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On the derivation of the Belomestnykh–Tesleva's formula

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The Belomestnykh–Tesleva's formula is interesting in that it establishes an unambiguous relationship between the Poisson's ratio and the Grüneisen's parameter. The derivation of this formula from the generally accepted Grüneisen's equation is discussed. The Belomestnykh–Tesleva's formula, obtained earlier from other assumptions, is derived using the theory of elasticity and the Leontiev's equation. For a number of silicate glasses and glassy metaphosphates of alkaline earth metals, the proposed approach finds a fairly satisfactory agreement with the experimental data.

Keywords: Grüneisen's equation, Grüneisen's parameter, Poisson's ratio, shear modulus, isothermal bulk modulus, acoustic wave velocities.

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The fact that parameters of elasticity theory (elastic moduli, Poisson's ratio) as harmonic linear values must not be related to anharmonism — with deviation of inter-atomic interaction force from linear dependence when an atom is displaced from equilibrium position, is considered common. At the same time papers appear in scientific literature that indicate presence of quite certain connection between elastic properties and anharmonism measure γ [1]:

$$\gamma = \frac{\beta V B}{C_V}, \tag{1}$$

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.

In papers by Belomestnykh and Tesleva [2] it is established that Grüneisen parameter γ is a single-valued function of Poisson's ratio μ— elastic theory parameter

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

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. They demonstrated that Grüneisen parameter was determined exclusively by velocities of longitudinal (v_L) and transverse (v_s) acoustic waves

$$\gamma = \frac{3}{2}\left[\frac{(v_L/v_s)^2 - 4}{(v_L/v_s)^2 + 2}\right]. \tag{3}$$

Belomestnykh and Tesleva [2], using in equation (3) the known ratios of physical acoustics [3]:

$$v_L = \sqrt{\frac{E(1-\mu)}{\rho(1+\mu)(1-2\mu)}},\ v_s = \sqrt{\frac{E}{2\rho(1+\mu)}}$$

in 2004 obtained equation (2), which unambiguously related Grüneisen parameter with Poisson's ratio. Notably, such comparatively simple equation (2) is in satisfactory agreement with Grüneisen equation (1) [2].

In this message it is proposed to produce equation of Belomestnykh–Tesleva (2) from Grüneisen equation (1).

Multiplying the numerator and the denominator of Grüneisen equation (1) by shear modulus G and taking into account the known interrelation between elastic moduli G and B [1,4]:

$$\frac{B}{G} = \frac{2}{3}\left(\frac{1+\mu}{1-2\mu}\right), \tag{4}$$

we obtain the following modification of Grüneisen equation (1)

$$\gamma = A\left(\frac{1+\mu}{1-2\mu}\right), \tag{5}$$

where designation is introduced

$$A = \frac{2}{3}\left(\frac{\beta V G}{C_V}\right). \tag{6}$$

Using Leontiev ratio [5]:

$$\frac{C_V}{\beta V} = \frac{2}{3}\rho v_k^2 \tag{7}$$

Table 1. Calculation of factor A by equations (8) and (11) for silicate glasses R_2O-SiO_2 ($R = Na, K$) [8] and vitreous metaphosphates of alkali-earth metals [9]

Item №	Compounds	μ	v_L, m/s	v_s, m/s	v_k, m/s	A (8)	A (11)
			Na_2O-SiO_2				
	Content of Na_2O, mol.% by synthesis:						
1	13	0.205	5233	3378	4091	0.68	0.64
2	16	0.218	5115	3275	3984	0.68	0.63
3	17	0.225	5054	3222	3929	0.67	0.62
4	20	0.235	12133	7705	9415	0.67	0.61
5	26	0.245	4835	3070	3752	0.67	0.60
6	30	0.255	4844	3052	3746	0.66	0.60
7	33.3	0.255	4906	3103	3800	0.67	0.60
			K_2O-SiO_2				
	Content of K_2O, mol.% by synthesis:						
1	13	0.230	4820	3073	3747	0.67	0.62
2	15	0.225	4759	3035	3700	0.67	0.62
3	20	0.250	4550	2889	3531	0.67	0.60
4	25	0.270	4463	2801	3445	0.66	0.58
			Vitreous metaphosphates of alkali-earth metals				
1	$0.51\ MgO \cdot 0.49\ P_2O_5$	0.233	5267	3110	3962	0.62	0.62
2	$0.50\ MgO \cdot 0.50\ P_2O_5$	0.233	5264	3108	3959	0.62	0.62
3	$0.49\ MgO \cdot 0.51\ P_2O_5$	0.233	5289	3121	3977	0.62	0.62
4	$0.51\ CaO \cdot 0.49\ P_2O_5$	0.264	5051	2858	3735	0.59	0.59
5	$0.50\ CaO \cdot 0.50\ P_2O_5$	0.267	5086	2869	3756	0.58	0.58
6	$0.49\ CaO \cdot 0.51\ P_2O_5$	0.265	5051	2857	3734	0.59	0.59
7	$0.51\ SrO \cdot 0.49\ P_2O_5$	0.274	4603	2568	3385	0.58	0.58
8	$0.50\ SrO \cdot 0.50\ P_2O_5$	0.273	4610	2577	3393	0.58	0.58
9	$0.49\ SrO \cdot 0.51\ P_2O_5$	0.271	4612	2584	3397	0.58	0.58
10	$0.50\ BaO \cdot 0.50\ P_2O_5$	0.288	4178	2278	3046	0.56	0.56
11	$0.49\ BaO \cdot 0.51\ P_2O_5$	0.286	4186	2291	3056	0.56	0.56

and shear modulus $G = \rho v_s^2$, let us present factor A (6) in the form of sound velocities ratio

$$A = \frac{v_s^2}{v_k^2}, \tag{8}$$

where v_k^2 — square of mean square sound velocity [5]:

$$v_k^2 = \frac{v_L^2 + 2v_s^2}{3}, \tag{9}$$

v_L and v_S — velocities of longitudinal and transverse elastic waves, respectively, ρ — density.

From equation (8) using equation (9) and known equation of elasticity theory [1,6]:

$$\left(\frac{v_L}{v_s}\right)^2 = \frac{2-2\mu}{1-2\mu} \tag{10}$$

we find relation of factor A with Poisson's ratio μ

$$A = \frac{3}{2}\left(\frac{1-2\mu}{2-3\mu}\right). \tag{11}$$

Calculation of parameter A using equations (8) and (11) shows agreed values (Table 1). For silicate glasses, values given in the Table and calculated using various equations are quite close. For vitreous metaphosphates of alkali-earth metals, values of coefficient A by equations (8) and (11) coincide to two decimals of the units, tangent of curve $A(8)-A(11)$ inclination angle is equal to one.

Notably, modified Grüneisen equation (5) may be transformed into Belomestnykh–Tesleva equation (2) with the use of relation (11)

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

Thus, Belomestnykh–Tesleva formula (2), which was derived by its authors from different basic assumptions [2], may be obtained from Grüneisen equation (1) by appealing to Leontiev's ratio (7) and the elasticity theory.

Let us note that coefficient A in equation (8) characterizes the proportion of mean interatomic interaction energy $\overline{U} = \rho v_k^2 V$ accounted for by elastic energy $\Delta U = \rho v_s^2 V$

Table 2. Comparison of results of Grüneisen parameter γ calculation using equations (1) and (2) (uses data [2,10])

№	Elements and compounds	μ	γ	
			Grüneisen (1)	Belomestnykh–Tesleva (2)
1	LiF	0.214	1.34	1.34
2	NaCl	0.243	1.46	1.47
3	Fe	0.292	1.68	1.72
4	Al	0.340	2.11	2.05
5	Ag	0.379	2.40	2.40
5	$NaNO_3$	0.257	1.31	1.53
7	Pd	0.374	2.40	2.35
8	Au	0.420	2.80	2.88

needed for shear deformation

$$A = \frac{v_s^2}{v_k^2} = \frac{\rho v_s^2 V}{\rho v_k^2 V} = \frac{GV}{\overline{U}} = \frac{\Delta U}{\overline{U}}. \qquad (12)$$

Equation (5) for vitreous solids has been obtained earlier with the following interpretation of factor A [7]:

$$A = \frac{2}{9} \ln\left(\frac{1}{f_g}\right), \qquad (13)$$

where f_g — the fraction of fluctuation free volume frozen at glass transition point T_g. Value f_g in vitreous systems of one and the same class is practically a universal constant $f_g \approx \text{const}$ [7]. Logarithm of this value is even weaker dependent on the composition of amorphous substances within the same class. Assessment of A using this equation (13) gives actually constant values, at least in glasses of one structural type, and by order of magnitude matches the results of calculation by ratios (8) and (11). For sodium-silicate Na_2O-SiO_2 and potassium-silicate K_2O-SiO_2 glasses, the value of volume fraction of fluctuation free volume $f_g \approx \text{const} \approx 0.028$, and value A, calculated according to equation (13), is approximately equal to 0.79.

Values of Grüneisen parameter for metals calculated using equation of Grüneisen (1) and Belomestnykh–Tesleva (2) are also in satisfactory agreement (Table 2).

Some deviations of values for solids are probably due to spread of values γ, produced by various researchers. The reason for such deviations also possibly lies in anisotropy of systems considered in Table 2, as more agreed data is observed for some quasiisotropic alkali-haloid crystals with central forces of interatomic interaction.

Thus, the suggested output of Belomestnykh–Tesleva equation (2) that establishes relation of Grüneisen parameter with Poisson's ratio, from Grüneisen equation finds quite satisfactory agreement with experimental data.

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Conflict of interest

The authors declare that they have no conflict of interest.

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