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# Quasi-transverse ultrasound absorption due to point defects and anharmonic scattering processes in cubic crystals with positive and negative anisotropies of the second-order elastic moduli

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## Abstract

The quasi-transverse ultrasound absorption in cubic crystals with positive and negative anisotropies of the second-order elastic moduli is analyzed. The scattering of the ultrasound by point defects and during anharmonic scattering processes is considered. The quasi-transverse ultrasound absorption is analyzed as a function of the wavevector direction in terms of the anisotropic continuum model. The Landau–Rumer mechanism is considered for anharmonic scattering processes. Known values of the second- and third-order elastic moduli are used to calculate parameters determining the ultrasound absorption. It is shown that the angular dependences of the quasi-transverse ultrasound absorption differ qualitatively if the anharmonic scattering processes dominate in cubic crystals with positive and negative anisotropies of the second-order elastic moduli. For the scattering by point defects and the anharmonic scattering processes, the angular dependences of the quasi-transverse ultrasound absorption exhibit the inverse behavior, making it possible to determine the dominating mechanism of the ultrasound relaxation in the crystals under study.

## 1. Introduction

A problem encountered in studies of the ultrasound absorption [1–4], the phonon transport [5, 6] and the thermal emf of the electron–phonon drag [7] in semiconductor and dielectric crystals is the correct consideration of the effect of the cubic anisotropy on the spectrum, the oscillation mode polarization and the phonon relaxation rates. When the temperatures are sufficiently low and the inequality  $\omega_{q\lambda} \tau_{\text{ph}}^{\lambda}(\mathbf{q}, T) \gg 1$  is fulfilled ( $\tau_{\text{ph}}^{\lambda}(\mathbf{q}, T) = 1/\nu_{\text{ph}}^{\lambda}(\mathbf{q}, T)$ ,  $\nu_{\text{ph}}^{\lambda}(\mathbf{q}, T)$  being the phonon relaxation rate and  $\omega_{q\lambda}$  the frequency of phonons with wavevector  $q$  and polarization  $\lambda$ ,  $T$  is the temperature), the dominant contribution to the volume

absorption of sound waves is due to the scattering by defects, including isotopic scattering, and normal processes of phonon–phonon scattering (see, e.g., [1, 4]). We shall restrict ourselves to their consideration in this paper. The isotropic medium approximation [4–6, 8–11], which is commonly used to estimate the probability of various scattering processes, is inadequate for germanium, silicon, diamond and other semiconductor crystals having cubic symmetry and a considerable anisotropy both of the second- and third-order elasticity moduli. The anisotropic continuum model provides a convenient solution to these problems. In this model, the harmonic energy of cubic crystals is expressed in term of three second-order elasticity moduli, while the anharmonic energy in term of six third-order elasticity moduli. Notice that the second- and third-order elasticity moduli have been determined experimentally for a considerable number of cubic crystals. Therefore, the phonon relaxation rates calculated in terms of this model present a reliable basis for the interpretation of experimental data on the ultrasound absorption and the phonon transport in cubic crystals.

In [12], a working formula for the inelastic energy of a cubic crystal associated with anharmonicity of lattice vibrations was derived in terms of experimentally determined second- and third-order elastic moduli (see section 2) and phonon relaxation rates were calculated for a number of anharmonic relaxation processes. The transverse ultrasound absorption in cubic Ge, Si and diamond crystals was discussed in [13]. If the cubic anisotropy in the matrix element describing three-phonon scattering processes was taken into account, the dependences of the relaxation rates on the wavevector of transverse phonons were shown to be qualitatively different from the classical linear Landau–Rumer dependence [14]. However, the analysis [12, 13] was performed in the isotropic approximation for the spectrum and the polarization of phonons: the effect of the cubic anisotropy on the phonon spectrum was disregarded in the energy conservation law. Moreover, the vibrational modes were assumed to be pure (purely longitudinal or purely transverse) modes. As is known [1, 15, 16], quasi-longitudinal or quasi-transverse vibrations propagate in cubic crystals, while pure modes propagate only in symmetric directions such as [100], [110] and [111].

The formal anisotropy factor  $A = 2c_{44}/(c_{11} - c_{12})$  (where  $c_{ij}$  denotes second-order elasticity moduli) was introduced in [17] for characterization of elastic anisotropy of cubic crystals. According to [18, 19], the crystals under study may be conveniently divided into two groups depending on whether the anisotropy parameter  $A$  is greater or less than unity. However, the detailed analysis of elastic waves in cubic crystals [20] demonstrated that the effect of the cubic anisotropy on the spectrum and polarization vectors of vibrational branches is determined by the dimensionless parameter  $k - 1 = \Delta C/(c_{11} - c_{44})$  (where  $\Delta C = c_{12} + 2c_{44} - c_{11}$ ). It is the parameter  $k - 1$  rather than the anisotropy factor  $A$  that enters naturally into the equations for the spectrum and polarization vectors of phonons in cubic crystals [20] (see also appendix A equations (A.2)–(A.6)). Since the parameters  $k - 1$  and  $\Delta C$  have the same sign, all cubic crystals can be classified into those with the positive ( $\Delta C > 0$ ) and the negative ( $\Delta C < 0$ ) anisotropy of the second-order elasticity moduli depending on the sign of  $\Delta C$  (see [20], table 1). This parameter is zero in isotropic media. The first type ( $\Delta C > 0$ ) includes Ge, Si, diamond, InSb, GaSb and GaAs crystals. KCl and NaCl crystals are referred to the second type ( $\Delta C < 0$ ). The form of the spectra of vibrational branches and the angular dependences of polarization vectors of quasi-transverse modes differ qualitatively in crystals of the first and second types; these characteristics differ just quantitatively in crystals of one type [20]. The question arises of how this difference influences the behavior of the relaxation characteristics of cubic crystals: will the angular dependences of the ultrasound absorption in the crystals of the first and second types have qualitative differences? In other words, will the ultrasound absorption anisotropy be determined predominantly by the anisotropy of the harmonic or the anharmonic energy?

**Table 1.** Thermodynamic elasticity moduli for the cubic crystals under study, in  $10^{12}$  dyn  $\text{cm}^{-2}$ . The data are adopted from [1, 27–29].

	Ge	Si	Diamond	InSb	GaSb	KCl	NaCl	GaAs [28]	GaAs [29]
$c_{11}$	1.289	1.657	10.76	0.672	0.885	0.398	0.487	1.1904	1.1877
$c_{12}$	0.483	0.638	1.25	0.367	0.404	0.062	0.124	0.5384	0.5372
$c_{44}$	0.671	0.796	5.758	0.302	0.433	0.0625	0.126	0.5952	0.5944
$\Delta C$	0.54	0.57	2.01	0.3	0.385	-0.211	-0.11	0.54	0.54
$c_{111}$	-7.10	-8.25	-62.6	-3.56	-4.75	-7.01	-8.8	-6.75	-6.22
$c_{112}$	-3.89	-4.51	-22.6	-2.66	-3.08	-0.571	-0.571	-4.02	-3.87
$c_{123}$	-0.18	-0.64	1.12	-1.0	-0.44	0.284	0.284	-0.04	-0.57
$c_{144}$	-0.23	0.12	-6.74	0.16	0.5	0.127	0.257	-0.7	0.02
$c_{155}$	-2.92	-3.10	-28.6	-1.39	-2.16	-0.245	-0.611	-3.2	-2.69
$c_{456}$	-0.53	-0.64	-8.23	-0.004	-0.25	0.118	0.271	-0.69	-0.39
$A_{\text{cub}}$	-0.084	0.71	-27.88	1.57	1.7	0.98	2.09	-1.84	0.8
$\tilde{c}_{155}$	-1.63	-1.9	-5.4	-1.54	-2.16	-0.61	-1.41	-1.12	-1.93
$\tilde{c}_{111}$	28.01	32.4	138.1	20.96	31.53	1.62	8.23	24.19	30.53
$\tilde{c}_{112}$	-3.25	-4.1	-10.24	-1.98	-3.64	-1.11	-1.37	-2.58	-3.34

Such analysis was performed [21] for the relaxation rates of quasi-transverse phonons in terms of the Landau–Rumer mechanism. Unlike earlier calculations, the analysis took into account exactly the effect of the cubic anisotropy on both the spectrum of the vibrational branches involved in the energy conservation law and the phonon polarization vectors. The contributions of the longitudinal components of quasi-transverse vibrations to the phonon relaxation rates were estimated for the two types of cubic crystals. It was shown that the quasi-isotropic approximation is not adequate for the quantitative description of the anisotropy of the relaxation rates of quasi-transverse phonons.

In what follows we shall analyze the angular dependences of the quasi-transverse ultrasound absorption in cubic crystals of the two types for the scattering by defects and in terms of the Landau–Rumer mechanism. As to the phonon polarization vectors involved in the Landau–Rumer mechanism, we shall restrict ourselves to the pure mode approximation for the quasi-longitudinal vibrations. It has been shown [20] that the error induced by this approximation is small for quasi-longitudinal phonons: less than 1% in Ge, Si and diamond crystals, and 3% in KCl. In the case of quasi-transverse phonons moving in directions other than symmetric ones, the maximum contribution of the longitudinal component to the transverse–longitudinal vibrations is 27% in KCl, 16.5% in Ge, 10% in Si and 8% in diamond [20]. Thus, we take into account explicitly the phonon polarization vectors for quasi-transverse phonons, but use the approximation of pure modes for quasi-longitudinal vibrations. Therefore, our calculations of the ultrasound absorption in an arbitrary direction of the wavevector will allow for the contribution of the longitudinal component to the transverse–longitudinal vibrations similarly to [21]. It will be shown that the angular dependences of the absorption of quasi-transverse vibrational modes are qualitatively different in cubic crystals with the positive and the negative anisotropy of the second-order elasticity moduli.

## 2. Absorption of transverse ultrasound in cubic crystals subject to competitive scattering on defects and anharmonic scattering processes

If the inequality  $\omega_{q\lambda} \tau_{\text{ph}}^{\lambda}(\mathbf{q}, T) \gg 1$  ( $\tau_{\text{ph}}^{\lambda}(\mathbf{q}, T) = 1/\nu_{\text{ph}}^{\lambda}(\mathbf{q}, T)$  and  $\omega_{q\lambda}$  being the frequency of a phonon with a wavevector  $q$  and a polarization  $\lambda$ ) is fulfilled, the ultrasonic wave absorption  $\alpha_{\lambda}(\mathbf{q})$  with a wavevector  $q$  and a polarization  $\lambda$  is proportional to the phonon relaxation rate

$\nu_{\text{ph}}^\lambda(\mathbf{q}, T)$  (see, e.g., [1–3]):

$$\alpha_\lambda(\mathbf{q}, T) = \frac{\nu_{\text{ph}}^\lambda(\mathbf{q}, T)}{2S_\lambda(\mathbf{q})}, \quad (1)$$

where  $S_\lambda(\mathbf{q}) = S_\lambda(\theta, \varphi)$  is the phonon phase velocity, which depends on the angular variables  $\theta$  and  $\varphi$  of the vector  $\mathbf{q}$ , and  $T$  is the temperature. Experimental studies of the ultrasound absorption [1, 22] demonstrated that the inequality  $\omega_{q\lambda} \tau_{\text{ph}}^\lambda(\mathbf{q}, T) \gg 1$  is fulfilled at sufficiently low temperatures. For example, it holds at temperatures below 50, 100 and 300 K for germanium, silicon and diamond crystals respectively. Therefore, in what follows we shall only consider the intervals of temperatures and wavevectors  $\mathbf{q}$  when this inequality is fulfilled. In this case, the dominant contribution to the volume absorption of acoustic waves is due to the scattering by defects, including the isotopic scattering, and normal processes of the phonon–phonon scattering (see, e.g., [1, 10]). We shall restrict ourselves to the consideration of these relaxation processes while analyzing the absorption of the long-wave transverse ultrasound ( $\hbar\omega_{qt} \ll k_B T$ ).

That fluctuation in the mass distribution throughout a crystal cause thermal resistance was first pointed out by Pomeranchuk [23], who quoted the correct frequency dependence of the phonon relaxation rate. More detailed consideration of the phonon scattering by static imperfection was made in [24]. In accordance with [25, 26], the expression for the phonon relaxation rate subject to the elastic scattering by point defects in cubic crystals is

$$\nu_{\text{phi}}(q_1, \lambda_1) = \pi G V_0 \omega_{q_1 \lambda_1}^2 \frac{1}{2V} \sum_{\mathbf{q}_2 \lambda_2} \delta(\omega_{q_1 \lambda_1} - \omega_{q_2 \lambda_2}) |(\mathbf{e}_{\mathbf{q}_1 \lambda_1} \mathbf{e}_{\mathbf{q}_2 \lambda_2}^*)|^2. \quad (2)$$

Here  $V_0$  is the volume per one atom,  $V$  is the system volume,  $\mathbf{e}_{\mathbf{q}\lambda}$  is the phonon polarization vector, and  $G$  characterizes the scattering intensity. In the case of the scattering by the isotopic disorder or impurities of the concentration  $N_i$ , the scattering intensity  $G$  has the form [24–26]

$$G = g = \sum_i C_i \left( \frac{\Delta M_i}{\bar{M}} \right)^2, \quad G = V_0 N_i [\sigma_1^2 + (\sigma_2 + \sigma_3)^2], \quad (3)$$

where  $g$  is the isotopic disorder factor,  $\Delta M = M_i - \bar{M}$ ,  $M_i$  is the mass of the  $i$ th isotope,  $\bar{M} = \sum_i C_i M_i$  is the average mass of the isotope composition,  $C_i$  is the concentration of the  $i$ th isotope, while  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  characterize the contributions from the change of the unit cell mass, the force constants and the lattice deformation to the scattering cross-section of phonons by impurities (for more information see [5, 24–26]). Expression (2) can be written in the form

$$\begin{aligned} \nu_{\text{phi}}(q_1, \lambda_1) &= \frac{G V_0 \omega_{q_1 \lambda_1}^4}{16\pi^2} \Phi_{q_1 \lambda_1}(\theta_1, \varphi_1), \\ \Phi_{q_1 \lambda_1}(\theta_1, \varphi_1) &= \sum_{\lambda_2} \int_{-1}^1 dx \int_0^{2\pi} d\varphi_2 \frac{|(\mathbf{e}_{\mathbf{q}_1}^{\lambda_1} \mathbf{e}_{\mathbf{q}_2}^{*\lambda_2})|^2}{(S_{\lambda_2}(\theta_2, \varphi_2))^3}, \quad x = \cos \theta_2. \end{aligned} \quad (4)$$

It is easy to show for the isotropic medium that

$$\Phi_{q_1 \lambda_1}(\theta_1, \varphi_1) = \frac{4\pi}{3} \left( \frac{1}{S_L^3} + \frac{2}{S_t^3} \right), \quad (5)$$

where  $S_L$  and  $S_t$  are velocities of longitudinal and transverse phonons. Using the data on phase velocities and polarization vectors of phonons [20], we found that in cubic crystals the function  $\Phi$  does not depend on either the polarization or the scattering angles of phonons:

**Table 2.** Parameters and the transverse ultrasound absorption in the cubic crystals under study.

	$B_0 \cdot 10^{24}$ ( $\text{cm}^4 \text{dyn}^{-2} \text{s}^{-1} \text{K}^{-5}$ ) [100]	$B_0^{TLL}$ ( $\text{s}^{-1} \text{K}^{-5}$ ) [100]	$\alpha_{TLL[001]} 10^5$ ( $dB/\text{cm}$ )	$\alpha_{TLLt2}^*$ [101]	$\alpha_{TLLt1}^*$ [101]	$\alpha_{TLLt1}^*$ [111]	$\alpha_{TLLt2}^*$ [111]	$\Phi$ , $10^{-16}$ ( $\text{s cm}^{-1}$ ) <sup>3</sup>
Ge	0.239	0.87	1.06	0.23	0.64	0.32	0.32	2.88
Si	0.026	0.071	$5.27 \times 10^{-2}$	0.33	0.73	0.37	0.37	0.615
Diamond	$1.3 \times 10^{-5}$	0.0057	$1.93 \times 10^{-3}$	0.11	0.798	0.31	0.31	0.052
InSb	5.23	2.43	4.61	0.47	0.86	0.39	0.39	11.66
GaSb	1.418	1.42	2.22	0.41	0.7	0.36	0.36	6.25
KCl	88.67	0.627	1.54	107	0.48	85	85	9.47
NaCl	19.32	1.13	2.03	37	1.37	25	25	5.28
GaAs [28]	0.333	1.81	2.35	0.157	0.65	0.29	0.29	3.6
GaAs [29]	0.333	0.91	1.18	0.27	0.67	0.33	0.33	3.6

$$\Phi_{q_1\lambda_1}(\theta_1, \varphi_1) = \Phi = \frac{4\pi}{3} \left( \left\langle \frac{1}{S_L^3} \right\rangle + \left\langle \frac{1}{S_{t1}^3} \right\rangle + \left\langle \frac{1}{S_{t2}^3} \right\rangle \right), \quad (5a)$$

$$\left\langle \frac{1}{S_\lambda^3} \right\rangle = \frac{1}{4\pi} \int \sin \theta \, d\theta \, d\varphi \frac{1}{(S_\lambda(\theta, \varphi))^3}.$$

The values of  $\Phi$  for the crystals under study are given in table 2. So, the relaxation rates of phonons during their elastic scattering by defects in cubic crystals are equal for longitudinal and transverse phonons and depend only on the scattered phonon energy:

$$\nu_{\text{phi}}(q_1, \lambda_1) = \frac{\pi}{6} G V_0 \omega_{q_1\lambda_1}^2 D(\omega_{q_1\lambda_1}), \quad (6)$$

$$D(\omega_{q_1\lambda_1}) = \frac{1}{V} \sum_{\mathbf{q}_2\lambda_2} \delta(\omega_{q_1\lambda_1} - \omega_{q_2\lambda_2}) = \frac{3}{(2\pi)^3} (\omega_{q_1\lambda_1})^2 \Phi.$$

Expression (6) can be written in the form

$$\nu_{\text{phi}} \approx B_i T_q^4, \quad T_q \equiv \hbar \omega_{q_i} / k_B, \quad B_i = G(\hbar/k_B)^4 (V_0 \Phi / 8\pi^2), \quad (6a)$$

where  $T_q$  is the ultrasonic quantum energy in Kelvin. Expression (6) for the scattering by the isotopic disorder in cubic crystals coincides with the equation derived in [25, 26].

In accordance with the prevailing concepts [1–6, 8–11], the main mechanism of the transverse phonon relaxation in normal three-phonon scattering processes is the Landau–Rumer mechanism [14] when the merging of the transverse and the longitudinal phonon produces a longitudinal phonon ( $T + L \rightarrow L$ ). The expression for the relaxation rate of phonons moving in an arbitrary direction relative to the crystallographic axes of crystals was obtained for this mechanism in terms of the anisotropic continuum model in [20]. Unlike earlier calculations, this expression exactly allows for the effect of the cubic anisotropy both on the spectrum of the vibrational branches involved in the energy conservation law and on the phonon polarization vectors. In the long-wave approximation, at temperatures much lower than the Debye temperature the relaxation rate has the form [21]

$$\nu^{TLL}(\theta_1, \varphi_1) = B_0^{TLL}(\theta_1, \varphi_1) T_q^4, \quad B_0^{TLL}(\theta_1, \varphi_1) = B_0 J(\theta_1, \varphi_1), \quad (7)$$

$$B_0 = \frac{\pi^3 k_B^5}{15 \hbar^4 \rho^3 S_t(\theta_1, \varphi_1) \langle S_L \rangle^8},$$

where

$$J(\theta_1, \varphi_1) = \int_{-1}^1 dx \frac{1}{\pi} \int_0^{2\pi} d\varphi_2 \delta(\cos \theta_{12} - S^{**}) \frac{I(\theta_2, \varphi_2, \theta_1, \varphi_1)}{(1 + \Delta_2)^8}, \quad x = \cos \theta_2, \\ S^{**} = \lim_{y \rightarrow 0} [S^*(1 - \Delta_2) + (\Delta_2 - \Delta_3)/y], \quad S^* = S_i(\theta_1, \varphi_1)/S_L \quad (8)$$

$$\cos \theta_{12} = \sin \theta_1 \cos(\varphi_2 - \varphi_1) \sin \theta_2 + \cos \theta_1 \cos \theta_2.$$

Here  $\rho$  is the density, while the variables  $\theta_1$  and  $\varphi_1$  determine the direction of the sound wavevector  $\mathbf{q}_1$  relative to the crystallographic axes. The spectrum and the polarization vectors of the vibration modes in an arbitrary direction of the wavevector were determined in a system of coordinates connected with the cube edges. The anisotropy of the spectra is associated with the anisotropy in the phonon phase velocities  $S^\lambda(\theta_i, \varphi_i)$ , which are functions of the angles  $\theta_i$  and  $\varphi_i$  of the vectors  $\mathbf{q}_i$  (see appendix A). The quantities  $\Delta_2^L(\theta_2, \varphi_2)$  and  $\Delta_3^L(\theta_3, \varphi_3)$  characterize the anisotropy of the phase velocity of longitudinal phonons with the wavevectors  $\mathbf{q}_2$  and  $\mathbf{q}_3$ :

$$\Delta_i^L(\theta_i, \varphi_i) = (S_i^L(\theta_i, \varphi_i) - 1)/S_L, \\ S_L = \langle S_L(\theta, \varphi) \rangle = \frac{1}{4\pi} \int \sin \theta d\theta d\varphi S_L(\theta, \varphi), \quad i = 2, 3. \quad (9)$$

Considering the law of phonon momentum conservation, the angular variables  $\theta_3$  and  $\varphi_3$  of the vector  $\mathbf{q}_3$  are expressed as the angular variables  $\theta_1, \varphi_1$  and  $\theta_2, \varphi_2$  of the wavevectors  $\mathbf{q}_1$  and  $\mathbf{q}_2$  (for more information see [21]). Then we find the cubic harmonics  $\xi_3$  and  $\eta_3$ :

$$\xi_3 = (1 - \psi_3)\psi_3 + \psi_4^2, \quad \eta_3 = \psi_3\psi_4^2, \\ \psi_3 = (\cos \theta_3)^2 = (\cos \theta_2 + y \cos \theta_1)^2 / (1 + y^2 + 2y \cos \theta_{12}), \quad y = q_1/q_2, \\ \psi_4 = (\sin \theta_3)^2 \sin \varphi_3 \cos \varphi_3 = \frac{(\sin \theta_2 \sin \varphi_2 + y \sin \theta_1 \sin \varphi_1)}{(1 + y^2 + 2y \cos \theta_{12})} (\sin \theta_2 \cos \varphi_2 + y \sin \theta_1 \cos \varphi_1). \quad (10)$$

The maximum  $|\Delta_L(\theta, \varphi)|$  values are 0.08, 0.07 and 0.04 for Ge, Si and diamond crystals respectively; therefore, the terms linear in  $\Delta_L(\theta, \varphi)$  alone can be taken into account, whereas the quadratic terms can be neglected. This approximation is accurate to within 1%. The explicit expression for the three-phonon matrix element is lengthy and is given in appendix B. The expression for the matrix element describing the three-phonon scattering of quasi-transverse phonons for the Landau–Rumer mechanism in the long-wave approximation has the form [21]

$$I(\theta_1, \varphi_1, \theta_2, \varphi_2) = \left(2 \frac{q_1 q_2^3}{q_3}\right)^{-2} |V_{q_1 q_2 q_3}^{TLL}|^2 = \{A_{\text{cub}}(\mathbf{e}_1 \mathbf{n}_2) \cos \theta_{12} + (2\tilde{c}_{155} - \Delta C)N_C \\ + 2\tilde{c}_{155}N_{155} + 0.5\tilde{c}_{111}N_{111} + \tilde{c}_{112}N_{112} \\ + (\mathbf{e}_1 \mathbf{n}_1)[0.5\tilde{c}_{112}\Delta N_{112} + 0.5\tilde{c}_{123} + (0.5c_{12} + c_{144})]\}^2, \quad (11)$$

where

$$A_{\text{cub}} = c_{12} + 3c_{44} + 2c_{144} + 4c_{456}, \quad y = \frac{q_1}{q_2} = \frac{z_1(1 + \Delta_2)}{z_2 S^*(\theta_1, \varphi_1)}, \\ N_C = \sum_i n_{1i} n_{2i}^2 [(\mathbf{e}_1 \mathbf{n}_2) n_{2i} + 0.5e_{1i}], \quad N_{112} = \sum_i e_{1i} n_{1i} n_{2i}^2, \\ N_{111} = \sum_i e_{1i} n_{1i} n_{2i}^4, \quad N_{155} = \sum_i e_{1i} n_{2i}^2 [n_{2i} \cos \theta_{12} + 0.5n_{1i}], \\ \Delta N_{112} = \sum_i n_{2i}^2 n_{2i}^2, \quad \Delta N_{155} = \sum_i n_{1i} n_{2i}^3, \\ \tilde{c}_{111} = c_{111} - 3c_{112} + 2c_{123} + 12c_{144} - 12c_{155} + 16c_{456}, \\ \Delta C = c_{12} + 2c_{44} - c_{11}, \\ \tilde{c}_{112} = c_{112} - c_{123} - 2c_{144}, \quad \tilde{c}_{155} = c_{155} - c_{144} - 2c_{456}, \quad (12)$$

where  $\mathbf{n} = \mathbf{q}/q = (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi), \cos(\theta))$  is the unit vector of a phonon,  $c_{ij}$  denotes the second-order elasticity moduli, and  $c_{ijk}$  stands for the third-order elasticity moduli. The first term proportional to  $A_{\text{cub}}$  in (10) corresponds to the isotropic scattering, while the other terms containing the third-order elasticity moduli  $\tilde{c}_{111}$ ,  $\tilde{c}_{112}$ ,  $\tilde{c}_{155}$  and  $\Delta C$  correspond to the anisotropic scattering. These terms distinguish cubic crystals from isotropic media: they turn to zero in the isotropic medium model [12]. In the case where the wavevector  $q_1$  is directed along the  $z$  axis ( $n_1 = [001]$ ) and the polarization vector is  $\mathbf{e}_1 = \{1, 0, 0\}$ , we have  $(e_1 n_1) = 0$  and  $e_{1i} n_{1i} = 0$  for any value of  $i$  and also we have  $N_{111} = N_{112} = 0$  and  $\cos \theta_{12} = \cos \theta_2$ . Then the explicit expression for the matrix element (see appendix B equation (B.1)) leads to the result ([12], equation (14))

$$V_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3}^{TLL} = 2 \frac{q_1 q_2^3}{q_3} \sin \theta_2 \cos \varphi_2 (0.5y + \cos \theta_2) \cdot \{A_{\text{cub}}(1 + y \cos \theta_2) + 2\tilde{c}_{155}(\sin \theta_2)^2(\cos \varphi_2)^2 + (2\tilde{c}_{155} - \Delta C) \cos \theta_2(y + \cos \theta_2)\}. \quad (13)$$

In the long-wavelength limit ( $y \ll 1$ ), expression (13) agrees with the result obtained by Simpson [18]. To check this agreement in terms of the function  $I_1(\theta)$  [18], we shall deduce the expression for the square of the matrix element averaged over the angle  $\varphi_2$ .

$$\int_0^{2\pi} d\varphi_2 |V_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3}^{TLL}|^2 = \left(\frac{q_1 q_2^3}{q_3}\right)^2 I_1(\theta), \quad (14)$$

$$I_1(\theta) = 4\pi (\sin \theta_2 \cos \theta_2)^2 (P_1 - M_1 (\sin \theta_2 \cos \theta_2)^2 - N_1 (\sin \theta_2)^2),$$

where the expressions for the coefficients  $P_1$ ,  $M_1$  and  $N_1$  in [18] are simpler in our notation:

$$P_1 = (c_{11} + c_{44} + 2c_{155})^2, \quad M_1 = 0.5 \cdot ((2\tilde{c}_{155} - \Delta C)^2 + (\Delta C)^2), \quad (15)$$

$$N_1 = P_1 \cdot (2\tilde{c}_{155} - \Delta C) - M_1.$$

Obviously, the coefficients  $M_1$  and  $N_1$  vanish at the transition to the isotropic medium model. It should be noted that in the arbitrary direction of the wavevector  $\mathbf{q}_1$ , unlike the [001] direction considered in [12], the matrix element (11) includes new terms proportional to the third-order elasticity moduli  $\tilde{c}_{111}$  and  $\tilde{c}_{112}$ , as well as the term proportional to  $(\mathbf{e}_1 \mathbf{n}_1)$ , which takes into account the longitudinal component of the transverse–longitudinal vibrations.

According to Matthiessen’s rule, the scattering by defects and the normal processes of the phonon scattering in the Landau–Rumer mechanism make an additive contribution to the transverse sound relaxation. Therefore, formulae (1) and (6)–(12) give for the absorption:

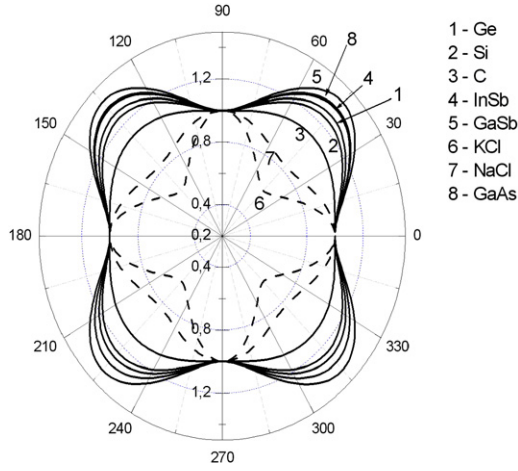
$$\alpha_T(\theta_1, \varphi_1, T) = 8.68(B_0^{TLL}(\theta_1, \varphi_1)T_q T^4 + B_i T_q^4)/2S_t(\theta_1, \varphi_1) \text{ (dB/cm)}. \quad (16)$$

It is seen from (16) that at  $T \ll T_q$  the coefficient  $\alpha_T$  tends to the constant, which is characteristic of the scattering on defects, while at  $T \gg T_q$  it follows the  $T^4$  dependence typical of the Landau–Rumer mechanism. Formulae (6)–(12) and (16) can be used to calculate dependences of the ultrasound absorption on the direction of the quasi-transverse wavevector when the cubic anisotropy is taken into account exactly in the energy conservation law subject to the competition between the anharmonic scattering processes and the scattering by defects. For analysis of these dependences, we shall introduce the dimensionless coefficient  $\alpha_T^*(\theta_1, \varphi_1)$  characterizing the change of the ultrasound absorption relative to the [001] direction:

$$\alpha_T^*(\theta_1, \varphi_1) = \frac{\alpha_T(\theta_1, \varphi_1)}{\alpha_{T[100]}(0, 0, T)} = \frac{S_{[100]}^t}{S_t(\theta_1, \varphi_1)} \frac{(B_0^{TLL}(\theta_1, \varphi_1)T^4 + B_i T_q^3)}{(B_{0[100]}^{TLL} T^4 + B_i T_q^3)}$$

$$= \left(\frac{S_{[100]}^t}{S_t(\theta_1, \varphi_1)}\right)^2 \frac{(J(\theta_1, \varphi_1)T^4 + B_i T_q^3 S_t(\theta_1, \varphi_1))}{(J_{[100]} T^4 + B_i T_q^3 S_{[100]}^t)}. \quad (17)$$





**Figure 1.** Angular dependences of the reduced ultrasound absorption  $\alpha_i^*(\theta_1, \varphi_1)$  for the quasi-transverse mode  $t_2$  in the case of the scattering by defects.

The ultrasound absorption in the [001] direction is defined as

$$\alpha_{T[100]} = (A_{[100]}^{TLL} T_q T^4 + A_{i[100]} T_q^4) \text{ (dB/cm)},$$

$$A_{[100]}^{TLL} = \frac{4.34}{S_{[100]}^t} B_{0[100]}^{TLL}, \quad A_{i[100]} = \frac{4.34}{S_{[100]}^t} B_i. \quad (18)$$

It follows from (17) that for the scattering by point defects the coefficient  $\alpha_i^*(\theta_1, \varphi_1)$  has the form

$$\alpha_i^*(\theta_1, \varphi_1) = S_{[100]}^t / S_t(\theta_1, \varphi_1). \quad (19)$$

In the case of the Landau–Rumer mechanism, the ultrasound absorption anisotropy  $\alpha_{TLL}^*(\theta_1, \varphi_1)$  is defined by the expression

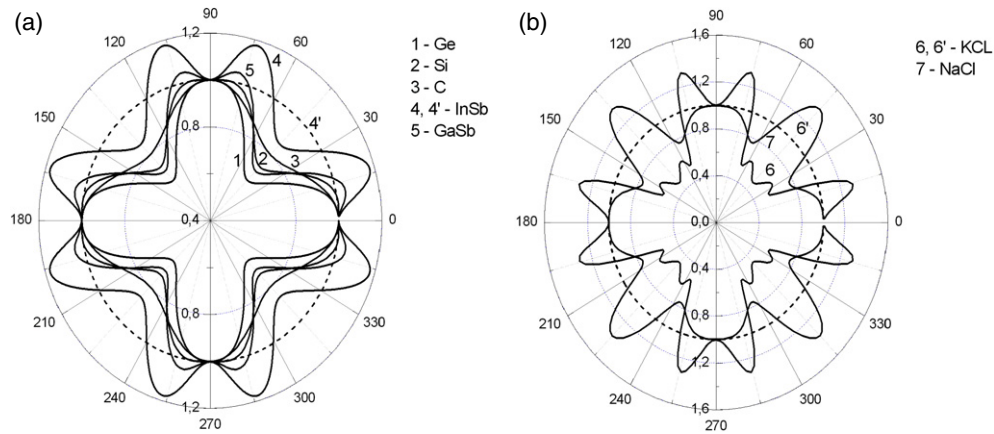
$$\alpha_{TLL}^*(\theta_1, \varphi_1) = \frac{S_{[100]}^t}{S_t(\theta_1, \varphi_1)} \frac{B_0^{TLL}(\theta_1, \varphi_1)}{B_{0[100]}^{TLL}} = \left( \frac{S_{[100]}^t}{S_t(\theta_1, \varphi_1)} \right)^2 \frac{J(\theta_1, \varphi_1)}{J_{[100]}}. \quad (20)$$

We shall show below that the ultrasound absorption anisotropies are considerably different for the aforementioned two cases.

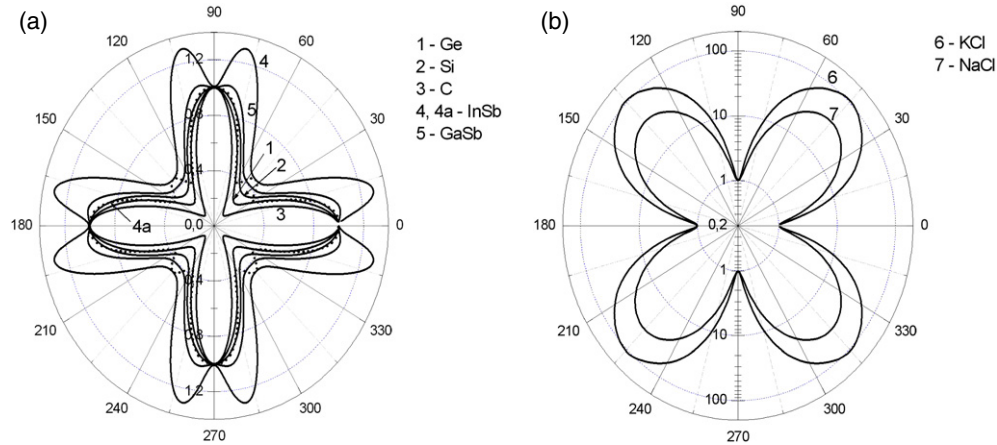
### 3. Results of numerical analysis of transverse ultrasound absorption in cubic crystals

Let us analyze the angular dependences of the acoustic wave absorption for the two most important cases: (1) the acoustic wavevectors  $q_1$  are in the cube face plane ( $\varphi_1 = 0$ ); (2) the acoustic wavevectors  $q_1$  are in the diagonal plane ( $\varphi_1 = \pi/4$ ). These dependences are shown in figures 1–5 for cubic crystals with the positive (Ge, Si, diamond, GaSb, InSb and GaAs) and the negative (KCl and NaCl) anisotropy of the second-order elasticity moduli. The calculations were made using experimental values of the thermodynamic elasticity moduli of the second  $c_{ik}$  and third  $c_{ijk}$  orders, which were adopted from [1, 27–29] (see table 1).

It should be noted first that in the case of the scattering by defects, the ultrasound absorption anisotropy is determined by the harmonic energy anisotropy. The angular dependences of the transverse ultrasound absorption in the cubic crystals of the first and second types are qualitatively different (see figure 1). For example, for a quasi-transverse mode  $t_2$ ,



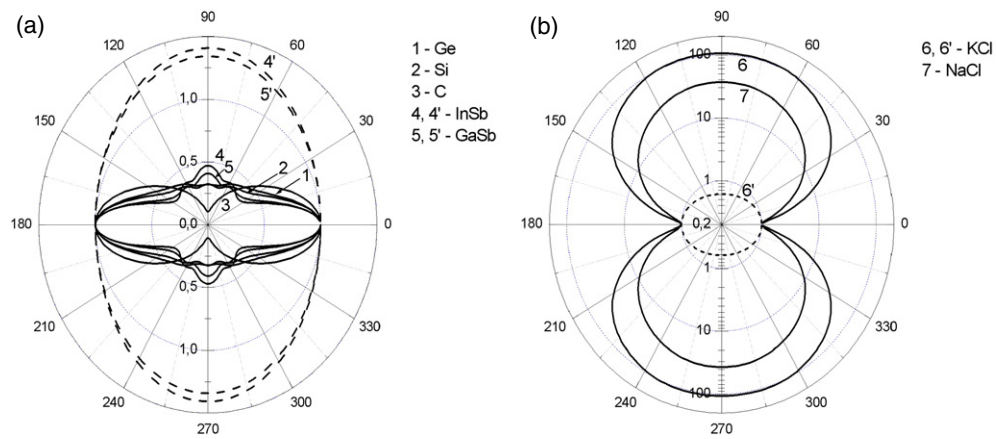
**Figure 2.** Angular dependences of the absorption  $\alpha_{TLL t1}^*(\theta_1, 0)$  for the pure mode  $t_1$  with the wavevector in the cube face plane and the polarization vector perpendicular to this plane in the case of the Landau–Rumer mechanism: (a) crystals of the first type; (b) crystals of the second type. Dashed curves 4', 6': scattering by defects.



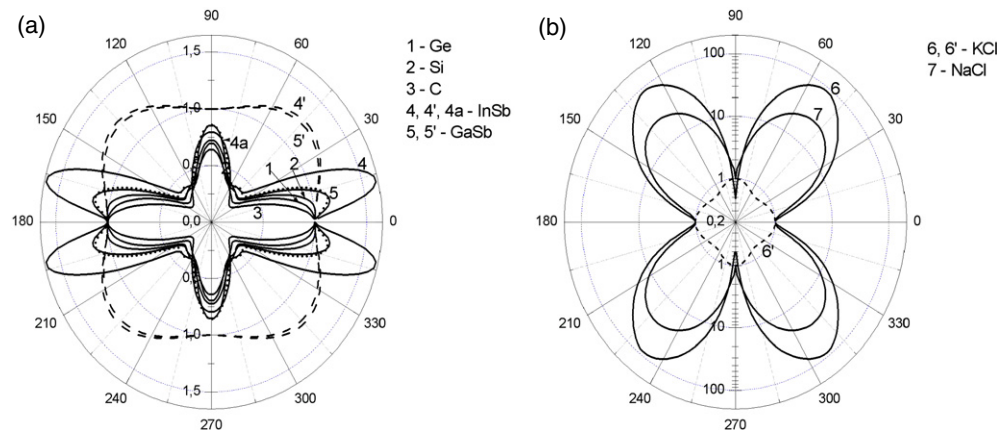
**Figure 3.** Angular dependences of the absorption  $\alpha_{TLL t2}^*(\theta_1, 0)$  for the quasi-transverse mode  $t_2$  with the wave and the polarization vector in the cube face plane for the case of the Landau–Rumer mechanism: (a) crystals of the first type; (b) crystals of the second type. Curve 4a: InSb in the pure mode approximation.

whose wave and polarization vectors are in the cube face plane ( $\varphi_1 = 0$ ), the absorption  $\alpha_{it2}^*(\theta_1, 0)$  is maximum and minimum in the [101] and [001] crystallographic directions respectively in the Ge, Si, diamond, InSb, GaSb and GaAs crystals. The absorption  $\alpha_{it2}^*(\pi/4, 0)$  is equal to 1.29, 1.25, 1.1, 1.41, 1.34 and 1.35 in the Ge, Si, diamond, InSb, GaSb and GaAs crystals, respectively. In the crystals of the second type (KCl, NaCl), these dependences exhibit the inverse behavior (the absorption maxima and minima exchange places): the absorption  $\alpha_{it2}^*(\theta_1, 0)$  is maximum in directions like [101] and minimum in directions like [001]. The absorption  $\alpha_{it2}^*(\pi/4, 0)$  is equal to 0.61 and 0.83 in KCl and NaCl, respectively.

If the anharmonic processes play the dominant role, the ultrasound absorption anisotropy is determined by both the harmonic energy anisotropy and the anharmonic energy anisotropy in the crystals. In this case, the angular dependences of the absorption  $\alpha_{TLL it2}^*(\theta_1, \varphi_1)$  are inverse



**Figure 4.** Angular dependences of the absorption  $\alpha_{TLLt1}^*(\theta_1, \pi/4)$  for the pure mode  $t_1$  with the polarization vector perpendicular to the diagonal plane in the case of the Landau–Rumer mechanism: (a) crystals of the first type; (b) crystals of the second type. Dashed curves 4', 5' and 6': scattering by defects in the InSb, GaSb and KCl crystals, respectively.



**Figure 5.** Angular dependences of the absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  for the quasi-transverse mode  $t_2$  with the wave and the polarization vector in the diagonal plane in the case of the Landau–Rumer mechanism: (a) crystals of the first type; (b) crystals of the second type. Curve 4a: InSb in the pure mode approximation. Dashed curves 4', 5' and 6': scattering by defects in the InSb, GaSb and KCl crystals, respectively.

to those for the scattering by defects. In the crystals of the first type (Ge, Si, diamond, InSb, GaSb and GaAs), the absorption  $\alpha_{TLLt2}^*(\theta_1, \varphi_1)$  is maximum in crystallographic directions like [100] (Ge, Si and diamond) and directions near [100] (InSb, GaSb and GaAs), while the minimum is observed in directions like [101] and [111]. On the contrary, in the crystals of the second type (KCl and NaCl), the absorption  $\alpha_{TLLt2}^*(\theta_1, \varphi_1)$  is maximum in crystallographic directions like [101] and [111], and minimum in directions like [001]. The maximum absorption in the ionic KCl and NaCl crystals proves to be two orders of magnitude larger than the maximum absorption in Ge, whereas these values are similar with respect to their order of magnitude in crystallographic directions like [100]. Thus, the angular dependences of the absorption are qualitatively different for the crystals of the first and second types. The

absorption decreases in the crystals of the first type by nearly one order of magnitude in going from Ge to Si and Si to diamond. This decrease is explained mainly by the change of the coefficient  $B_0$  (see formula (7)), which depends on the second-order elasticity moduli (see table 1). The coefficient  $B_0$  decreases by one order of magnitude in going from Ge to Si and by three orders of magnitude in going from Si to diamond. However, the two orders of magnitude are compensated in the diamond crystals by large values of the third-order elasticity moduli, which determine the probability of the anharmonic scattering processes (see table 1). The growth of the absorption by two orders of magnitude in KCl is due mainly to the change of the parameter  $B_0$ , which depends on the second-order elasticity moduli (see table 2). They are significantly smaller than the moduli in the Ge and InSb crystals (see table 1). Notice that values of the second-order moduli and those of the sound velocity, given in [1] for GaAs, are incorrect. In this section we use values of the second- and third-order elasticity moduli obtained in [29] for GaAs. In this connection the results, obtained in [20, 21] for GaAs, are incorrect.

Let us consider in more detail the dominant role of the anharmonic scattering processes for the acoustic wavevectors  $\mathbf{q}_1$  in the cube face plane ( $\varphi_1 = 0$ ). The isotropic mode  $t_1(S_{t_1}(\theta_1, 0) = \sqrt{c_{44}/\rho} = \text{const})$ , whose polarization vector is perpendicular to the cube face at hand, is a fast mode in the crystals of the first type and a slow mode in the crystals of the second type. In the case of the scattering by defects, the absorption  $\alpha_{it_1}^*(\theta_1, 0)$  of this mode is isotropic in the crystals of both the first and second types. In terms of the Landau–Rumer mechanisms, the absorption  $\alpha_{TLLt_1}^*(\theta_1, 0)$  changes little with the angle  $\theta_1$  in the Ge, Si, diamond, InSb and GaSb crystals (see figure 2(a), curves 1–5). The absorption  $\alpha_{TLLt_1}^*(\theta_1, 0)$  reaches its minimum in [101] directions ( $\theta_1 = \pi/4$ ) in compounds of the first group. The  $\alpha_{TLLt_1}^*(\pi/4, 0)$  values are 0.64, 0.73, 0.8, 0.85, 0.7 and 0.67 for Ge, Si, diamond, InSb, GaSb and GaAs, respectively. The  $\alpha_{TLLt_1}^*(\theta_1, 0)$  values are maximum in [001] directions in the Ge and diamond crystals. Unlike in Ge and diamond, local minima are observed in [001] directions in InSb, GaSb, GaAs and Si. The absorption  $\alpha_{TLLt_1}^*(\theta_1, 0)$  is maximum at the angles  $\theta_1 = n\pi/2 \pm 0.3$ ,  $n\pi/2 \pm 0.19$ ,  $n\pi/2 \pm 0.16$  and  $n\pi/2 \pm 0.13$  ( $n = 0, 1, 2$  etc) and is equal to 1.18, 1.05, 1.09 and 1.002 for InSb, GaSb, GaAs and Si crystals, respectively (see figure 2(a), curves 2, 4 and 5). The ratio between the minimum and maximum values is 0.73, 0.67, 0.68 and 0.73 in InSb, GaSb, GaAs and Si, respectively. These specific features of the absorption in the InSb, GaSb, GaAs and Si crystals are due mainly to the anharmonic energy anisotropy. The point is that in the case of the pure mode  $t_1$  with  $\mathbf{n}_1 = \{\sin \theta_1, 0, \cos \theta_1\}$  and the polarization vector  $\mathbf{e}_1 = \{0, 1, 0\}$ ,  $(\mathbf{e}_1 \mathbf{n}_1) = 0$  and  $e_{1i}n_{1i} = 0$  at all  $i$ , while  $N_{111} = N_{112} = 0$ . Therefore, the matrix element (11) only contains the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$ :

$$I(\theta_1, \varphi_1, \theta_2, \varphi_2) = n_{2y}^2 [(A_{\text{cub}} + 2\tilde{c}_{155}n_{2y}^2) \cos \theta_{12} + (2\tilde{c}_{155} - \Delta C)(n_{1x}n_{2x}^3 + n_{1z}n_{2z}^3)]^2. \quad (21)$$

The moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  have opposite signs in these crystals (see table 1). Therefore, the contributions of the isotropic ( $A_{\text{cub}}$ ) and anisotropic ( $\tilde{c}_{155}$ ) scatterings to the absorption are mutually compensated to a large extent, unlike in Ge and diamond, where this compensation is absent. Since the compensation is larger in InSb than in GaSb and Si, the dependence  $\alpha_{TLLt_1}^*(\theta_1, 0)$  has a deeper minimum in directions like [100]. Thus, the local minima in the dependences  $\alpha_{TLLt_1}^*(\theta_1, 0)$  for the [100] directions in the InSb, GaSb, GaAs and Si crystals appear due to the mutual compensation of the terms proportional to the elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  in the matrix element of the three-phonon scattering processes.

For the Landau–Rumer mechanism, the angular dependences of the ultrasound absorption,  $\alpha_{TLLt_1}^*(\theta_1, 0)$ , are more complicated in the KCl and NaCl crystals of the second type than they are in the crystals of the first type (see figure 2(b)). The absorption  $\alpha_{TLLt_1}^*(\theta_1, 0)$  has the maximum value of 1.32 in the KCl crystal at the angle  $\theta_1 \cong n\pi/2 \pm 0.25$  and the minimum value of  $\alpha_{TLLt_1}^*(\pi/4, 0) = 0.48$  at the angle  $\theta_1 = \pi/4$ . At the angles  $\theta_1 = 0$ ,

$\theta_1 \cong 0.44$ ,  $\theta_1 \cong 1.13$  and  $\theta_1 = \pi/2$  the function  $\alpha_{TLLt_1}^*(\theta_1, 0)$  has four local minima. The maximum values of  $\alpha_{TLLt_1}^*(\theta_1, 0)$  at the angles  $\theta_1 \cong n\pi/2 \pm 0.25$  are nearly three times as large as the minimum values of  $\alpha_{TLLt_1}^*(\pi/4, 0)$ . In the NaCl crystal the maximum absorption  $\alpha_{TLLt_1}^*(\theta_1, 0)$  equal to 1.37 is observed in directions like [101] ( $\theta_1 = \pi/4$ ), while the minimum  $\alpha_{TLLt_1}^*(\theta_1, 0) = 0.76$  is achieved at the angles  $\theta_1 \cong 0.44$  and 1.13. In directions like [001] ( $\theta_1 = 0, \pi/2$ ) the function  $\alpha_{TLLt_1}^*(\theta_1, 0)$  has two local maxima. The angular dependences  $\alpha_{TLLt_1}^*(\theta_1, 0)$  are different in the crystals of the second group because the elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  have opposite signs in the KCl and NaCl crystals and their contributions to the absorption are mutually compensated to a greater (KCl) or lesser (NaCl) extent.

In the case of the quasi-transverse mode  $t_2$  with the wave and polarization vectors in the cube face plane and the anharmonic scattering processes playing the dominant role, the absorption  $\alpha_{TLLt_2}^*(\theta_1, 0)$  in the crystals of the first and second types changes to a greater degree than in the case of the pure mode  $t_1$  (see figures 3(a) and (b)). In the crystals with the positive anisotropy of the second-order elasticity moduli, the absorption  $\alpha_{TLLt_2}^*(\theta_1, 0)$  is minimum in [101] directions ( $\theta_1 = \pi/4$ ). Here  $\alpha_{TLLt_2}^*(\pi/4, 0)$  equals 0.23, 0.33, 0.11, 0.47, 0.4 and 0.27 in Ge, Si, diamond, InSb, GaSb and GaAs, respectively. The maximum  $\alpha_{TLLt_2}^*(\theta_1, 0)$  values are achieved in [001] directions in the Ge, Si and diamond crystals, whereas local minima are observed in these directions in InSb, GaSb and GaAs. The maximum values of the absorption  $\alpha_{TLLt_2}^*(\theta_1, 0)$  are achieved at the angles  $\theta_1 \cong n\pi/2 \pm 0.19$ ,  $n\pi/2 \pm 0.1$  and  $n\pi/2 \pm 0.07$  ( $n = 0, 1, 2$  etc) and are equal to 1.3, 1.02 and 1.007 in InSb, GaSb and GaAs, respectively (see figure 2(a), curves 4 and 5). The ratio of the minimum to maximum values of the absorption  $\alpha_{TLLt_2}^*(\theta_1, 0)$  is 0.36, 0.39 and 0.26 in InSb, GaSb and GaAs, respectively. As distinct from the pure mode  $t_1$  discussed above, all the terms of the matrix element (11) contribute to the absorption of the quasi-transverse mode  $t_2$ . The symmetric maxima, which appear in the dependences  $\alpha_{TLLt_2}^*(\theta_1, 0)$  in directions like [001] in the InSb, GaSb and GaAs crystals, are due to both the anisotropy of the anharmonic and the harmonic energy of the crystals. The anisotropy of the harmonic energy of the crystals gives rise to the longitudinal component of the quasi-transverse mode  $t_2$ , which plays a dominant role in the formation of the symmetric maxima. Figure 3(a) (dashed line 4a) presents the dependence of the mode  $t_2$  absorption in InSb as an approximation of the pure mode, i.e. when the polarization vector of the quasi-transverse mode is replaced by the polarization vector of the pure mode ( $e_0^{\prime 2} = (\cos \theta_1, 0, -\sin \theta_1)$ ). In this case, the local minima near directions like [001] vanish for the pure mode  $t_2$  in the InSb, GaSb and GaAs crystals. It should be noted that the anisotropy of the anharmonic energy of InSb, GaSb and GaAs is also important for the realization of this specific feature. The point is that in Ge the maximum contribution of the longitudinal component to the mode  $t_2$  is 15.5%, which differs little from 15–16% in InSb, GaSb and GaAs. However, the dependence  $\alpha_{TLLt_2}^*(\theta_1, 0)$  exhibits a clear-cut maximum in the [100] direction in the Ge crystal. As indicated above, the absorption of the ultrasound propagating along the cube edges is contributed only by the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  (see formula (21)), which have opposite signs in the InSb, GaSb and GaAs [29] crystals (see table 1). Consequently, their contributions are mutually compensated to a great extent and, therefore, the ultrasound absorption in these directions is considerably smaller than the absorption in Ge, where this compensation is absent. Since the compensation is more complete in InSb than in GaSb and GaAs, a deeper minimum is formed in the dependences  $\alpha_{TLLt_2}^*(\theta_1, 0)$ . Thus, the appearance of local maxima in  $\alpha_{TLLt_2}^*(\theta_1, 0)$  near [100] directions in the InSb, GaSb and GaAs crystals is due to both the longitudinal component of the quasi-transverse mode  $t_2$  and the mutual compensation of the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  in the matrix element of the three-phonon scattering processes. According to relevant estimates, the maximum contribution of the longitudinal component to the absorption of quasi-

transverse modes is 50% in InSb, 36% in GaAs, 34% in GaSb, 30% in Ge and Si and 6% in diamond. The comparison of figures 1 and 2(a) shows that in the case of the scattering by defects the angular dependences of the absorption,  $\alpha_{it2}^*(\theta_1, 0)$ , in the crystals of the first type are inverse to the corresponding dependences observed in the case of the anharmonic scattering processes.

For the quasi-transverse mode  $t_2$ , the angular dependences of the ultrasound absorption in the crystals of the second type (KCl and NaCl) are inverse to the corresponding dependences in the crystals of the first type (see figure 3(b), curves 6 and 7). The absorption  $\alpha_{TLLt2}^*(\theta_1, 0)$  in KCl and NaCl increases sharply from the minimum at  $\theta_1 = 0$ , reaches the maximum at  $\theta_1 = \pi/4$  and decreases to the initial value at  $\theta_1 = \pi/2$ . The dependence  $\alpha_{TLLt2}^*(\theta_1, 0)$  includes maxima in [001] and [100] directions, and minima in the [101] direction. The absorption  $\alpha_{TLLt2}^*(\pi/4, 0)$  is 107 and 37 in KCl and NaCl, respectively. The maximum contribution of the longitudinal component to the absorption of the mode  $t_2$  is 22% in KCl and 3% in NaCl. The comparison of figures 1 and 3(b) demonstrates that the angular dependences of the ultrasound absorption in KCl and NaCl observed for the scattering by defects are inverse to those in the case of the anharmonic scattering processes: the positions of the maxima and the minima are reversed.

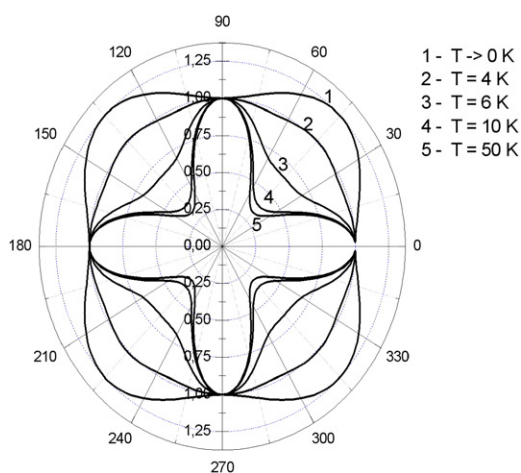
For the pure mode  $t_1$  with the wavevector in the diagonal plane ( $\varphi_1 = \pi/4$ ) and the polarization vector perpendicular to this plane, the absorption  $\alpha_{TLLt1}^*(\theta_1, \pi/4)$  is maximum in the [001] direction in Ge, Si, diamond, InSb, GaSb and GaAs (see figure 4(a), curves 1–5). As the angle  $\theta_1$  decreases, the absorption diminishes to its minimum value in the [110] direction ( $\theta_1 = \pi/2$ ) in the Ge, Si and diamond crystals and equals 0.32, 0.33 and 0.11, respectively (see figure 4(a), curves 1–3). In InSb, GaSb and GaAs the absorption reaches its minimum values at angles near  $\theta_1 \cong \pi/4$ , while a local maximum appears in the [110] direction in these crystals (see figure 4(a), curves 4 and 5). Notice that the relationship  $\alpha_{TLLt1}^*(\pi/2, \pi/4) = \alpha_{TLLt2}^*(\pi/4, 0)$  holds for the absorption referring to different modes. The situation is reverse in the crystals of the second group (KCl and NaCl): the absorption  $\alpha_{TLLt1}^*(\theta_1, \pi/4)$  is minimum in the [001] direction ( $\theta_1 = 0$ ), increases monotonically with the angle  $\theta_1$  and becomes maximum in the [110] direction (see figure 4(b), curves 1 and 2). The absorption  $\alpha_{TLLt1}^*(\pi/2, \pi/4)$  is 107 and 37 in KCl and NaCl, respectively. In the case of the scattering by defects, in contrast to the anharmonic scattering processes, the absorption becomes maximum in the [110] direction and minimum in the [001] direction in the crystals of the first group (see figure 4(a), curves 4' and 5'). The situation is reverse in the crystals of the second group. The absorption  $\alpha_{it2}^*(\pi/2, \pi/4)$  equals 1.20, 1.17, 1.07, 1.26, 1.23, 1.19, 0.68 and 0.87 for Ge, Si, diamond, InSb, GaSb, GaAs, KCl and NaCl, respectively.

For the quasi-transverse mode  $t_2$  with the polarization vector in the diagonal plane ( $\varphi_1 = \pi/4$ ), the absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  in the Ge, Si and diamond crystals is also considerably different from the absorption in the InSb, GaSb and GaAs crystals (see figure 5(a), curves 1–5). The absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  has minimum values in the crystals of the first group at angles  $\theta_1 \cong \pi/4$  and equals 0.27, 0.33, 0.23, 0.38, 0.34 and 0.29 for Ge, Si, diamond, InSb, GaSb and GaAs, respectively. In Ge, Si and diamond the absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  decreases from the maximum value in the [001] direction ( $\theta_1 = 0$ ), becomes minimum at angles  $\theta_1 \approx \pi/4$ , increases again and then at  $\theta_1 = \pi/2$  approaches the value of  $\alpha_{TLLt1}^*(\pi/4, 0)$ , which corresponds to the fast mode in the cube face plane at  $\theta_1 = \pi/4$  (see figure 5(a), curves 1–3). Local minima appear in the [100] direction in InSb, GaSb and GaAs, unlike in the Ge, Si and diamond crystals. The absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  is maximum at angles  $\theta_1 = n\pi/2 \pm 0.22$ ,  $n\pi/2 \pm 0.16$  and  $n\pi/2 \pm 0.15$  and equals 1.6, 1.15, 1.09 for InSb, GaSb and GaAs, respectively (see figure 5(a), curves 4 and 5). The ratio of the minimum to maximum values of the absorption  $\alpha_{TLLt2}^*(\theta_1, \pi/4)$  is 0.36, 0.39 and 0.27 for InSb, GaSb and GaAs, respectively. As noted

above, local maxima in the dependence  $\alpha_{TLLt_2}^*(\theta_1, \pi/4)$  near the [100] direction in the InSb, GaSb and GaAs crystals appear due to both the longitudinal component of the quasi-transverse mode  $t_2$  and the mutual compensation of the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  in the matrix element of the three-phonon scattering processes. The calculation of the absorption of the quasi-transverse mode  $t_2$  in the approximation of the pure mode (the polarization vector of the mode  $t_2$  is replaced by the polarization vector of the pure mode  $e_0^t = (\cos \theta/\sqrt{2}, \cos \theta/\sqrt{2}, -\sin \theta)$ ) shows that in the case of the pure mode  $t_2$  the local maxima considerably diminish near directions like [001] in InSb and GaSb and become as low as 1.14 and 1.01, respectively (see figure 5(a), curve 4a). According to relevant estimates, the maximum contribution of the longitudinal component to the absorption  $\alpha_{TLLt_2}^*(\theta_1, \pi/4)$  of the quasi-transverse modes is 35% in InSb, 27% in GaAs, 20% in Ge, Si and GaSb and 11% in diamond. If the scattering by defects is concerned, the angular dependences of the absorption change qualitatively (see figure 5(a), curves 4' and 5'): the absorption  $\alpha_{it_2}^*(\theta_1, \pi/4)$  is minimum in the [001] and [110] directions and is maximum at angles  $\theta_1 = \pi/4$ . The absorption  $\alpha_{it_2}^*(\pi/4, \pi/4)$  equals 1.20, 1.17, 1.07, 1.26, 1.23 and 1.24 for Ge, Si, diamond, InSb, GaSb and GaAs, respectively.

For the same mode, the angular dependences of the absorption  $\alpha_{TLLt_2}^*(\theta_1, \pi/4)$  in KCl and NaCl and the crystals of the first group differ qualitatively for both the scattering by defects and the Landau–Rumer relaxation mechanism. In the case of the scattering by defects, the absorption  $\alpha_{it_2}^*(\theta_1, \pi/4)$  peaks in directions like [001] and becomes minimum at angles  $\theta_1 = \pi/4$  in the KCl and NaCl crystals (see figure 5(b), curve 6'). The absorption  $\alpha_{it_2}^*(\pi/4, \pi/4)$  equals 0.67 and 0.87 in KCl and NaCl, respectively. In the case of the anharmonic scattering processes, the absorption  $\alpha_{TLLt_2}^*(\theta_1, \pi/4)$  reaches its maximum values in directions like [111] and its minimum values in the [001] and [011] directions in the KCl and NaCl crystals. The maximum absorption  $\alpha_{TLLt_2}^*(\theta_{[111]}, \pi/4)$  is 87 and 27 in KCl and NaCl respectively. It should be noted that in KCl the absorption  $\alpha_{TLLt_2}^*(\theta_{[111]}, \pi/4)$  proves to be a factor of 1.2 smaller than  $\alpha_{TLLt_2}^*(\pi/4, 0)$ , while the minimum absorption  $\alpha_{TLLt_2}^*(\pi/2, \pi/4)$  for this mode is 2.1 times smaller than  $\alpha_{TLLt_2}^*(0, \pi/4)$ . Therefore, the ultrasound absorption for this mode in KCl diminishes 182-fold on transition from the [111] direction to [110]. Thus, the anisotropy of the absorption for the quasi-transverse mode  $t_2$  is one order of magnitude larger in NaCl and two orders of magnitude larger in KCl than it is in the Ge, Si and diamond crystals. The maximum contribution of the longitudinal component to the absorption of the mode  $t_2$  equals 50 and 8% in KCl and NaCl, respectively.

Let us consider how the angular dependences of the ultrasound absorption  $\alpha_{Tt_2}^*(\theta_1, 0)$  change with the temperature in the presence of the competition between isotopic and anharmonic scattering processes. We shall take  $^{\text{nat}}\text{Si}$  crystals with the natural isotopic composition ( $g = 2.01 \times 10^{-4}$ ) as an example. It is seen from figure 6 (curves 1–5) that as the temperature rises from 4 to 50 K in  $^{\text{nat}}\text{Si}$  crystals, the isotopic scattering lets the anharmonic scattering processes have the dominant role and the angular dependences of the absorption  $\alpha_{Tt_2}^*(\theta_1, 0)$  change qualitatively. The change is most abrupt over the temperature interval of  $4 \text{ K} < T < 10 \text{ K}$  when  $T_q = 4.8 \text{ K}$  (corresponding to the ultrasound frequency of 100 GHz) is comparable with the temperature. Curve 5 in this figure, which was calculated at  $T = 50 \text{ K}$ , practically coincides with the results obtained for the Landau–Rumer mechanism. It should be noted that in Si crystals enriched to 99.983% in the  $^{28}\text{Si}$  isotope ( $g = 3.2 \times 10^{-7}$ ) the anharmonic scattering processes make the dominant contribution to the ultrasound absorption at  $T_q = 4.8 \text{ K}$  over the temperature interval of 4 to 50 K, while the angular dependences of the absorption  $\alpha_{Tt_2}^*(\theta_1, 0)$  are described by curve 5. Obviously, from the analysis of the ultrasound absorption anisotropy in cubic crystals it is possible to determine the dominating mechanism



**Figure 6.** Angular dependences of the absorption for the quasi-transverse mode  $t_2$  with the wave and the polarization vector in the cube face plane in the  $^{nat}\text{Si}$  ( $g = 2.01 \times 10^{-4}$ ) crystals in the presence of the competition between isotopic and anharmonic scattering processes for a fixed energy of ultrasonic quantum  $T_q = 4.8$  K and different temperatures.

of ultrasound relaxation at a given temperature. For this purpose, one has only to measure the absorption for the quasi-transverse mode  $t_2$  with the polarization vector in the cube face plane in the [100] and [101] directions and find the coefficient  $\alpha_{Tt_2}^*(\pi/4, 0)$ . If the inequality  $1 \leq \alpha_{Tt_2}^*(\pi/4, 0) \leq 1.25$  is fulfilled, the isotopic scattering makes the major contribution to the ultrasound relaxation in Si crystals. If  $\alpha_{Tt_2}^*(\theta_1, 0)$  is less than unity and tends to 0.33, the dominant contribution to the ultrasound relaxation in Si crystals is due to the anharmonic scattering processes.

#### 4. Discussion

The analysis demonstrated that the anisotropy of the absorption of quasi-transverse modes in the crystals of the first type is a maximum in diamond. This maximum anisotropy is due mainly to the anisotropy of the third-order elasticity moduli since the anisotropy of the second-order elasticity moduli decreases in going from Ge to Si and then to diamond [20]. The anomalously large anisotropy of the absorption of quasi-transverse modes in the KCl and NaCl crystals is caused by the anisotropy of the anharmonic energy of the crystals. The point is that the absorption of the ultrasound propagating along the cube edges is contributed only by the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  (see formula (21)), which have opposite signs in these crystals (see table 1). Therefore, their contributions are mutually compensated to a large extent and, as a result, the ultrasound absorption in these directions should be anomalously small as compared to the absorption in Ge where such compensation is not realized. However, the second-order elasticity moduli and, correspondingly, the sound velocity are much smaller in these crystals than those in Ge. For this reason, the coefficient  $B_0$  in KCl and NaCl is nearly two orders of magnitude larger than  $B_0$  in Ge. These two opposing factors have the effect that the ultrasound absorption in this direction in the KCl, NaCl and Ge crystals is of the same order of magnitude (see table 2). On the other hand, the absorption of the quasi-transverse modes propagating in directions like [101] and [111] is contributed not only by the terms proportional to the third-order elasticity moduli  $A_{\text{cub}}$  and



$\tilde{c}_{155}$ , but also by those proportional to the moduli  $\tilde{c}_{111}$  and  $\tilde{c}_{112}$  (see formula (11)). Therefore, in crystallographic directions like [101] and [111] such compensation is not realized in the matrix element of the three-phonon scattering processes (see table 1) and, because of the coefficient  $B_0$ , the ultrasound absorption in these directions in KCl and NaCl is two orders of magnitude higher than in Ge.

It should be noted that the angular dependences of the ultrasound absorption  $\alpha_{TLL}^*(\theta, \varphi)$  in GaAs, which are calculated using values of the third-order elasticity moduli from [28, 29], differ qualitatively. This behavior of the ultrasound absorption in GaAs is explained by a different character of the anharmonic energy anisotropy, which is determined using the data [28, 29]. The point is that the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  have the same (negative) signs according to [28] and are opposite in sign according to [29] (see table 1). Therefore, angular dependences of the ultrasound absorption, which are calculated from the data [28], have the same shape for all transverse modes in GaAs as in Ge crystals (see figures 2(a)–4(a), curves 1). In this case, a sharp maximum is realized in directions like [100], while the values are minimum in directions like [101] and [111]. By contrast, the third-order elasticity moduli  $A_{\text{cub}}$  and  $\tilde{c}_{155}$  have opposite signs according to [29] and angular dependences of the ultrasound absorption have the same shape for transverse modes in GaAs as in InSb and GaSb crystals (see figures 2(a)–4(a), curves 4 and 5). In this case, local minima occur in directions like [100], while the ultrasound absorption reaches its maximum values at the angles  $\theta_1 \cong n\pi/2 \pm \beta_t$  ( $n = 0, 1, 2$ ), where  $\beta_t \ll 1$ . Thus, at small  $\theta_1$  the ultrasound absorption in GaAs is a decreasing function of the angle  $\theta_1$  as calculated from the data [28] and an increasing function of the angle  $\theta_1$  as calculated from the data [29]. It should be noted that values of the ultrasound absorption in [100] directions differ by a factor of nearly two as calculated from the data [28, 29] (see table 2). Anisotropies of the ultrasound absorption by transverse modes are different too: for example, for mode  $t_2$  with the wavevector in the cube face plane the absorption  $\alpha_{TLL t_2}^*(\pi/4, 0)$  is 0.16 and 0.27 as calculated from the data [28, 29] respectively. The aforementioned behavior of the ultrasound absorption, which is calculated using values reported in [28, 29], calls for experimental verification of the third-order elasticity modulus values determined in [28, 29]. Thus, a conclusion follows from the above analysis that the characteristic types of angular dependences of the ultrasound absorption in cubic crystals are determined not only by values of the second-order elasticity moduli, but also by the relation of values and signs of the third-order elasticity moduli, which determine the anharmonic energy of the crystals.

In this study we only consider the volume absorption of transverse long-wave ultrasound. The boundary scattering of phonons is always present in samples of finite dimensions. This scattering is important for relaxation of the acoustic wave momentum at low temperatures: it makes a temperature-independent contribution to the ultrasound absorption. If this contribution is larger than the contribution from the scattering by defects at low temperatures, the specific features of the ultrasound absorption, which are related to the relaxation mechanisms under study, will not be observed in these crystals. The role of the boundary scattering is discussed more comprehensively in [13].

## 5. Conclusion

We have analyzed angular dependences of the quasi-transverse ultrasound absorption in cubic crystals with positive and negative anisotropies of the second-order elasticity moduli. The effect of the cubic anisotropy on the spectrum and polarization vectors of vibration modes was taken into account. Two most important cases—wavevectors of phonons are in the cube face plane or the diagonal planes—were considered in terms of the anisotropic continuum

model. Known values of the second- and third-order elasticity moduli were used to calculate parameters determining the ultrasound absorption in the crystals under study. The anisotropy of the transverse ultrasound absorption in the presence of the competition between the point defect and anharmonic scattering processes was analyzed. It was shown that the angular dependences of the transverse ultrasound absorption are inverse for the anharmonic scattering processes and the scattering by defects. Therefore, the dominant mechanism of ultrasound relaxation can be determined by analyzing the ultrasound absorption anisotropy in cubic crystals. The analysis demonstrated that the angular dependences of the transverse ultrasound absorption in cubic crystals with positive (Ge, Si and diamond) and negative (KCl, NaCl) anisotropies of the second-order elasticity moduli differ qualitatively for the Landau–Rumer relaxation mechanism. The absorption anisotropy in the crystals of the second type is one order (NaCl) and two orders of magnitude (KCl) larger than it is in Ge, Si and diamond. It was shown that the angular dependences of the ultrasound absorption in GaAs, which are calculated using values of the third-order elasticity moduli from [28, 29], differ qualitatively. This behavior of the ultrasound absorption in GaAs is explained by a different character of the anharmonic energy anisotropy, which is determined using the data [28, 29]. The contributions of longitudinal components of quasi-transverse vibrations to the absorption of quasi-transverse modes were estimated. They are in qualitative agreement with results of the analysis of polarization vectors performed in [20].

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### Appendix A

Let us consider the phonon spectrum of a cubic crystal using the anisotropic continuum model [1, 2]. This model implies that a phonon wavevector  $\mathbf{q}$  is much smaller than the Debye wavevector  $\mathbf{q}_d$  and that the spectrum of phonons with polarization can be written as

$$\omega_q^\lambda = S^\lambda(\theta, \varphi)q. \quad (\text{A.1})$$

The spectrum anisotropy is determined by the anisotropy of the phase velocity  $S^\lambda(\theta, \varphi)$ , which depends on the angles  $\theta$  and  $\varphi$  of the vector  $\mathbf{q}$ . In the coordinates measured along the cube edges, the polarization vector components  $e_j$  and the phonon spectrum of a cubic crystal can be determined from a set of equations [1] which, in the Simons designations [30], can be written in the form

$$\sum_j e_j \{ (n_i n_j - \varepsilon \delta_{ij}) + (k - 1) n_i n_j (1 - \delta_{ij}) \} = 0. \quad (\text{A.2})$$

Here,  $n_j = q_j/q$  are the projections of the phonon unit vector  $\mathbf{n} = (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi), \cos(\theta))$  onto the coordinate axes,  $k = \frac{c_{12} + c_{44}}{c_{11} - c_{44}}$ ,  $\varepsilon = \frac{S(\theta, \varphi)^2 \rho - c_{44}}{c_{11} - c_{44}}$ ,  $c_{ij}$  are the second-order elastic moduli. The parameter  $k - 1$  characterizes the elastic anisotropy of cubic crystals. From the condition of existence of a nonzero solution to the set of equations (A.2),

$$\varepsilon^3 - \varepsilon^2 - (k^2 - 1)\varepsilon\xi - (k - 1)^2(2k + 1)\eta = 0 \quad (\text{A.3})$$

(where  $\xi = n_1^2 n_2^2 + n_1^2 n_3^2 + n_2^2 n_3^2$ , and  $\eta = n_1^2 n_2^2 n_3^2$  are cubic harmonics), we can find the phase velocity for the acoustic branches of the phonon spectrum:

$$S_\lambda(\theta, \varphi) = \sqrt{\frac{c_{44}}{\rho}} \left( 1 + \frac{c_{11} - c_{44}}{c_{44}} \varepsilon_\lambda \right)^{1/2}, \quad \varepsilon_\lambda = \frac{1}{3} + z_\lambda. \quad (\text{A.4})$$

For longitudinal ( $L$ ) and transverse ( $t_1, t_2$ ) phonons, the quantities  $z$

$$z_L = 2r \cos \frac{Q}{3}, \quad z_{t_1, t_2} = 2r \cos \left( \frac{Q}{3} \mp \frac{2\pi}{3} \right), \quad (\text{A.5})$$

$$r = \frac{1}{3} \sqrt{1 + 3(k^2 - 1)\xi}, \quad \cos Q = \left\{ \frac{1 + 4.5(k^2 - 1)\xi + 13.5\eta(1 - 3k^2 + 2k^3)}{\sqrt{(1 + 3(k^2 - 1)\xi)^3}} \right\}.$$

The solutions  $\varepsilon_{t1}$  and  $\varepsilon_{t2}$  to the cubic equation (A.3) given by equations (A.4) and (A.5) correspond to fast and slow transverse vibrational modes (upper and lower branches, respectively). Substituting equations (A.4) and (A.5) into the set of equations (A.2), we can determine the phonon polarization vectors of various vibrational branches to be

$$e_j^\lambda = \frac{1}{A_\lambda} \left\{ \begin{array}{c} n_j \\ \psi_j^\lambda \end{array} \right\} \quad A_\lambda = \pm \sqrt{\sum_j \frac{n_j^2}{(\psi_j^\lambda)^2}}, \quad (\mathbf{e}^\lambda \mathbf{n}) = \frac{1}{A_\lambda} \sum_j \frac{n_j^2}{\psi_j^\lambda}, \quad (\text{A.6})$$

$$\psi_j^\lambda = \varepsilon_\lambda + (k - 1)n_j^2.$$

It is easy to verify that the polarization vectors satisfy the relations

$$(e^\lambda, e^{\lambda'}) = \delta_{\lambda, \lambda'}.$$

It follows from equations (A.2)–(A.6) that the dimensionless parameter  $k - 1 = \Delta C / (c_{11} - c_{44})$  (where  $\Delta C = c_{12} + 2c_{44} - c_{11}$ ) determines the influence of elastic anisotropy of cubic crystals on the spectrum and polarization vector of the phonon in cubic crystals [20]. These results have been used to compute ultrasonic absorption in cubic crystals.

## Appendix B

The expression for the elastic energy of cubic crystals up to the third order terms with respect to the deformation tensor components is obtained in [31]. We transform it analogously to [2]. Then the matrix element  $V_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3}^{\lambda_1 \lambda_2 \lambda_3}$ , determining the probabilities of various three-phonon scattering processes in terms of the elastic moduli of the second and third order, can be written [12]

$$V_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3}^{\lambda_1 \lambda_2 \lambda_3} = \tilde{c}_{111} \sum_i e_{1i} q_{1i} e_{2i} q_{2i} e_{3i} q_{3i} + c_{123} (\mathbf{e}_1 \mathbf{q}_1) (\mathbf{e}_2 \mathbf{q}_2) (\mathbf{e}_3 \mathbf{q}_3) + \tilde{c}_{112} \sum_i [(e_1 \mathbf{q}_1) e_{2i} q_{2i} e_{3i} q_{3i} + (\mathbf{e}_2 \mathbf{q}_2) e_{1i} q_{1i} e_{3i} q_{3i} + (\mathbf{e}_3 \mathbf{q}_3) e_{1i} q_{1i} e_{2i} q_{2i}] + c_{144} [(\mathbf{e}_1 \mathbf{q}_1) (\mathbf{e}_2 \mathbf{q}_3) (\mathbf{e}_3 \mathbf{q}_2) + (\mathbf{e}_2 \mathbf{q}_2) (\mathbf{e}_1 \mathbf{q}_3) (\mathbf{e}_3 \mathbf{q}_1) + (\mathbf{e}_3 \mathbf{q}_3) (\mathbf{e}_1 \mathbf{q}_2) (\mathbf{e}_2 \mathbf{q}_1)] + (c_{12} + c_{144}) [(\mathbf{e}_1 \mathbf{q}_1) (\mathbf{e}_2 \mathbf{e}_3) (\mathbf{q}_3 \mathbf{q}_2) + (\mathbf{e}_2 \mathbf{q}_2) (\mathbf{e}_1 \mathbf{e}_3) (\mathbf{q}_3 \mathbf{q}_1) + (\mathbf{e}_3 \mathbf{q}_3) (\mathbf{e}_1 \mathbf{e}_2) (\mathbf{q}_1 \mathbf{q}_2)] + c_{456} [(\mathbf{e}_1 \mathbf{q}_3) (\mathbf{e}_2 \mathbf{q}_1) (\mathbf{e}_3 \mathbf{q}_2) + (\mathbf{e}_1 \mathbf{q}_2) (\mathbf{e}_2 \mathbf{q}_3) (\mathbf{e}_3 \mathbf{q}_1)] + (c_{44} + c_{456}) [(\mathbf{e}_1 \mathbf{q}_2) (\mathbf{q}_1 \mathbf{q}_3) (\mathbf{e}_2 \mathbf{e}_3) + (\mathbf{e}_2 \mathbf{q}_3) (\mathbf{q}_1 \mathbf{q}_2) (\mathbf{e}_1 \mathbf{e}_3) + (\mathbf{e}_3 \mathbf{q}_1) (\mathbf{q}_2 \mathbf{q}_3) (\mathbf{e}_1 \mathbf{e}_2) + (\mathbf{e}_1 \mathbf{q}_3) (\mathbf{q}_1 \mathbf{q}_2) (\mathbf{e}_2 \mathbf{e}_3) + (\mathbf{e}_2 \mathbf{q}_1) (\mathbf{q}_2 \mathbf{q}_3) (\mathbf{e}_1 \mathbf{e}_3) + (\mathbf{e}_3 \mathbf{q}_2) (\mathbf{q}_1 \mathbf{q}_3) (\mathbf{e}_1 \mathbf{e}_2)] + \tilde{c}_{155} \sum_i \{ e_{1i} e_{2i} e_{3i} (q_{1i} (\mathbf{q}_2 \mathbf{q}_3) + q_{2i} (\mathbf{q}_1 \mathbf{q}_3) + q_{3i} (\mathbf{q}_1 \mathbf{q}_2)) \}$$

$$\begin{aligned}
& + e_{1i}q_{1i}[e_{2i}q_{3i}(\mathbf{e}_3\mathbf{q}_2) + e_{3i}q_{2i}(\mathbf{e}_2\mathbf{q}_3)] \\
& + e_{2i}q_{2i}[e_{1i}q_{3i}(\mathbf{e}_3\mathbf{q}_1) + e_{3i}q_{1i}(\mathbf{e}_1\mathbf{q}_3)] + e_{3i}q_{3i}[e_{1i}q_{2i}(\mathbf{e}_2\mathbf{q}_1) + e_{2i}q_{1i}(\mathbf{e}_1\mathbf{q}_2)] \\
& + [\tilde{c}_{155} - \Delta C] \sum_i q_{1i}q_{2i}q_{3i}[e_{1i}(\mathbf{e}_2\mathbf{e}_3) + e_{2i}(\mathbf{e}_1\mathbf{e}_3) + e_{3i}(\mathbf{e}_1\mathbf{e}_2)] \quad (\text{B.1})
\end{aligned}$$

where  $c_{ijk}$  are the thermodynamic moduli of the third order in the normalization introduced by Brugger [32]. The contributions containing the elasticity moduli  $\tilde{c}_{111}$ ,  $\tilde{c}_{112}$ ,  $\tilde{c}_{155}$  and  $\Delta C$  are typical of cubic crystals and distinguish them from the isotropic medium. Equality to zero of these moduli provides a transition to the isotropic medium model. In this case one can obtain the expression for the energy density for the isotropic medium caused by anharmonic lattice vibration (see formula (4.22) of [2]).

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