = \exp(-3\gamma_3^2)$ is the asymptotic form of $K_3(r)$ when $r \longrightarrow \infty$.

According to these equations, effective correlation radii of the SL can be introduced for the 1D and 3D cases, respectively:

$$r_1 = (\gamma_1^2 k_\parallel)^{-1}, \quad r_3 = (\gamma_3^2 k_0)^{-1}. \quad (13)$$

One can see that the effective correlation radii of the SL depend not only on the correlation radii $k_\parallel^{-1}$ or k_0^{-1} of the corresponding modulating functions u_1 or u_3 but also on the rms fluctuations of these functions, γ_1 or γ_3.

3. Dispersion law and damping of waves. We consider the equation for waves in the superlattice in the form

$$\nabla^2\mu + (\nu - \varepsilon\rho(\mathbf{x}))\nu = 0, \quad (14)$$

where the expressions for the parameters ε and ν and the variable μ are different for waves of different natures. For spin waves, when the parameter of the superlattice $A(\mathbf{x})$ in Eq. (1) is the value of the magnetic anisotropy $\beta(\mathbf{x})$, we have [15] $\nu = (\omega - \omega_0)/\alpha g M$, $\varepsilon = \gamma\beta/\alpha$, where ω is the frequency, $\omega_0 = g(H + \beta M)$, g is the gyro-magnetic ratio, α is the exchange parameter, H is the magnetic field strength, M is the value of the magnetization, β is the average value of the anisotropy, and γ is its relative rms variation. For elastic waves in the scalar approximation, we have $\nu = (\omega/V)^2$, $\varepsilon = \gamma\nu$, where γ is the rms fluctuation of the density of the material and V is the wave velocity. For an electromagnetic wave in the same approximation, we have $\nu = \epsilon_e(\omega/c)^2$, $\varepsilon = \gamma\nu$, where ϵ_e is the average value of the dielectric permeability, γ is its rms deviation, and c is the speed of light.

Laws of the dispersion and damping of the averaged waves are determined by the equation for the complex frequency $\nu = \nu' + i\xi$, which follows from the vanishing of the denominator of the Green's function of Eq. (14). In the Bourret approximation [24], this equation has the form [15]

$$\nu - k^2 = \varepsilon^2 \int \frac{S(\mathbf{k} - \mathbf{k}_1)d\mathbf{k}_1}{\nu - k_1^2}, \quad (15)$$

where $S(\mathbf{k})$ is the spectral density of the function $\rho(\mathbf{x})$:

$$S(\mathbf{k}) = \frac{1}{(2\pi)^3}\int K(\mathbf{r})e^{-i\mathbf{kr}}d\mathbf{r}. \quad (16)$$

Substituting Eq. (5) into Eq. (16), then Eq. (16) into Eq. (15), and approximating $K_1(r_z)$ and $K_3(r)$ by Eqs. (11) and (12), we obtain an exactly integrable expression. Upon integrating this expression with respect to $\mathbf{k}_1$ and $\mathbf{r}$, we obtain an explicit form of the equation for ν:

$$\begin{aligned} \nu - k^2 \\ = \frac{\varepsilon^2}{2}\Bigg\{(1-L)\frac{P_{13}}{P_3}\left[\frac{1}{P_{13}^2 - (k-q)^2} + \frac{1}{P_{13}^2 - (k+q)^2}\right] \\ + L\frac{P_1}{\sqrt{\nu}}\left[\frac{1}{P_1^2 - (k-q)^2} + \frac{1}{P_1^2 - (k+q)^2}\right]\Bigg\}, \end{aligned} \quad (17)$$

where

$$\begin{aligned} P_1 = \sqrt{\nu} - ik_\parallel\gamma_1^2, \quad P_3 = \sqrt{\nu} - ik_0\gamma_3^2, \\ P_{13} = \sqrt{\nu} - i(k_\parallel\gamma_1^2 + k_0\gamma_3^2). \end{aligned} \quad (18)$$

We consider this equation at the Brillouin zone boundary $k = k_r \equiv q/2$. Under the conditions that ε, $(k_\parallel\gamma_1^2)^2$, and $(k_0\gamma_3^2)^2$ are much smaller than $\nu_r = k_r^2$, we obtain Eq. (17) in the form of a cubic equation in ν:

$$\begin{aligned} \nu - k_r^2 = \frac{\varepsilon^2}{2}\Bigg[\frac{1-L}{\nu - 2ik_r(k_\parallel\gamma_1^2 + k_0\gamma_3^2) - k_r^2} \\ + \frac{L}{\nu - 2ik_r k_\parallel\gamma_1^2 - k_r^2}\Bigg]. \end{aligned} \quad (19)$$

Both limiting cases of this equation, corresponding to 1D ($\gamma_1 \neq 0$, $\gamma_3 = 0$) and 3D ($\gamma_1 = 0$, $\gamma_3 \neq 0$) inhomogeneities, were considered in our previous works.

The equation (19) for the mixture of 1D and 3D inhomogeneities has been investigated by numerical methods. The results of this investigation are shown in Figs. 1 and 2 by solid curves. Dotted and dashed curves in these figures correspond to the limiting cases of the presence of only 1D or 3D inhomogeneities, respectively. All figures correspond to the same correlation wave numbers for 1D ($\eta_1 \equiv k_\parallel q/\Lambda = 4$, where $\Lambda = \sqrt{2}\varepsilon$) and 3D ($\eta_3 \equiv k_0 q/\Lambda = 4$) inhomogeneities. Different situations are shown in these figures.

Figure 1a shows the decrease of the gap $\Delta\nu = \nu'_+ - \nu'_-$ with the increase of γ_1^2 or γ_3^2. If $\gamma_3 = 0$, the increase in γ_1^2 leads to the closing of the gap at $\gamma_1^2 = 0.25$ (dotted curve). Simultaneously the damping of both eigenfrequencies increases linearly till the point $\gamma_1^2 = 0.25$ (dot-

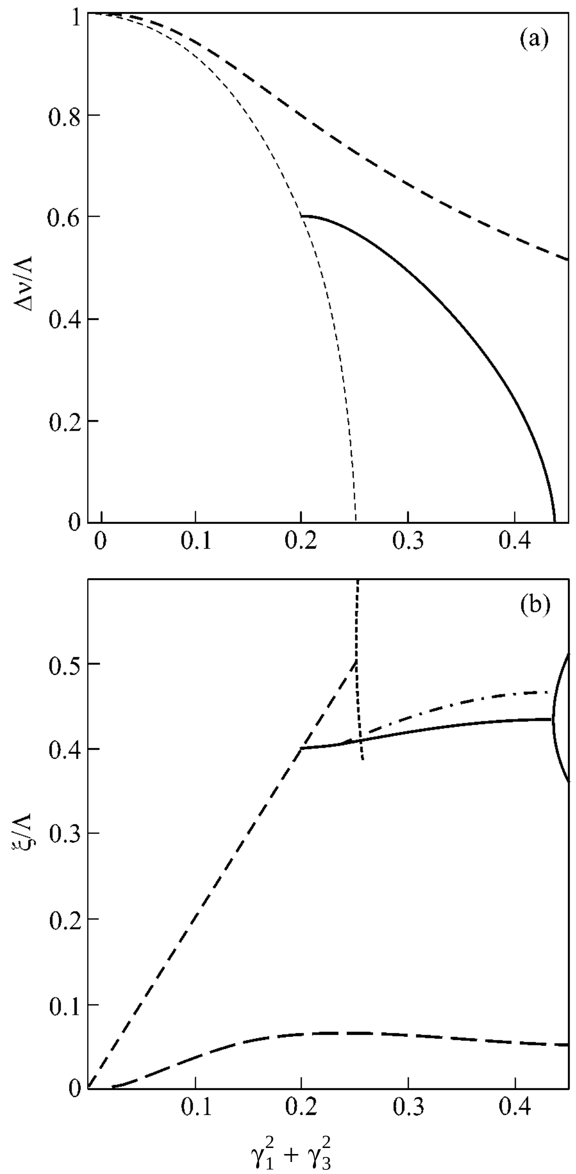

Fig. 1. The width of the (a) gap and (b) damping as functions of the sum $\gamma_1^2 + \gamma_3^2$ for different situations: $\gamma_1^2 \neq 0$, $\gamma_3^2 = 0$ (dotted curves); $\gamma_1^2 = 0$, $\gamma_3^2 \neq 0$ (dashed curves); $\gamma_1^2 = 0.2$, $\gamma_3^2 \neq 0$ (solid curves). The explanation of the dotted-dashed curve in Fig. 1b is given in the text.

ted curve in Fig. 1b). For $\gamma_1^2 > 0.25$, two degenerate eigenfrequencies $\nu'_+ = \nu'_-$ exist with different dampings, $\xi_+ \neq \xi_-$. If $\gamma_1^2 = 0$ the increase of γ_3^2 also leads to the decrease of the gap (dashed curve in Fig. 1a) but significantly more slowly than under the action of the 1D inhomogeneities. For example, a large gap exists for $\gamma_3^2 = 0.25$, while the gap closes when γ_1^2 has the same value. In line with this, the damping increases very

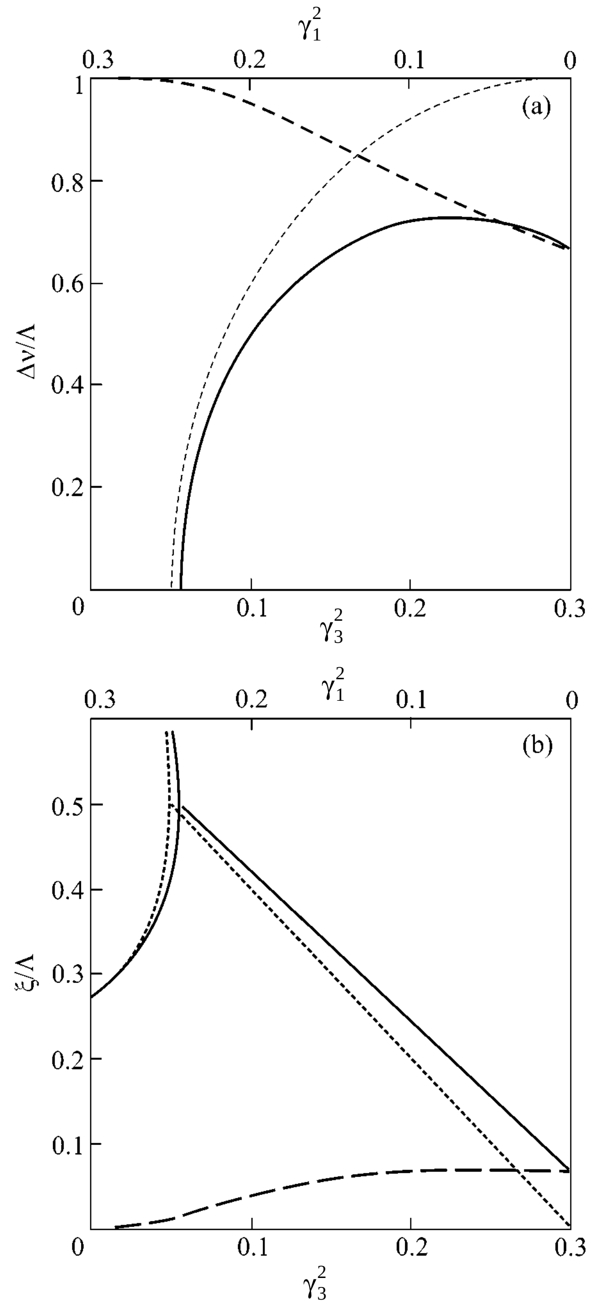

Fig. 2. The width of the (a) gap and (b) damping under the condition $\gamma_1^2 + \gamma_3^2 = 0.3$ (solid curves) and for the situations when γ_3^2 increases for $\gamma_1^2 = 0$ (dashed curves, the scale is under the picture), and when γ_1^2 decreases for $\gamma_3^2 = 0$ (dotted curves, the scale is above the picture).

slightly with the increase in γ_3^2 (dashed curve in Fig. 1b).

To show the effects of the mixture of inhomogeneities of different dimensionalities, the following situation is depicted in Figs. 1. Let us have only 1D inhomogeneities with $\gamma_1^2 = 0.2$ and, correspondingly, let the spectrum gap be $\Delta\nu/\Lambda = 0.6$. Then we add 3D inhomogeneities increasing γ_3^2 and keeping $\gamma_1^2 = 0.2$. One can see that the gap decreases slowly and closes at $\gamma_1^2 + \gamma_3^2 = 0.45$ (solid curve in Fig. 1a). Simultaneously, the increase in the damping slows down (solid curve in Fig. 1b). The dashed-dotted curve in Fig. 1b corresponds to the unreal situation that would have been realized if the damping of the mixture of 1D inhomogeneities with $\gamma_1^2 = 0.2$ and 3D inhomogeneities with γ_3^2 were equal to the simple sum of the damping of the components of the mixture. One can see that in reality the additional contribution to the damping due to 3D inhomogeneities in the presence of the 1D inhomogeneities is approximately two times smaller than in the absence of the latter.

Quite another situation is shown in Figs. 2 by the solid curves. We assume here that the sum $\gamma_1^2 + \gamma_3^2$ remains constant (and equal to 0.3 in these graphs) when γ_1^2 and γ_3^2 are varied. In other words, we consider a gradual replacement of the 1D inhomogeneities by 3D inhomogeneities with the same values of rms fluctuations. For comparison, the functions $\Delta\nu$ and ξ are shown in Figs. 2 separately for the 1D and 3D inhomogeneities. The origin of the coordinates corresponds to $\gamma_3^2 = 0$ (the scale is under the picture) and $\gamma_1^2 = 0.3$ (the scale is above the picture). The width $\Delta\nu$ of the gap is equal to zero for the 1D inhomogeneities and to Λ for the 3D inhomogeneities. The dashed curve in Fig. 2a shows the decrease in $\Delta\nu$ when γ_3^2 increases for $\gamma_1^2 = 0$. The dotted curve in this figure shows the opening and increase of $\Delta\nu$ when γ_1^2 decreases for $\gamma_3^2 = 0$. The solid curve shows the dependence of $\Delta\nu$ on γ_3^2 under the condition $\gamma_1^2 + \gamma_3^2 = 0.3$. One can see that the maximum of $\Delta\nu$ corresponds to some point corresponding to the presence of both components of the mixture ($\gamma_1^2 \neq 0$, $\gamma_3^2 \neq 0$) but not to the absence of the 1D inhomogeneities ($\gamma_1^2 = 0$, $\gamma_3^2 = 0.3$), as might be expected from the general point of view.

4. The method of the random spatial modulation of the superlattice period [15] permits developing the CF of a SL with 1D random modulation (which models random displacements of the interfaces from their initial periodic arrangement), 3D modulation (which models random deformations of the interfaces), and the simultaneous presence of both kinds of modulation (which models the mixture of the 1D and 3D inhomogeneities of the SL structure).

The decreasing part of the CF of the SL in the presence of the mixture of the 1D and 3D inhomogeneities has the form of the product of the decreasing parts of the CFs of the components of the mixture $K_1(r_z)$ and $K_3(\mathbf{r})$.

The widths of the gap in the spectrum and damping of waves at the boundary of the first Brillouin zone have the following behavior depending on the relationship between rms fluctuations γ_1 and γ_3 of the 1D and 3D inhomogeneities. On addition of the 3D inhomogeneities to the SL containing only 1D inhomogeneities, the damping of waves increases. But this additional damping is approximately half as large as the damping that is due to the inhomogeneities with the same value of γ_3^2 in the absence of the 1D inhomogeneities. The situation has also been considered when a gradual replacement of inhomogeneities of one dimensionality by inhomogeneities of the other dimensionality subject to the condition $\gamma_1^2 + \gamma_3^2 = \text{const}$ occurs. It has been shown that the maximum value of the gap corresponds to some relationship between γ_1^2 and γ_3^2 but not to $\gamma_1^2 = 0$, as one could expect from general considerations. This phenomenon, as well as the phenomenon of the reduction of the damping induced by the 3D inhomogeneities in the presence of 1D inhomogeneities, is due to the fact that the decreasing parts of the CFs of the components of the mixture $K_1(r_z)$and $K_3(\mathbf{r})$, as for the mixture of any phase inhomogeneities, enter into the CF of the SL in the form of a product, not a sum.

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