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Elastic properties and anharmonicity of solids

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The squares of the velocities of the longitudinal and transverse acoustic waves separately are practically not associated with anharmonicity, and their ratio (v_L^2/v_S^2) turns out to be a linear function of the Grüneisen parameter γ — the measure of anharmonicity. The obtained dependence of (v_L^2/v_S^2) on γ is in satisfactory agreement with the experimental data. The relationship between the quantity (v_L^2/v_S^2) and anharmonicity is explained through its dependence on the ratio of the tangential and normal stiffness of the interatomic bond λ, which is a single-valued function of the Grüneisen parameter $\lambda(\gamma)$. The relationship between Poisson's ratio μ and Grüneisen parameter γ, established by Belomestnykh and Tesleva, can be substantiated within the framework of Pineda's theory. Attention is drawn to the nature of the Leont'ev formula, derived directly from the definition of the Grüneisen parameter by averaging the frequency of normal lattice vibration modes. The connection between Grüneisen, Leontiev and Belomestnykh–Tesleva relations is considered. The possibility of a correlation between the harmonic and anharmonic characteristics of solids is discussed.

Keywords: elastic properties, Grüneisen parameter, formulas of Belomestnykh–Tesleva, Leont'ev, Grüneisen equation, tangential and normal stiffness of interatomic bond, crystals, glasses.

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1. Introduction

It is known that an atom in solids shifted slightly from its equilibrium position by x undergoes harmonic oscillations with parabolic potential $U(x)$, which corresponds to a linear dependence of interatomic interaction force $f(x)$ on displacement x. Anharmonicity manifests itself at significantly large values of x: force $f(x)$ deviates from a linear dependence, and an atom undergoes anharmonic oscillations with a cubic potential. Anharmonically oscillating atoms and groups of atoms produce a considerable contribution to the thermal expansion, thermal conductivity, and other physical properties of solids [1–6]. The nonlinearity of the interatomic and intermolecular interaction force plays a significant part at almost all stages of deformation and fracture of amorphous polymers and other materials. The emergence of fracture nuclei in solids is associated primarily with anharmonicity [3,4].

The Grüneisen parameter is the measure of anharmonicity. This parameter is defined by the variation of frequency of normal modes of lattice oscillations ν_i with volume of a body

$$\gamma_i = -\frac{V}{\nu}\left(\frac{d\nu_i}{dV}\right) = -\frac{d\ln\nu_i}{d\ln V}. \qquad (1)$$

The following approximation with all normal modes of oscillations having the same dependences of frequency on volume is used in most cases: $\gamma = -d\ln\nu/d\ln V$.

The Grüneisen equation (law, formula) is the primary relation for the experimental determination of γ [1]:

$$\gamma = \frac{\beta V B}{C_V}, \qquad (2)$$

where β is the coefficient of volume thermal expansion, V is the molar volume, B is the isothermal bulk compression modulus, and C_V is the molar heat capacity at constant volume. This relation is derived from the equation of state of a solid that contains Grüneisen parameter γ as a measure of nonlinearity of the interatomic interaction force and anharmonicity of lattice oscillations.

It is generally assumed that the parameters of elasticity theory (elastic moduli and Poisson's ratio), being harmonic linear quantities, should not normally be related to anharmonicity. Specifically, the harmonic and anharmonic coefficients of the Taylor expansion of the potential lattice energy are usually regarded as independent parameters. However, studies hinting at a certain relation between the harmonic and anharmonic properties of solids are still published from time to time [7–15].

The interest in the relation between elastic properties and the Grüneisen parameter has been on the rise lately [7–13]. For example, Belomestnykh and Tesleva [7] have found relatively recently that Poisson's ratio μ is a single-valued function of Grüneisen parameter γ

$$\gamma = \frac{3}{2}\left(\frac{1+\mu}{2-3\mu}\right), \tag{3}$$

and it is worth mentioning that their approach is fairly rigorous and relies on well-known postulates of the elasticity theory, thermodynamics, and physical acoustics. Notably, Belomestnykh–Tesleva formula (3) is in satisfactory agreement with Grüneisen equation (2) [7–10] (see, e.g., Fig. 1). The best fit is observed for quasi-isotropic alkali-haloid crystals with central particle interaction forces. Slight deviations for certain bodies [7–9] are probably attributable to the spread of γ values determined by different research groups. For example, Grüneisen parameter (2) for aluminum was estimated at 2.11, 2.43, and 2.34 in three different studies [8]. It is not improbable that the anisotropy of certain crystals plays a role here.

Bodryakov et al. [11] have proposed a thermodynamic generalization of the Grüneisen parameter concept. The generalized version of this quantity is also related to elastic properties (specifically, the Poisson's ratio).

Relying on the elasticity theory, molecular physics, thermodynamics, and physical acoustics, Leont'ev [12] has averaged the frequency of normal modes of lattice oscillations ν_i and derived the following formula for γ directly from the definition of Grüneisen parameter (1):

$$\gamma = \frac{3}{2}\left(\frac{B_A}{\rho v_k^2}\right), \tag{4}$$

where ρ is the density, B_A is the adiabatic bulk compression modulus, and v_k^2 is the mean-square sound velocity squared

$$v_k^2 = \frac{v_L^2 + 2v_S^2}{3}, \tag{5}$$

where v_L and v_S are the velocities of longitudinal and transverse acoustic waves, respectively. Leont'ev formula (4) is in satisfactory agreement with Grüneisen equation (2) [10].

The relations of Belomestnykh–Tesleva (3) and Leont'ev (4) have an advantage over Grüneisen equation (2) in that they allow one to calculate γ based on more readily available experimental data. At the same time, it is noteworthy that anharmonicity measure γ is at the left-hand sides of these equalities, while the right-hand parts appear to contain only harmonic (linear) characteristics of solids (ρ, B_A, v_k^2, μ). Thus, an apparent contradiction arises.

The present study is focused on the relation between elastic properties and the Grüneisen parameter as an example of interconnection between harmonic and anharmonic characteristics of solids. We develop further the idea that the right-hand parts of Belomestnykh–Tesleva and Leont'ev formulae depend on anharmonicity via the dependence of the ratio of squares of sound velocities (v_L^2/v_S^2) on the Grüneisen parameter. In addition to novel insights, little-known but poignant studies focused on the matter in question are discussed briefly.

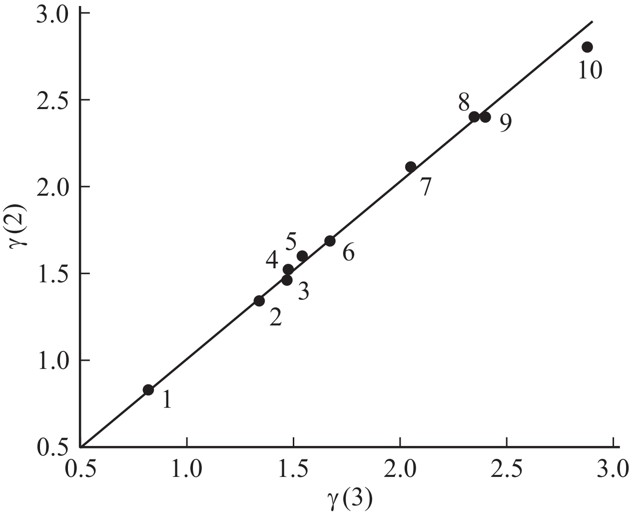

Figure 1. Linear correlation between the values of γ determined using Grüneisen equation (2) and Belomestnykh–Tesleva formula (3) for different crystals (the data from [7-9] were used). *1* — Be, *2* — LiF, *3* — NaCl, *4* — LiCl, *5* — KCl, *6* — KBr, *7* — Al, *8* — Ag, *9* — Pb, *10* — Au.

2. Linear dependence of (v_L^2/v_S^2) on the Grüneisen parameter

If one examines formulae (3) and (4), it becomes apparent that their right-hand sides are functions of the ratio of squares of propagation velocities of longitudinal and transverse acoustic waves (v_L^2/v_S^2). For example, quantity v_κ^2 in Leont'ev equation (4) makes its right-hand side a function of the mentioned ratio $(v_L/v_S)^2$ (see relation (5))

$$v_\kappa^2 = \frac{v_S^2}{3}\left[\left(\frac{v_L}{v_S}\right)^2 + 2\right].$$

According to the well-known formula from the elasticity theory [16], Poisson's ratio μ at the right-hand side of Belomestnykh–Tesleva equation (3) is also a function of the ratio of squares of sound velocities (v_L^2/v_S^2)

$$\mu = \frac{2-(v_L/v_S)^2}{2-2(v_L/v_S)^2}. \tag{6}$$

This feature of the discussed formulae suggests that their right-hand sides may depend on anharmonicity via the ratio of squares of velocities of longitudinal and transverse acoustic waves (v_L^2/v_S^2). Our examination of a number of metal and ionic and molecular crystals (Table 1) did indeed demonstrate [10] that while Grüneisen parameter γ and the squares of velocities v_L^2 and v_S^2 are not individually related in any specific way (Fig. 2), their ratio (v_L^2/v_S^2) is a linear function of Grüneisen parameter γ, which is a measure of anharmonicity (Fig. 3). Vitreous solids [17] also feature a similar linear correlation between the ratio of squares of velocities of acoustic waves and the Grüneisen parameter (Fig. 4, Table 2).

Table 1. Sound velocities, Poisson's ratio, and Grüneisen parameter of inorganic substances at standard conditions ($p = 10^5$ Pa and $T = 298$ K)

№	Elements and compounds	Sound velocity, m/s		Ratio of velocities squared, $(v_L/v_S)^2$	Poisson's ratio, μ	Grüneisen parameter, γ	A	$\overline{D}_I$
		v_L	v_S				(14)	(16)
1	LiF	7323	4518	2.627	0.200	1.34	0.63	1.5
2	NaCl	4666	2755	2.869	0.243	1.46	0.59	1.7
3	LiCl	5260	3058	2.959	0.245	1.52	0.61	1.6
4	NaBr	3284	1885	3.35	0.270	1.56	0.55	1.7
5	KCl	4090	2312	3.130	0.259	1.60	0.58	1.7
6	KI	2623	1469	3.188	0.265	1.63	0.58	1.7
7	W	5233	2860	3.348	0.283	1.62	0.56	1.8
8	Fe	6064	3325	3.326	0.292	1.68	0.56	1.8
9	KF	4641	2587	3.218	0.274	1.73	0.57	1.7
10	RbI	2245	1198	3.512	0.309	1.73	0.53	1.9
11	Co	5827	3049	3.652	0.357	1.87	0.53	1.9
12	Cu	4726	2298	4.229	0.350	2.00	0.48	2.1
13	Ag	3686	1677	4.831	0.379	2.40	0.45	2.2
14	Pt	3960	1670	5.623	0.390	2.54	0.40	2.5
15	Pb	2158	860	6.30	0.372	2.93	0.43	2.3

Table 2. Density ρ, propagation velocities of longitudinal (v_L) and transverse (v_S) acoustic waves, bulk compression modulus B_A, Poisson's ratio μ, and Grüneisen parameter γ for $Na_2O-Al_2O_3-SiO_2$ glasses (data from [17] were used)

№	Synthesis composition, mol.%			ρ, kg/m^3	v_L, m/s	v_S, m/s	$B_A \cdot 10^{-8}$, Pa	μ	γ	A	$\overline{D}$
	Na_2O	Al_2O_3	SiO_2							(14)	(16)
1	15	0	85	2339	5430	3340	342	0.196	1.28	0.65	1.5
2	15	5	80	2358	5570	3390	370	0.206	1.31	0.64	1.6
3	15	10	75	2410	5697	3510	386	0.194	1.26	0.65	1.5
4	15	15	70	2465	5737	3469	416	0.212	1.34	0.63	1.6
5	15	20	65	2428	5850	3540	425	0.211	1.34	0.63	1.6
6	15	25	60	2472	6000	3568	470	0.226	1.40	0.62	1.6
7	25	0	75	2439	5280	3140	359	0.226	1.40	0.62	1.6
8	25	5	70	2455	5480	3240	394	0.231	1.41	0.62	1.6
9	25	10	65	2461	5610	3330	411	0.228	1.40	0.62	1.6
10	25	20	55	2470	5680	3450	405	0.208	1.32	0.64	1.6
11	25	25	50	2499	5790	3490	432	0.215	1.35	0.63	1.6
12	25	30	45	2519	6026	3556	490	0.233	1.43	0.62	1.6
13	35	0	65	2497	5340	3070	398	0.253	1.52	0.60	1.7
14	30	5	65	2486	5500	3200	413	0.244	1.47	0.61	1.6
15	20	15	65	2450	5670	3490	390	0.195	1.28	0.65	1.5
16	17.5	17.5	65	2447	5746	3458	418	0.216	1.35	0.63	1.6

3. Theoretical version of the dependence of (v_L^2/v_S^2) on γ

Figures 3 and 4 demonstrate linear correlations between the values of (v_L^2/v_S^2) and γ obtained empirically based on experimental data. It is of some interest to establish the relation between these quantities using the already known relevant theoretical equations.

A formula for the dependence of ratio (v_L^2/v_S^2) on Grüneisen parameter γ may be derived from Belomestnykh–Tesleva equation (3) and formula (6) of the elasticity theory. We use this formula to determine (v_L^2/v_S^2) and rewrite it in the following form [16]:

$$\left(\frac{v_L}{v_S}\right)^2 = \frac{2-2\mu}{1-2\mu}. \tag{7}$$

Using Belomestnykh–Tesleva equation (3) to obtain an expression for Poisson's ratio μ as a function of γ and inserting this expression in formula (7) of the elasticity theory, we

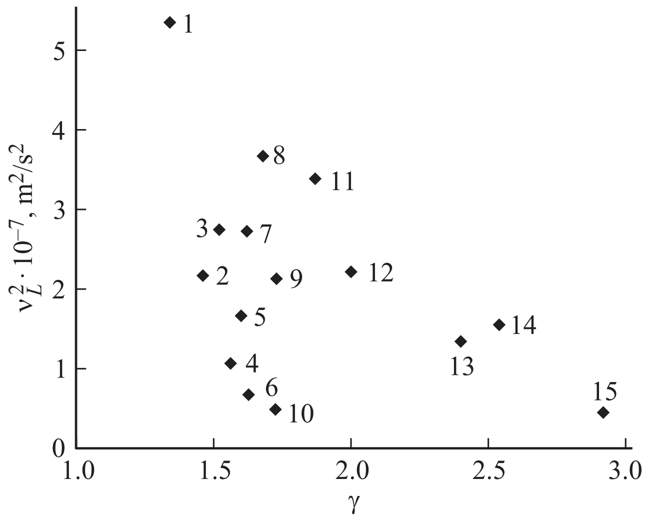

Figure 2. Square of velocity of a longitudinal acoustic wave v_L^2 vs Grüneisen parameter γ. Numbers at points correspond to the numbers of crystals in Table 1.

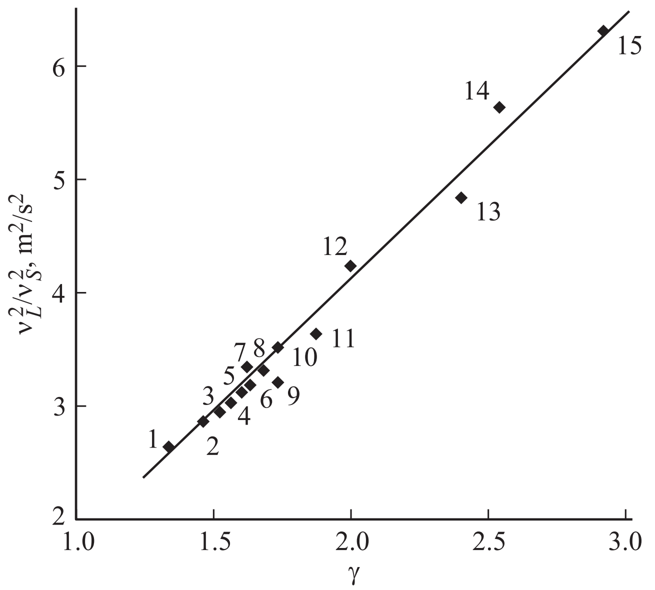

Figure 3. Linear correlation between the ratio of squares of longitudinal and transverse sound velocities (v_L^2/v_S^2) and Grüneisen parameter γ for the crystals from Fig. 2. Numbers at points correspond to the numbers of substances in Table 1.

arrive at the following dependence of ratio (v_L^2/v_S^2) on γ:

$$\left(\frac{v_L}{v_S}\right)^2 = 4\left(\frac{3+\gamma}{9-2\gamma}\right). \tag{8}$$

The same result may be derived from the Belomestnykh formula for the acoustic Grüneisen parameter [8].

Theoretical dependence (8) agrees with the experimental data for glasses: the straight line plotted in coordinates of Eq. (8) goes through the origin and has a slope equal to unity (Fig. 5). The studied crystals (Table 1) largely follow dependence (8), but they are divided into two groups with respect to this dependence. One of these groups is characterized by an equation of line that does not go through the origin of coordinates (Figs. 6, *a*, *b*),

$$\left(\frac{v_L}{v_S}\right)^2 = a_1\left(\frac{3+\gamma}{9-2\gamma}\right) + b_1,$$

where a_1 and b_1 are constants.

This naturally poses the question how relation (8) may be coordinated with the empirical linear correlation between (v_L^2/v_S^2) and γ (Figs. 3 and 4). It turns out that a linear dependence of (v_L^2/v_S^2) on γ may be derived from

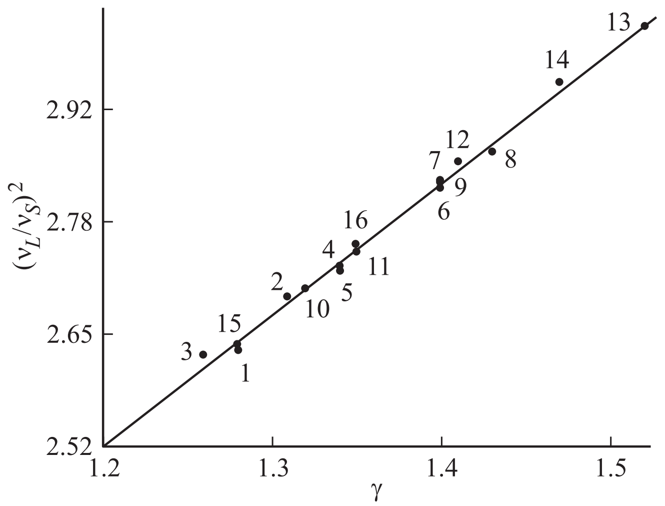

Figure 4. Linear correlation between the ratio of squares of longitudinal and transverse sound velocities (v_L^2/v_S^2) and Grüneisen parameter γ. Sodium aluminosilicate glasses with different concentrations of oxides. Numbers at points correspond to the numbers of glasses in Table 2.

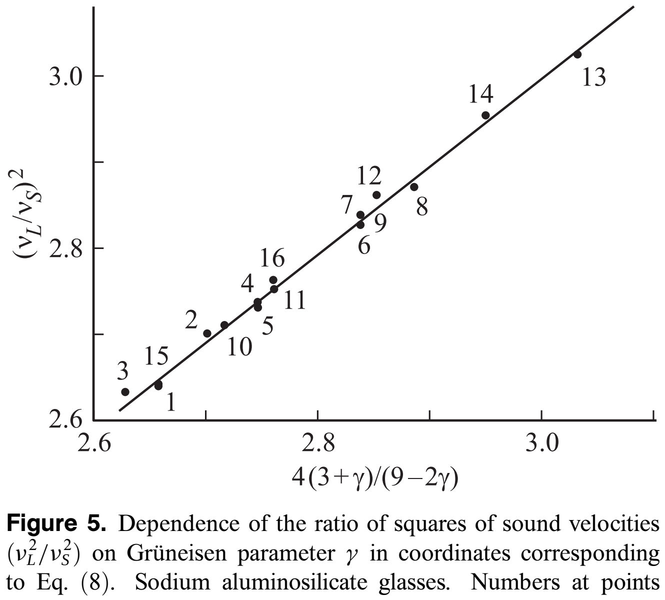

Figure 5. Dependence of the ratio of squares of sound velocities (v_L^2/v_S^2) on Grüneisen parameter γ in coordinates corresponding to Eq. (8). Sodium aluminosilicate glasses. Numbers at points correspond to the numbers of glasses in Table 2.

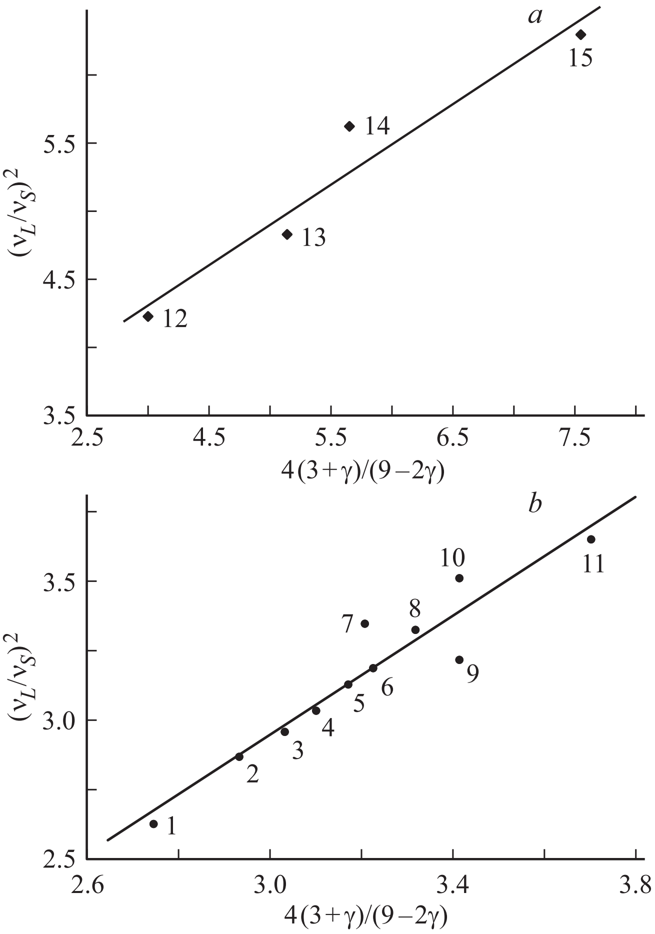

Figure 6. Dependence of (v_L^2/v_S^2) on Grüneisen parameter γ in coordinates corresponding to Eq. (8). Crystalline solids. Numbers at points correspond to the numbers of crystals in Table 1.

formula (8) under condition that $2\gamma \ll 9$

$$\left(\frac{v_L}{v_S}\right)^2 \approx 1.3 + 0.4\gamma. \tag{9}$$

While this condition is suitable for the studied glasses with $\gamma \approx 1.2{-}1.5$ (Table 2), it is hardly satisfactory for some of the studied crystals (Table 1). This issue warrants further study with the application of approaches developed in [5–15,18].

Note that condition $(9 - 2\gamma) > 0$ is satisfied according to formula (8). Therefore, $\gamma < 4.5$, which agrees with the maximum Grüneisen parameter in polymorphic transformations in crystals. For example, when the cubic phase of a rubidium cyanide crystal RbCN is cooled within the interval from $T = 380\,\mathrm{K}$ to values in the vicinity of polymorphic transformation temperature $T_c = 110\,\mathrm{K}$, the Grüneisen parameter increases from $\gamma \approx 2$ to limit value $\gamma_c = 4.5$ [19].

4. On the interrelation between the Grüneisen, Leont'ev, and Belomestnykh–Tesleva equations

The study of Leont'ev [12] was aimed primarily at establishing the relation between elastic and thermal properties of matter. His formula (4) for the Grüneisen parameter was intended to be used in solving this problem.

Relying on the fundamental principles of thermodynamics, elasticity theory, molecular physics, and physical acoustics, Leont'ev managed to establish the relation between thermal characteristics β and C_V and the velocities of propagation of longitudinal and transverse elastic waves (see definition (5) of v_k^2):

$$\frac{C_V}{\beta V} = \frac{2}{3}\rho v_k^2. \tag{10}$$

This relation agrees with the experimental data [10,12]. We took note of the fact that Leont'ev formula (4) may be derived from Grüneisen equation (2) with the use of equality (10):

$$\gamma = \frac{\beta V B}{C_V} = \left(\frac{\beta V}{C_V}\right) B = \frac{3}{2}\left(\frac{B}{\rho v_k^2}\right) \cong \frac{3}{2}\left(\frac{B_A}{\rho v_k^2}\right).$$

The known $B \approx B_A$ approximation was used here. Note that Leont'ev [12] derived his formula (4) for γ in a more rigorous fashion without the use of Grüneisen relation (2).

Let us demonstrate how Belomestnykh–Tesleva formula (3) may be derived from Grüneisen equation (2). Multiplying the numerator and the denominator of Eq. (2) by shear modulus G and taking into account the known relation between elastic moduli [16],:

$$\frac{B}{G} = \frac{2}{3}\left(\frac{1+\mu}{1-2\mu}\right),$$

we obtain the following modification of Grüneisen equation (2):

$$\gamma = A\left(\frac{1+\mu}{1-2\mu}\right), \tag{11}$$

where

$$A = \frac{2}{3}\left(\frac{BVG}{C_V}\right). \tag{12}$$

Using Leont'ev relation (10) and expression $G = \rho v_S^2$ for the shear modulus, we present factor A (12) as a ratio of squares of sound velocities

$$A = \frac{v_S^2}{v_k^2}. \tag{13}$$

We then use expression (5) for v_k^2 and formula (7) to derive the relation between A and Poisson's ratio *mu* from equality (13)

$$A = \frac{3}{2}\left(\frac{1-2\mu}{2-3\mu}\right). \tag{14}$$

Notably, modified Grüneisen equation (11) may be transformed into Belomestnykh–Tesleva formula (3) with the use of relation (14)

$$\gamma = \left[\frac{3}{2}\left(\frac{1-2\mu}{2-3\mu}\right)\right]\left(\frac{1+\mu}{1-2\mu}\right) = \frac{3}{2}\left(\frac{1+\mu}{2-3\mu}\right).$$

Thus, Belomestnykh–Tesleva formula (3), which was derived by its authors from different basic assumptions [7], may be obtained from Grüneisen equation (2) by appealing to the elasticity theory.

Let us focus on the physical meaning of factor A in Eq. (11).

We note first that coefficient A in expression (13) characterizes the proportion of mean interatomic interaction energy $\overline{U} = \rho v_k^2 V$ accounted for by elastic energy $\Delta U = \rho v_S^2 V$, needed for shear deformation

$$A = \frac{v_S^2}{v_k^2} = \frac{\rho v_S^2 V}{\rho v_k^2 V} = \frac{GV}{\overline{U}} = \frac{\Delta U}{\overline{U}}.$$

The behavior of a body being deformed is governed by the processes of formation and evolution of dissipative structures that scatter the supplied energy [20,21]. These structures are characterized by a universal hierarchy of spatial scales (structure levels) that is established due to the fundamental property of a solid: its shear resistance that specifies the difference between the characteristic spatial scales of regions of localization and scattering of energy supplied to a body being deformed under an external influence.

The ratio between the spatial scales of dissipative structures on neighboring levels (i.e., dimension D_f of the regions of energy localization) is defined by relation (7) [20,21]:

$$D_f = \frac{L_{i+1}}{L_i} = \frac{L_l}{L_S} = \frac{v_L^2}{v_S^2} = \frac{2(1-\mu)}{(1-2\mu)}, \tag{15}$$

where $L_i \sim \rho \cdot v_L^2$ is the characteristic size of the regions of energy localization and $L_S \sim \rho \cdot v_S^2$ is the characteristic scale of the regions of energy dissipation (shear stresses are solely responsible for the energy dissipation in a body being deformed [22]).

If we substitute quantity $L_l \sim \rho \cdot v_L^2$ in formula (15) with an averaged characteristic size of the regions of energy localization $\overline{L}_l \sim \rho \cdot v_K^2$, where v_K is mean-square sound velocity (5), a certain average dimension is obtained instead of $D_f = v_L^2/v_S^2$ (see (13) and (14)):

$$\overline{D}_f = \frac{v_K^2}{v_S^2} = \frac{2}{3}\left(\frac{2-3\mu}{1-2\mu}\right). \tag{16}$$

It follows from the comparison of Eqs. (13) and (16) that factor A has the meaning of a reciprocal value of the average dimension of the localization regions of energy supplied to a body:

$$A = \frac{v_S^2}{v_K^2} = \frac{1}{\overline{D}_f}. \tag{17}$$

If we assume that the value of μ of different solids varies approximately within the $0.165 \leq \mu \leq 0.475$ range [20], the range of variation of $\overline{D}_f$ is $1.5 \leq \overline{D}_f \leq 7.7$, which is quite acceptable. The range of D_f variation is wider: $2.5 \leq \overline{D} \leq 21$.

Thus, coefficient A in equality (11) may be regarded as a reciprocal value of the average dimension of the localization regions of energy supplied to bodies being deformed. It is equal to the fraction of energy dissipated in the process of deformation.

It is easy to see that the results of determination of A with the use of formulae (13) and (14) are the same. Since the numerator and the denominator of expression (14) for factor A vary with the Poisson's ratio symbatically, the value of A is almost independent of the nature of a solid and remains almost constant ($A \approx \text{const}$) within a group of solids of the same structural type. For example, sodium aluminosilicate glasses have (Table 2)

$$A \approx \text{const} \approx 0.62{-}0.64,$$

and the average dimension of the regions of localization of stored energy is

$$\overline{D}_f \approx \text{const} \approx 1.6{-}1.7.$$

The studied crystals (Table 1) may be divided tentatively into two groups according to their values of $\overline{D}_f = 1/A$: (1) halide alkali salts with the structure of NaCl, which have $\overline{D}_f \approx 1.7$ ($\mu = 0.200{-}0.270$), and (2) metals with a face-centered cubic structure and $\overline{D}_f \approx 2.1$ ($\mu = 0.309{-}0.390$).

It is noteworthy that average dimensions $\overline{D}_f$ of the regions of localization of stored energy for a number of ionic crystals (Table 1) and inorganic glasses (Table 2) are the same. This agrees with Anderson's notion [23] of similarity of the atomic dynamics in glasses and ionic salts.

As was expected, the dependence of Grüneisen parameter γ on function $(1+\mu)/(1-2\mu)$ of the Poisson's ratio

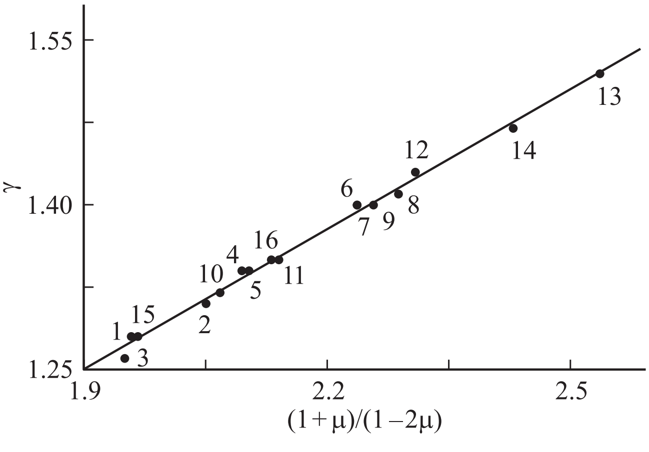

Figure 7. Linear dependence of Grüneisen parameter γ on function $(1+\mu)/(1-2\mu)$ of the Poisson's ratio for sodium aluminosilicate glasses. Numbers at points correspond to the numbers of glasses in Table 2.

is, in accordance with Eq. (11), linear at $A = \text{const}$ (Fig. 7). This fact verifies the approximate constancy of factor A in Eq. (11).

Using formula (5) for the mean-square sound velocity squared $\langle v_k^2 \rangle$ and the above relations from the elasticity theory, one may derive Belomestnykh–Tesleva formula (3) from Leont'ev equation (4) [10].

5. On early approaches to the relation between the Poisson's ratio and the Grüneisen parameter

An interrelation similar to (11) between the Poisson's ratio and the Grüneisen parameter has been established for the first time in 1978 with the use of formulae for internal pressure p_i induced by the interatomic interaction forces [24]. The value of p_i is defined by the derivative of internal energy with respect to volume at $T = \text{const}$ and represents the elastic response of a lattice to bulk compression or strain. Therefore, the internal pressure is closely related to the elastic moduli and the lattice deformation [25].

It follows from an approximation of the Hooke's law and the elastic limit deformation of an interatomic bond that p_i is given by [25]

$$p_1 \cong \left(\frac{1}{6\gamma}\right) E, \tag{18}$$

where E is the elastic modulus under uniaxial deformation. A similar formula is derived based on the Mie potential and the relation between the Poisson's ratio and the parameters of this potential [24,26]:

$$p_1 \cong \frac{1-2\mu}{6(1+\mu)} E. \tag{19}$$

Comparing these two equalities, one arrives at an approximate relation between the Grüneisen parameter and the Poisson's ratio [24,26]:

$$\gamma \approx \frac{1+\mu}{1-2\mu}. \tag{20}$$

For example, ionic cubic crystals have $\mu \sim 0.20{-}0.25$, and the corresponding $\gamma \approx 2$ estimate obtained using this formula agrees in a first approximation with the results of calculation of γ in accordance with the Grüneisen equation.

It is evident that formula (20) is a particular case of (11) at $A \approx 1$. Equation (11) for vitreous solids has been obtained earlier with the following interpretation of factor A [5,6,27]:

$$A \approx \frac{2}{9} \ln\left(\frac{1}{f_g}\right),$$

where $f_g = (V_f/V)_{T=T_g}$ is the fraction of fluctuation free volume frozen at glass transition point T_g. The value of f_g depends only weakly on the glass nature. Within one and the same class of vitreous systems, it is practically a universal constant ($f_g \approx \text{const}$) [26,28,29]. The estimate of A obtained using this formula agrees in the order of magnitude with the results of calculations performed in accordance with relations (13) and (14).

6. Microscopic interpretation of the Grüneisen parameter. Limit deformation of an interatomic bond

Let us consider a linear chain of coupled atoms (oscillators). Let l be the „lattice period" (i.e., the distance between neighboring atoms). At $l = l_0$, an atom is in an equilibrium position. The harmonic and anharmonic coefficients of the series expansion of pairwise potential $U(r)$ are denoted as a_0 and b_0, respectively. Here, r is the interatomic distance in a two-atom (pair) model. Coefficients a_0 and b_0 are defines by the second and the third derivatives of $U(r)$ at equilibrium point $r = r_0$.

One may sum up the potential curves characterizing the interaction of an atom with its left and right neighbors (U_- and U_+) to gain a qualitative understanding of the potential within which the atoms of a linear chain are moving. Although each of these curves has its own minimum (at $r = r_0$) in the vicinity of which

$$U = U_0 + \frac{a_0}{2}(r - r_0)^2 - \frac{b_0}{6}(r - r_0)^3 + \ldots, \tag{21}$$

they add up to potential $\Phi = U_- + U_+$, which is symmetric in displacement from the position equidistant from both neighbors [25,26,30]. Restoring force F applied to this atom is also the sum of forces acting on it from the left and from the right: $F = f_- + f_+$. Both of them are defined by the same derivative of pairwise potential $f(r) = dU/dr$. Using expansion (21), one may find that function $f(r)$ near a lattice site is expressed as [25]

$$\begin{aligned} f(r) &\approx a_0(r - l_0) - \frac{b_0}{2}(r - l_0)^2 \\ &\approx c(l - l_0)^2 + a(r - l) - \frac{b}{2}(r - l)^2, \end{aligned} \tag{22}$$

where $c = a_0 - b_0(l - l_0)/2$, $b = b_0$,

$$a = a_0 - b_0(l - l_0). \tag{23}$$

In the general case, $\Delta l = (l - l_0) \neq 0$, since a lattice may be either compressed or strained. $\Delta l/l_0$ is usually so small that the mismatch of U_- and U_+ minima does not preclude one from obtaining a parabolic shape, which is typical of a harmonic potential, after summation. Therefore, the motion of atoms in a solid is of the same nature as harmonic oscillations about the equilibrium position. As was demonstrated by Debye (see [2,25]), the frequencies of oscillations vary within the range from 0 to maximum frequency ν_m that is written as

$$\nu_m = \frac{1}{\pi}\sqrt{\frac{a}{m}}. \qquad (24)$$

Here, m is the mass of an atom, and a is defined by relation (23).

The Grüneisen parameter is expressed in the Debye theory in terms of characteristic temperature $\theta_D = h\nu_m$ (h is the Planck constant):

$$\gamma = -\frac{d\ln\theta_D}{d\ln V} = -\frac{d\ln(h\nu_m)}{d\ln V}.$$

Let us insert maximum frequency ν_m from relation (24) into this formula:

$$\gamma = -\frac{d\ln\theta_D}{d\ln V} = -\frac{1}{2}\frac{d\ln a}{d\ln V} = -\frac{V}{2a}\frac{da}{dV}. \qquad (25)$$

If the deformation is isotropic, we have $dV/V = 3(dl/l)$. Performing differentiation in (25) with this equality and expression (23) for a taken into account, we arrive at the following formula for the Grüneisen parameter:

$$\gamma = -\frac{l}{6a}\frac{da}{dl} = \frac{lb_0}{6a}.$$

Since equality $l/a = l_0/a_0$ holds true, the final form of the microscopic interpretation of γ is [2,25,31]:

$$\gamma = \frac{l_0 b_0}{6a_0}. \qquad (26)$$

As was expected, Grüneisen parameter γ is proportional to anharmonic coefficient b_0; at $b_0 = 0$, it is also equal to zero ($\gamma = 0$).

These results remain valid after switching to a three-dimensional solid body. Ya.I. Frenkel' [30, p. 171] has proposed a formula for the coefficient of thermal expansion of a three-dimensional solid body that includes the parameters already known to us (a_0, b_0, and l_0):

$$\beta = \frac{b_0 k}{2a_0 l_0^2 B}.$$

Multiplying the right-hand side of this equation by $(3N_A l_0/3N_A l_0)$, we present it in the following form [31]:

$$\beta = \left(\frac{l_0 b_0}{6a_0}\right)\frac{C_V}{BV},$$

where $C_V = 3N_A k = 3R$ is the molar heat capacity, $V = N_A l_0^3$ is the molar volume, N_A is the Avogadro number, k is the Boltzmann constant, R is the gas constant, and B is the isothermal bulk compression modulus.

Comparing this relation to Grüneisen equation (2)

$$\beta = \gamma\frac{C_V}{BV},$$

we find the above microscopic interpretation of Grüneisen parameter (26) [31] $\gamma = l_0 b_0/6a_0$, which turns out to be valid for a three-dimensional solid body.

Let us turn our attention to estimating the limit deformation of an interatomic bond $\Delta l_m = (l_m - l_0)$ in solids. At $l = l_m$, interatomic interaction force $f = -dU/dr$ reaches its maximum at the point of inflection of the potential curve:

$$\left.\frac{df}{dr}\right|_{r=l_m} = 0.$$

Using dependence $f(r)$ in the form of a series expansion (22), one finds easily that the maximum relative elongation of a bond between neighboring atoms is given by equality

$$\frac{\Delta l_m}{l_0} = \frac{a_0}{l_0 b_0},$$

which assumes the following form if we take the microscopic interpretation of Grüneisen parameter (26) into account [25,26,32,33]:

$$\frac{\Delta l_m}{l_0} = \frac{1}{6\gamma}. \qquad (27)$$

The limit deformation of an interatomic bond $(1/6\gamma)$ is included into formula (18) for the internal pressure.

If we take dependence $\gamma(\mu)$ in the form given by Belomestnykh–Tesleva (3) into account, limit deformation (27) becomes a single-valued function of Poisson's ratio μ

$$\frac{\Delta l_m}{l_0} = \frac{2-3\mu}{9(1+\mu)}. \qquad (28)$$

The results of calculations in accordance with this formula for, e.g., inorganic glasses (Table 3) [34,35]

$$\frac{\Delta l_m}{l_0} \cong 0.09{-}0.13$$

agree with the results provided by other methods of estimating this deformation [4,6,25,26].

7. Discussion

(1) Let us consider the obtained results using the model of randomly packed spherical atoms that interact with each other at the contact point via two mutually perpendicular forces: central forces (normal to the contact plane) $f_n = k_n x_n$ and friction forces (tangential) $f_t = k_t x_t$. The Poisson's ratio in this Berlin–Rothenburg–Bathurst (BRB) model [36,37] is defined by ratio $\lambda = (k_t/k_n)$ of tangential k_t and normal k_n stiffness values of an interatomic bond (BRB formula):

$$\mu = \frac{1-\lambda}{4+\lambda}. \qquad (29)$$

It follows from equalities (7) and (29) that the ratio of squares of sound velocities (v_L^2/v_S^2) is also defined by microscopic parameter λ

$$\left(\frac{v_L^2}{v_S^2}\right) = \frac{2(3+\lambda)}{2+3\lambda}. \qquad (30)$$

Table 3. Characteristics of inorganic glasses (the data from [34,35] were used)

Glass	μ	γ	$\Delta l_m/l_0$
Potassium borate glasses			
$K_2O-B_2O_3$			
K_2O, mol. %			
1.1	0.292	0.72	0.10
2.5	0.293	1.73	0.10
3.9	0.293	1.73	0.10
8.5	0.293	1.73	0.10
13.0	0.295	1.74	0.10
18.0	0.301	1.78	0.09
22.8	0.295	1.74	0.10
28.2	0.288	1.70	0.10
33.5	0.303	1.79	0.09
Sulphate-phosphate glasses			
$NaPO_3$	0.294	1.74	0.10
$NaPO_3-Na_2SO_4$			
Na_2SO_4, mol. %			
10	0.299	1.77	0.09
20	0.292	1.72	0.10
30	0.288	1.70	0.10
$NaPO_3-K_2SO_4$			
K_2SO_4, mol. %			
10	0.316	1.88	0.09
20	0.316	1.88	0.09
30	0.313	1.86	0.09
$0.4NaPO_3 \cdot 0.6Na_2SO_4$	0.320	1.90	0.09
Alkali-silicate glasses			
Li_2O-SiO_2			
Li_2O, mol. %			
10	0.187	1.24	0.13
25	0.223	1.38	0.12
33.3	0.232	1.42	0.12
Na_2O-SiO_2			
Na_2O, mol. %			
13	0.205	1.31	0.13
26	0.245	1.48	0.11
33.3	0.255	1.52	0.11
K_2O-SiO_2			
K_2O, mol. %			
13	0.230	1.41	0.12
25	0.270	1.60	0.10
32	0.250	1.50	0.11

According to (3) and (29), parameter λ is, in turn, related to anharmonicity (γ)

$$\gamma = \frac{3}{2(1+\lambda)}. \tag{31}$$

If we follow this line of reasoning, the relation between (v_L^2/v_S^2) and anharmonicity is attributable to the dependence of this ratio on relative tangential stiffness $\lambda = (k_t/k_n)$ of an interatomic bond, which is a single-valued function of Grüneisen parameter γ (31).

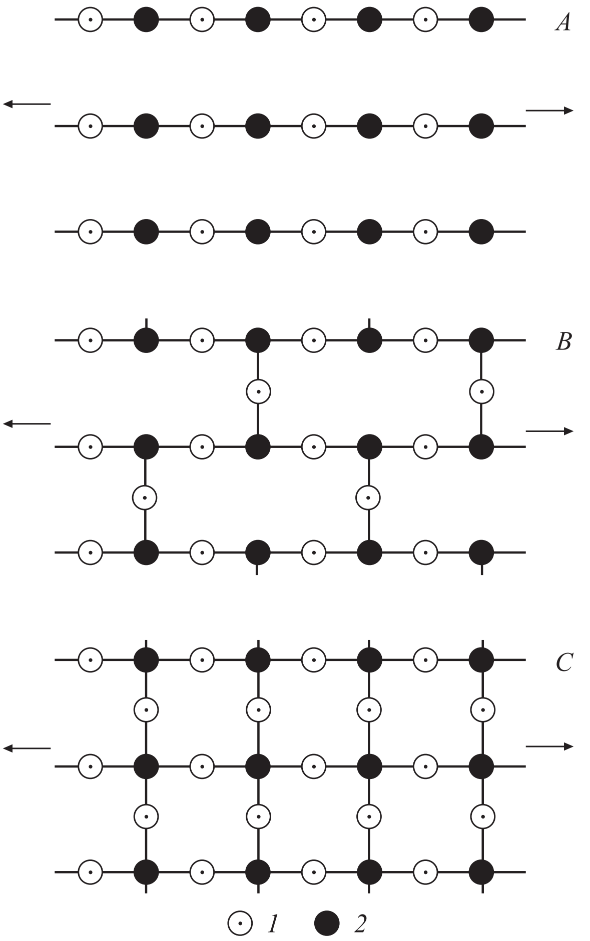

Figure 8. Diagrams of linear (A), linear-branched (B), and network (C) structures of amorphous substances [38]. *1* — anions, *2* — cations. A — $n = 0$, $\mu \approx 0.4$; B — $n = 1$, $\mu \approx 0.3$; C — $n = 2$, $\mu \approx 0.15$. n is the density of transverse bonds. Arrows denote tension stresses.

In the case of amorphous organic polymers and inorganic glasses, the dependence of parameter λ on the density of transverse interatomic bonds, which is defined as number n of valence bonds per a single cation (Fig. 8), is evident [38]. Linear structures (polyvinyl chloride, rubber, selenium) with a connectivity of 2 (two anions bound to a cation along a chain) have $n = 0$ and $\mu \approx 0.4$, linear-branched structures with a connectivity of 3 (B_2O_3, P_2O_5, As_2O_3) have $n = 1$ and $\mu \approx 0.3$, and structural networks with a connectivity of 4 (SiO_2, GeO_2) have $n = 2$ and $\mu \approx 0.15$.

It is evident that the nonlinearity of the interatomic interaction force becomes less pronounced, anharmonicity γ decreases, and, according to (31), relative tangential stiffness λ of an interatomic bond increases as density n of transverse valence bonds grows (Fig. 8). According to BRB formula (29), an increase in λ translates into a reduction in transverse deformation coefficient μ.

Lateral branches of the backbone chain of a macromolecule („lateral pendants“ of the backbone chain) exert a significant influence on the values of μ and γ in amorphous polymers. Polyethylene with a light hydrogen atom being its lateral pendant has the minimum values of μ and γ. When hydrogen is substituted with a larger and heavier fluorine atom in transition from polyethylene to polytetrafluorethylene, μ increases from 0.25 to 0.33, and γ increases accordingly from 3 to 4 [39].

If light atoms are substituted with larger and heavier atoms in the lateral (and end) regions of the chain, the nonlinearity of the intermolecular interaction force and anharmonicity of lattice oscillations become more pronounced, and Grüneisen parameter γ increases. According to relation (31) between λ and γ, this should result in a reduction in relative tangential bond stiffness $\lambda = (k_t/k_n)$ and, consequently, lead to an increase in Poisson's ratio μ (see BRB formula (29)).

Thus, μ and γ naturally depend on the specifics of the atomic and molecular structure of vitreous solids, and this dependence is mediated primarily via microscopic parameter λ.

The following values of the Poisson's ratio and the Grüneisen parameter correspond to central forces ($k_n \gg k_t$, $\lambda \approx 0$):

$$\mu = \frac{1-\lambda}{4+\lambda} = 0.25 \quad \text{and} \quad \gamma = \frac{3}{2(1+\lambda)} = 1.5.$$

The other limit value of λ ($k_n \ll k_t$, $\lambda \approx \infty$) corresponds to

$$\mu = \frac{1-\lambda}{4+\lambda} \cong -1, \quad \gamma = \frac{3}{2(1+\lambda)} \approx 0.$$

By definition, Poisson's ratio μ is the ratio of the relative transverse deformation of a body ($\Delta r/r$) to its relative longitudinal elongation ($\Delta l/l$) under uniaxial strain [16]:

$$\mu = -\frac{\Delta r/r}{\Delta l/l}. \tag{32}$$

When a body (rod) is subjected to uniaxial strain, it normally undergoes transverse compression: $\Delta r < 0$. Therefore, $\mu > 0$. In accordance with the definition of μ (32), negative Poisson's ratio $\mu < 0$ implies that a body extends in the transverse direction ($\Delta r > 0$) under uniaxial strain. Generally speaking, this runs counter to common sense. However, it has to be noted that several papers confirming the existence of isotropic bodies with a negative transverse deformation coefficient μ have been published recently [36,37,40].

(2) Product ρv_k^2, which has the characteristic features of elastic moduli, in Leont'ev formula (4) is called the effective elastic modulus [32,41]: $K = \rho v_k^2$. Relations of the elasticity theory for cubic crystals (see, e.g., [12])

$$B = \frac{C_{11} + 2C_{12}}{3} \quad \text{and} \quad \rho v_k^2 = \frac{C_{11} + 2C_{44}}{3}$$

demonstrate that effective elastic modulus $K = \rho v_k^2$ is equal to the bulk compression modulus ($K = B$) if Cauchy condition $C_{12} = C_{44}$ is satisfied (when central forces act between uniformly deformed regions of a cubic lattice). In any other case, it differs from B. Here, C_{11}, C_{12}, and C_{44} are the second-order elastic constants.

According to Leont'ev formula (4), the Grüneisen parameter is defined by the ratio of the bulk compression modulus and the effective elastic modulus.

$$\gamma = \frac{3}{2}\left(\frac{B}{K}\right). \tag{33}$$

With Cauchy condition $K = B$ satisfied, the Grüneisen parameter is equal to 1.5, and a solid body is in the central force field; if $K \neq B$, deviations from this field (from $\gamma = 1.5$) are observed.

It follows from Leont'ev (4) and Belomestnykh–Tesleva (3) relations that ratio B/K is, just as the ratios of other elastic moduli, a single-valued function of Poisson's ratio μ [16],

$$\frac{B}{K} = \frac{1+\mu}{2-3\mu}. \tag{34}$$

This expression agrees with the experimental data both for crystals and for vitreous solids (Figs. 9 and 10 [42]). It can also be seen that individual elastic moduli are harmonic characteristics of solids, while their ratios (e.g., B/G) are single-valued functions of Grüneisen parameter γ, which is a measure of anharmonicity [see first the dependence of (B/G) on μ and then the dependence of μ on γ] (Figs. 11 and12). In contrast to isotropic glasses (Fig. 11), the studied crystals are divided into two groups with respect to the dependence of (B/G) on γ (Fig. 12).

(3) Pineda [13] has studied theoretically the influence of structural changes on the elastic properties of metallic glasses. His analysis is based on the following three assumptions: (1) the interatomic interaction potential includes harmonic and anharmonic parts,

$$U(r) = a(r-r_0)^2 - b(r-r_0)^3, \tag{35}$$

where a and b are the harmonic and anharmonic coefficients, respectively, and r_0 is the interatomic distance corresponding to the potential minimum; (2) the distribution of distances between nearest-neighbor atoms is Gaussian; (3) the elastic properties are defined by the first coordination sphere (the immediate surroundings of atoms).

The resulting (rather cumbersome) formulae for instantaneous bulk compression B and shear G moduli include dimensionless parameters

$$s = \frac{\delta}{r_1}, \quad \Delta = \frac{\delta_1}{r_0}, \quad \gamma_1 = \frac{br_0}{a},$$

where $\delta = (r_1 - r_0)$, r_1, δ_1 are the average radius and width of the first coordination sphere, respectively. The values of s and δ characterize the deviation of the interatomic distance from its equilibrium value r_0 and the average variance near r_0. Parameter γ_1 characterizes the degree of anharmonicity of the potential and is proportional to Grüneisen parameter $\gamma = br_0/6a$ (26).

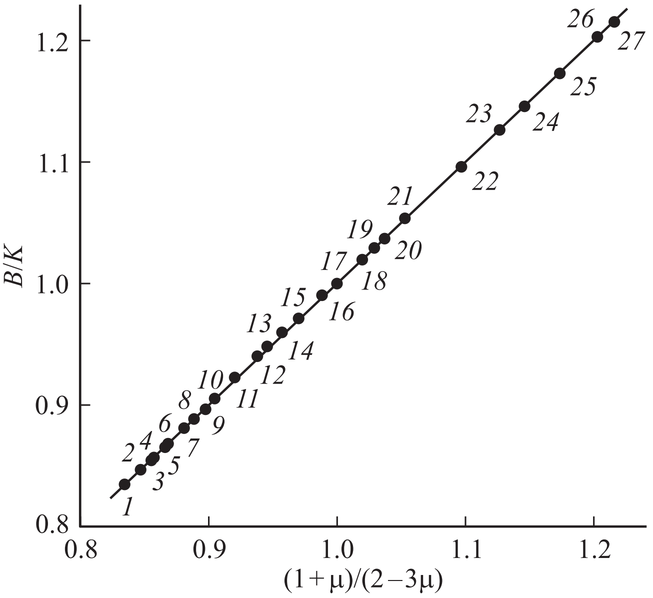

Figure 9. Dependence of the ratio of the bulk compression modulus and the effective elastic modulus (B/K) on function $(1+\mu)/(2-3\mu)$ of the Poisson's ratio for multicomponent optical glasses: *1* — LK7, *2* — KF6, *3* — F6, *4* — KF7, *5* — K14, *6* — LF5, *7* — K8, *8* — KF4, *9* — F13, *10* — K19, *11* — F4, *12* — TF1, *13* — BK6, *14* — BF21, *15* — BF8, *16* — BK10, *17* — TF7, *18* — FK14, *19* — TK13, *20* — TK23, *21* — BF11, *22* — TK17, *23* — OF2, *24* — STK7, *25* — STK9, *26* — LK4, *27* — TBF4. The data were taken from handbook [42].

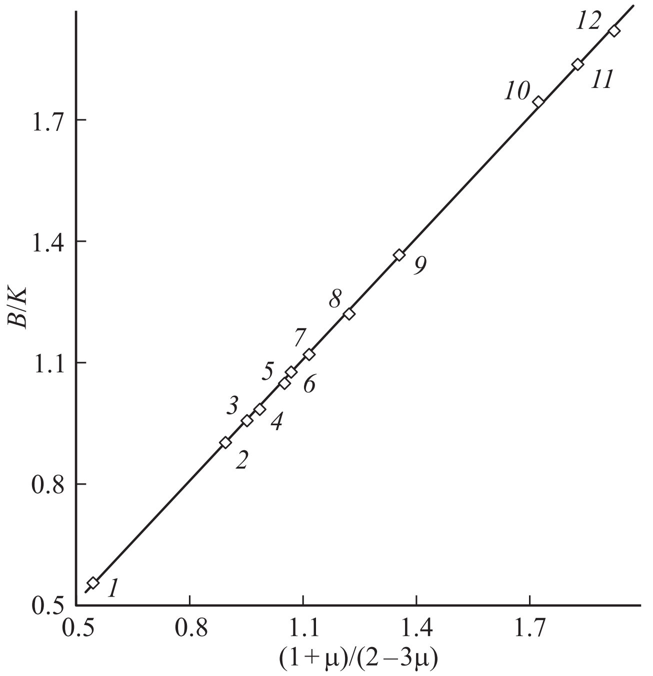

Figure 10. Dependence of (B/K) on function $(1+\mu)/(2-3\mu)$ of the Poisson's ratio for crystals (data from [23] were used). *1* — Be, *2* — LiF, *3* — NaF, *4* — LiCl, *5* — LiI, *6* — NaClO$_3$, *7* — KBr, *8* — RbI, *9* — Ta, *10* — AgBr, *11* — AgCl, *12* — Au.

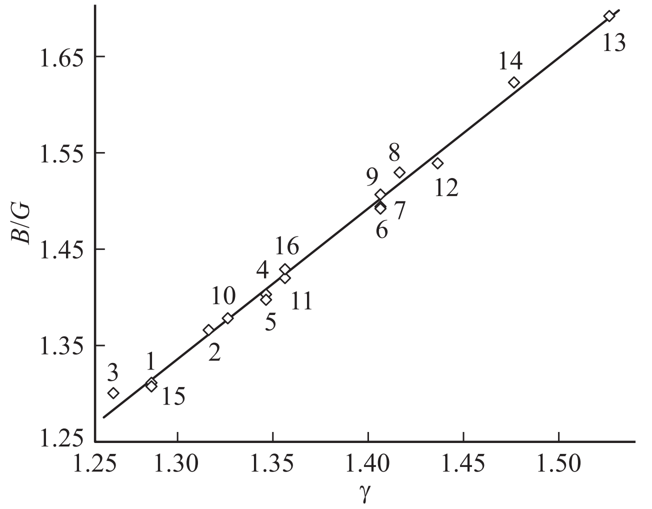

Figure 11. Linear correlation between the ratio of elastic moduli (B/G) and Grüneisen parameter γ. Sodium aluminosilicate glasses $Na_2O{-}Al_2O_3{-}SiO_2$ with different concentrations of oxides. Numbers at points correspond to the numbers of glasses in Table 2. B is the bulk compression modulus and G is the shear modulus.

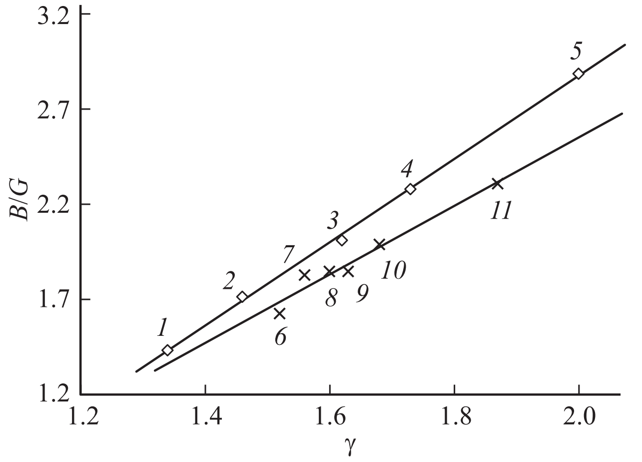

Figure 12. Dependence of the ratio of elastic moduli (B/G) on Grüneisen parameter γ for a number of crystals. B is the bulk compression modulus and G is the shear modulus. *1* — LiF, *2* — NaCl, *3* — W, *4* — RbI, *5* — Cu, *6* — LiCl, *7* — NaBr, *8* — KCl, *9* — KI, *10* — Fe, *11* — Co. The data provided by Belomestnykh and Tesleva [7] were used.

This theory was applied by Pineda to interpret the results of experiments on structural relaxation and triaxial compression of metallic glasses. It provides a generally correct qualitative description of changes in the elastic characteristics occurring in these experiments.

We used the Pineda theory to verify the dependence of ratio (B/G) of elastic moduli and, consequently, Poisson's ratio μ on anharmonicity parameter γ_1. The theory demonstrates that such a dependence exists. Indeed, it follows from the formulae that elastic moduli B and G are proportional to harmonic coefficient a (the interatomic potential parameter), while their ratio (B/G) is almost independent of a and is defined primarily by anharmonicity parameter γ_1. This implies that Poisson's ratio μ depends on Grüneisen parameter γ (measure of anharmonicity). It is known [16] that μ is a single-valued function of ratio (B/G) of elastic moduli.

Thus, the Pineda theory provides a certain justification for Belomestnykh–Tesleva equation (3) that establishes the relation between the Poisson's ratio and the Grüneisen parameter.

(4) The single-valued correspondence between the Poisson's ratio and the Grüneisen parameter is not the only example of this kind; e.g., the empirical Barker rule [43] characterizes the relation between elastic modulus E and the thermal expansion coefficient: $E\beta^2 = \text{const}$.

The approach of Kontorova [14,15] to interpreting the interrelation between linear (harmonic) and nonlinear (anharmonic) quantities is not without interest. As was already noted, harmonic a and anharmonic b coefficients are defined by the second and the third derivatives of function $U(r)$ at $r = r_0$, respectively (see Section 6). Using $U(r)$ in the form of Mie potential ($U = -Ar^{-m} + Br^{-n}$) in these derivatives, Kontorova [14] has found the following relation between coefficients a and b:

$$b = \frac{m+n+3}{2r_0}a. \tag{36}$$

The discussed phenomenon is then attributed to the existence of a relation between a and b of the indicated type and the functional dependence (also obtained by Kontorova) of linear and nonlinear properties of solids on a and b.

Thus, the studies of Kontorova [14,15] and Pineda [13] demonstrate the possibility of existence of certain correlations between harmonic and anharmonic characteristics of solids.

(5) According to the definitions of μ and γ, Poisson's ratio μ and Grüneisen parameter γ characterize, first and foremost, the volume change of a body being deformed. For example, Poisson's ratio function $(1-2\mu)$ and, consequently, transverse deformation coefficient μ itself are related to the volume change of a solid body under uniaxial deformation [44]:

$$\frac{\Delta V}{V} = \varepsilon_x(1-2\mu). \tag{37}$$

where ε_x is the relative uniaxial deformation.

Kuz'menko [18] believes that the Poisson's ratio characterizes the ability of solids to resist changes in their volume. The higher the transverse deformation coefficient, the smaller the change in volume of a solid being deformed. The upper limit of $\mu = 0.5$ corresponds to the condition that the change in volume in the process of deformation is compensated completely by the counteraction of matter $(\Delta V = 0)$. This condition is relevant to liquids. Since solid bodies do not compensate the change in volume completely, they have $\mu < 0.5$.

It is, in fact, evident from (37) that the higher the Poisson's ratio of a given body is, the smaller is its relative volume deformation $(\Delta V/V)$. At $\mu = 0.5$, $\Delta V/V = 0$.

Similar reasoning may be applied to the Grüneisen parameter. It follows from the definition of γ that the higher the Grüneisen parameter is, the smaller is the volume change of a body needed to alter the oscillation frequency (in the process of deformation).

$$\frac{\Delta V}{V} = -\frac{1}{\gamma}\left(\frac{\Delta\nu}{\nu}\right). \tag{38}$$

Viewed in this way, the Grüneisen parameter is similar to the Poisson's ratio in that it characterizes the ability of a solids to resist changes in its volume. It follows from Belomestnykh–Tesleva formula (3) that the maximum value of transverse deformation coefficient $\mu = 0.5$ corresponds to the limit value of Grüneisen parameter $\gamma_{\max} = 4.5$. As was noted in Section 3, the Grüneisen parameter may reach its maximum value of 4.5 in the process of structural transformations (specifically, polymorphic transformations in crystals).

(6) We have discussed the obtained results on a qualitative level by appealing to the currently available theoretical approaches relevant to the matter under investigation. Note that certain questions without a definitive answer arise in discussion of the problems under consideration. First, why does a linear (harmonic) quantity and a parameter of the elasticity theory μ turn out to be a single-valued function of a purely nonlinear (anharmonic) quantity γ? Second, why do certain isotropic solid bodies have negative values of the Poisson's ratio? This implies, counterintuitively, that a body undergoes transverse extension under uniaxial strain. Third, why do formulae derived for anisotropic cubic crystals remain valid for isotropic vitreous solids? An universally recognized microscopic theory of mechanical and thermal properties of crystalline and vitreous solids is needed to answer such questions in full.

8. Conclusion

We developed further the idea that the right-hand parts of Leont'ev (4) and Belomestnykh–Tesleva (3) formulae depend on anharmonicity via the dependence of the ratio of squares of longitudinal and transverse sound velocities on the Grüneisen parameter.

A formula for the dependence of the ratio of squares of sound velocities (v_L^2/v_S^2) on Grüneisen parameter γ was derived. This formula agrees with experimental data (at least for vitreous solids). The Berlin–Rothenburg–Bathurst model provides an explanation for the dependence of (v_L^2/v_S^2) on anharmonicity (γ): it is attributable to the dependence of this ratio on relative tangential stiffness λ of an interatomic bond, which is a single-valued function of Grüneisen parameter $\lambda(\gamma)$.

It was demonstrated that the Leont'ev and Belomestnykh–Tesleva formulae may be derived from the

Grüneisen equation. Coefficient A in modified Grüneisen equation (11) characterizes the proportion of the mean interatomic interaction energy accounted for by the elastic energy needed for shear deformation. The relation between Poisson's ratio μ (parameter of the elasticity theory) and Grüneisen parameter γ (measure of anharmonicity) was examined as an example of a specific correlation between harmonic and anharmonic characteristics of solids. The Pineda theory provides a qualitative justification for the single-valued correspondence between the Poisson's ratio and the Grüneisen parameter.

The microscopic representation of the Grüneisen parameter was used to demonstrate that the limit elastic deformation of an interatomic bond is a single-valued function of the Poisson's ratio.

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Conflict of interest

The author declares that he has no conflict of interest.

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