ORIENTATIONAL ANHARMONICITY OF INTERATOMIC INTERACTION IN CUBIC MONOCRYSTALS

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Abstract

Anharmonicity of interatomic interaction from a position of physical acoustics under the standard conditions is investigated. It is shown that the measure of anharmonicity of interatomic interaction (Grüneisen parameter) is explicitly expressed through velocities of sound. Calculation results of orientation anharmonicity are shown on the example of 116 cubic monocrystals with different lattice structural type and type of chemical bond. Two types of anharmonicity interatomic interaction anisotropy are determined.

Key words: *acoustics, orientational anharmonicity, Grüneisen parameter, velocity of sound.*

1. ANHARMONICITY AND VELOCITY OF SOUND IN ELASTIC ISOTROPIC MEDIUMS

As it is known [1] the potential curve of particle (atom, molecule) interaction within a solid body is asymmetrical when close to their equilibrium position. Asymmetry of atomic force interaction appears under (due to) great shifts and approaches when repulsion forces grow quicker than those of attraction. Asymmetry grows together with the growth of total energy of a particle. At the same time the particle will accomplish non-linear anharmonic oscillations which cause such anharmonic effects as thermal expansion, heat conductivity, temperature dependence of the elastic properties, sound absorption, etc. The measure of anharmonicity is Grüneisen parameter γ. It is included into the Mi-Grüneisen equation of state and reflects the peculiarities of the phonon specter of the crystal [1]:

$$p = -\left(\frac{\partial E_0}{\partial V}\right)_T + \frac{\gamma}{V}(U - E), \quad (1)$$

where p – pressure; V – volume; $E_o = U_o + \sum_{j=1}^{3N} h\nu_j$; U_o – potential energy of the crystal in the equilibrium state; E – total energy; h – Planck's constant. The volumetric dependence of the solid body frequencies ν_j is used to calculate the microscopical Grüneisen parameter:

$$\gamma = -\frac{d\ln\nu_j}{d\ln V} = -\frac{V}{\nu_j}\left(\frac{d\nu_j}{dV}\right). \quad (2)$$

The main formula for the experimental calculation of the macroscopic (thermodynamic) Grüneisen parameter γ_D is the Grüneisen equation (law, formula), in which γ_D depends on the four directly measured quantities:

$$\frac{\alpha}{\chi} = \gamma_D \rho c_v, \quad (3)$$

where α – coefficient of the thermal expansion; χ – volume compressibility; c_V – heat capacity under the constant volume. The values of γ_D for the majority of real elastic isotropic solid bodies are between 0.8-3.5. (Notice that for a "harmonic" solid body $\gamma_D = 0$). A theoretical work by S.Sh. Suleiman [2] calculates thermodynamic properties of ionic crystals in various approximations and suggests using this calculation for quantitative evaluation of the anharmonic effects in the given type of crystals. Recently, from the viewpoint of physical acoustics a new approach was suggested for evaluating interatomic interaction anharmonism in a solid body and new correlation was received in which the Grüneisen parameter was called acoustic γ_{ac} [3]. For that Grüneisen equation was transformed into a more convenient

$$\gamma_D = \frac{\beta B^T}{\rho c_V}, \quad (4)$$

where β – temperature coefficient of volumetric expansion, B^T – isothermal volumetric modulus of uniform compression ($B^T = 1/\chi$). In the physical acoustic of crystals adiabatic modulus of uniform compression B^S, shear modulus are most reliably evaluated experimentally and in thermal physics - specific (molar) heat capacity under the constant pressure c_p (C_p). That's why in (4) we pass from B^T, c_V to B^S, c_p using the well-known correlation

$$B^T \cdot c_p = B^S \cdot c_V. \quad (5)$$

As a result the formula takes on the following form

$$\gamma_D = \frac{\beta B^s \mu}{C_p \rho}. \quad (6)$$

Besides, according to the elasticity theory formulas for isotropic spatially unlimited elastic medium, showing the correlation between the acoustic and elastic characteristics of a solid body [4, 5]

$$\rho \upsilon_L^2 = B^S + 4/3 \cdot G, \qquad \rho \upsilon_t^2 = G, \quad (7)$$

we come to correlation between Grüneisen parameter and velocity of elastic waves transmission

$$\gamma = \frac{\beta}{c_p}\left(\upsilon_L^2 - 4/3 \cdot \upsilon_t^2\right). \quad (8)$$

Having used the notion of root-mean-square velocity as in work [6]:

$$\upsilon_{rms} = \left(\frac{\upsilon_L^2 + 2\upsilon_t^2}{3}\right)^{1/2} \quad (9)$$

and $\mu \upsilon_{кв}^2 = \frac{3}{2}\frac{C_p}{\beta}$ (μ – molar mass), as shown in the same work [3] we get the formula for γ as velocity of sound function:

$$\gamma_{ac} = \frac{9}{2}\left(\frac{\upsilon_L{}^2 - 4\upsilon_t^2/3}{\upsilon_L^2 + 2\upsilon_t^2}\right). \quad (10)$$

Here υ_L – velocity of longitudinal wave transmission in isotropic spatially unlimited elastic medium, υ_t – velocity of transverse wave transmission. Thermodynamic and acoustic values of Grüneisen parameter for a number of metals, ion, ion-molecule compounds are given in tab. 1

Table 1

Grüneisen parameter for solid bodies[3]

Elements and compounds	Velocity of sound, m/s		Grüneisen parameter	
	υ_L	υ_t	γ_{ac}	γ_D
1	2	3	4	5
Ag	3686	1677	2.30	2.4 [1]; 2.4; 2.5 [7]
Al	6422	3235	1.98	2.34 [1]; 2.43 [8]; 2.11 [9]
Au	3361	1239	2.90	3.0 [1]; 2.80 [9]
Cu	4726	2298	2.09	2.00 [1]; 1.96; 1.9 [7]; 2.06 [9]

Continuation of the table 2

Ni	5894	3219	1.70	1.88; 2.2 [7]; 1.73 [9]
Pd	4954	1977	2.47	2.23; 2.4 [7]
Pb	2158	860	2.69	2.9 [9]
W	5233	2860	1.70	1.62; 1.7 [7]
Be	13003	8967	0.84	0.83 [9]
Co	5827	3049	1.85	1.87; 2.1 [7];
Mg	5898	3276	1.64	1.41 [8]
Fe	6064	3325	1.68	1.60; 1.68 [7]; 1.66 [8];
Pt	3960	1670	2.53	2.54; 3.3 [7];
Ta	4147	2039	2.06	1.73
Th	2900	1583	1.70	1.54
Y	4106	2383	1.48	1.25
Zn	4117	2350	1.54	2.00
U	3422	2105	1.29	1.62
LiF	7323	4518	1.26	1.34; 1.75 [10]
NaF	5666	3330	1.44	1.72 [10]
KF	4641	2587	1.63	1.45; 1.73 [10];
RbF	3948	2132	1.74	1.41 [10]
LiCl	5260	3058	1.48	1.52; 1.78 [10]
NaCl	4666	2755	1.42	1.62; 1.74 [10];1.46
KCl	4090	2312	1.58	1.60 [10]
RbCl	3077	1658	1.75	1.53 [10]
LiBr	3621	2072	1.53	1.70; 2.02 [10]
NaBr	3284	1885	1.52	1.56; 1.81 [10]
KBr	3075	1695	1.67	1.68; 1.58 [10]
RbBr	2591	1403	1.73	1.37; 1.50 [10]
LiI	2846	1608	1.58	2.22 [10]
NaI	2889	1639	1.56	1.90 [10]
KI	2623	1469	1.61	1.63; 1.72 [10]
RbI	2245	1198	1.78	1.41; 1.73 [10]
AgCl	3145	1207	2.79	2.02
AgBr	2845	1159	2.63	2.33
TlCl	2265	1153	1.94	2.60
TlBr	2133	1085	1.94	2.47
NaCN	3600	960	3.57	
KCN	3340	1170	3.04	
NaN_3	3460	1350	2.75	4.25

$NaClO_3$	4240	2380	1.65	1.36
$NaClO_4$	3970	2200	1.65	
$NaNO_2$	3880	2400	1.25	
$NaNO_3$	4510	2580	1.53	
$KBrO_3$	3280	1780	1.16	
NH_4ClO_4	3800	2130	1.61	1.81

Note: 1. Velocity values were taken from [4, 5, 11, 12].

2. γ_D parameter was calculated by the authors. Values β, B^s, C_p and ρ were taken from reference books [4, 13–15].

The results given in table 1 show quite a satisfactory agreement between γ_{ac} и γ_D for the substances under research. Here is a subject for analysis. For example, values of Grüneisen parameter for sodium azide (NaN_3) seem relatively high at the first glance. But it is known that [16], standard conditions are critical for the given azide as at $T_c = 292.7$ K (atmospheric pressure) a diffused lattice transformation takes place, which gives the λ peak on the thermal curve $C_P(T)$. For the substances with Grüneisen parameter reasonably defined by the formula (10) it becomes possible to study the orientation dependence γ_{ac}, Grüneisen parameter changes under external energy exposure as well as other aspects by means of the acoustic experiment only. At the same time it would be naive to suppose that (10) could be directly used for evaluating γ_{ac} of all solid body varieties. Preliminary investigations in this direction show a significant difference between γ_{ac} and γ_D in a number of objects. This group consists, on the one hand, from rare-earth elements (γ_{ac} is average twice as big compared to γ_D) and on the other hand it includes such elements as bismuth, cadmium, zinc (γ_{ac} is average 1,5 as little compared to γ_D). Though here we can also mark out some groups of substances where γ_a/γ_D remains constant. A more substantial check of correlation (10) has been carried out by D.S Sanditov, A.A. Mashanov and M.D. Darmayev [17].

2. ORIENTATIONAL ANHARMONOCITY IN CUBIC MONOCRYSTALS

Using the acoustic method for calculation the Grüneisen parameter not only expands the way of estimation of this important for anharmonic effects quantity but also makes the given approach perspective for the solid body theory in general. One of the advantages of its practical use (10) is the possibility of studying anharmonicity anisotropy in crystals. It is known [18] that cubic crystals have only three preferential directions – [100], [110], [111], along which purely longitudinal or transversal waves can transmit (fig. 1). The velocity of these waves transmission is correlated with components of elasticity tensor of a cubic monocrystal c_{ij} as follows [18]:

$$\rho\upsilon^2_{L[100]} = c_{11}, \qquad 2\rho\upsilon^2_{L[110]} = c_{11} + c_{12} + 2c_{44}, \qquad 3\rho\upsilon^2_{L[111]} = c_{11} + 2c_{12} + 4c_{44},$$

$$\rho\upsilon^2_{t[100]} = c_{44}, \qquad 3\rho\upsilon^2_{t[111]} = c_{11} + c_{44} - c_{12},$$

$\rho\upsilon^2_{t_1[110]} = c_{44}$ (the wave is polarized in $[00\bar{1}]$),

$2\rho\upsilon^2_{t_2[110]} = c_{11} - c_{12}$ (the wave is polarized in $[1\bar{1}0]$). (11)

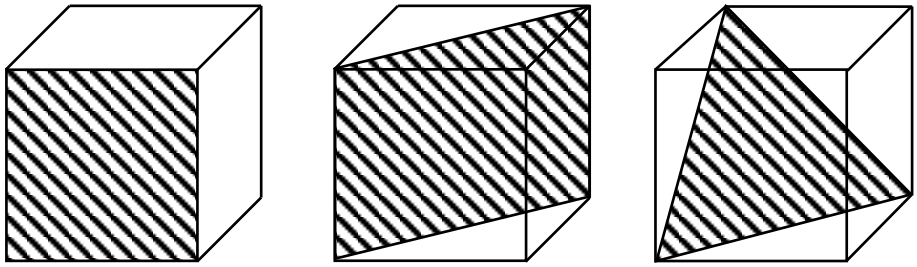


Fig 1. The basic planes in cubic monocrystals

Table 2 provides the results of sound velocity anisotropy under the standard conditions (in most cases) for 116 metallic, ion, covalent, ion-covalent and molecular cubic monocrystals with various structural lattice types (cubic volume-centered, cubic face-centered, NaCl, CsCl, diamond, sphalerite, fluorite, pyrite and others).

On the basis of these data and information on c_{ij} elastic anisotropy factor A, Koshi correlation Δ and orientational Grüneisen parameters $\gamma_{[hkl]}$, have been calculated and included into table 3.

Table 2

Sound velocities along the specific directions in cubic monocrystals (m/s)

Substance	Direction					
	[100]		[110]		[111]	
	υ_L	υ_t	υ_L	υ_{t2}	υ_L	υ_t
1	2	3	4	5	6	7
Li (78 K)	5211	4452	6698	1453	7125	2831
CuZn	3877	3097	4847	1063	5130	1980
BN	15350	11744	16824	9514	17287	10311
Na	2761	2080	3366	786	3545	1362
K (83 K)	2312	1739	2802	723	2947	1165
LiF	6548	4888	7318	3650	7558	4107
C (diamond)	17504	12804	18301	11636	18560	12038
MgO	9128	6616	9960	5281	10223	5761
Ge	4929	3553	5415	2755	5581	3044
LiCl	4830	3465	5315	2663	5467	2955
Ne (24.3 K)	901	645	1037	391	1078	490
Ni (4 K)	5397	3832	6136	2482	6363	3000
α-Fe	5561	3938	6305	2584	6535	3102

GaAs	4731	3346	5240	2475	5399	2795
GaP	5808	4080	6374	3123	6552	3472
LiBr	3468	2405	3833	1764	3947	1841
Si	8431	5844	9132	4673	9354	5093
Kr (77 K)	1189	824	1362	488	1415	620
InAs	3832	2642	4239	1831	4418	2136
LiI	2649	1823	2925	1336	3012	1516
$(CH_2)_6N_4$	3437	2348	3549	2174	3586	2233
AlSb	4528	3085	4984	2277	5127	2575
LSAT*	2152	1445	2311	1175	2361	1271
InSb	3407	2284	3767	1701	3880	1623
ZnSe	4011	2689	4484	1792	4632	2133
Cu	4335	2901	4959	1620	5150	2134
C_{60}	2961	1970	3294	1339	3398	1578
$Ba(NO_3)_2$**	2997	1980	3404	1149	3529	1479
$Mg(BrO_3)_2{\cdot}6H_2O$	2902	1910	3144	1477	3221	1634
$Zn(BrO_3)_2{\cdot}6H_2O$	2924	1864	3132	1488	3199	1623
$SrTiO_3$	7849	4912	8059	4558	8120	4679
$Co(BrO_3)_2 \cdot 6H_2O$	2945	1835	3133	1480	3200	1604
$Cu(BrO_3)_2 \cdot 6H_2O$	2950	1836	3135	1499	3194	1619
$LaGaO_3$	1927	1189	2015	1032	2043	1087
$LiBaF_3$	1574	965	1616	892	1630	917
$Ni(BrO_3)_2 \cdot 6H_2O$	3016	1847	3190	1527	3243	1641
$Sr(NO_3)_2$	3773	2306	4162	1494	4284	1806
Ag	3432	2092	3834	1205	3959	1558
Cr_2FeO_4	8513	5121	8866	4482	8981	4705

Continuation of the table 2

Fe_3O_4	7260	4330	7438	4015	7497	4122
MnO	2027	1206	2148	974	2187	1057
Cu_3Au	3952	2330	4348	1465	4472	1800
$Y_3Al_5O_{12}$	8568	5030	8615	4948	8631	4975
ZnS (sphalerite)	4947	2889	5339	2075	5464	2377
Re	5397	3130	5411	3105	5416	3113
$KAl(SO_4)_2$	3810	2191	3888	2049	3913	2098

$Y_3Ga_5O_{12}$	7081	4061	7189	3865	7225	3931
Pd	4324	2429	4741	1456	4872	1838
Ta	3986	2232	4206	1783	4277	1944
Pb	2026	1126	2246	571	2315	800
CuBr	3122	1722	3399	1722	3486	1329
CuCl	3570	1963	3933	1963	4046	1428
Nb	4682	2547	5010	1820	5114	2090
$Pb(NO_3)_2$	3211	1739	3425	1265	3494	1440
$Mg_3Al_2(SO_4)_3$	7239	3894	7303	3773	7325	3814
BaF_2	4322	2285	4337	2257	4342	2266
Al	6305	3238	6453	2932	6502	3037
Au (0 K)	3216	1526	3445	904	3516	1150
$AgPO_3$	3043	1416	3045	1413	3045	1414
$CeRu_2$	3889	1485	3986	573	4196	974
$Ni(NH_3)_6(NO_3)_2$	2508	815	2589	501	2616	623
PbSe	3635	1267	2947	2476	2677	2150
KI	2974	1090	2500	1945	2320	1709
NH_4I	3120	977	2584	2004	2378	1731
RbBr	3382	1171	2828	2193	2617	1914
RbCl	3956	1305	3080	2364	2861	2399
KBr	3551	1358	3016	2314	2815	2046
RbI	2719	888	2333	1788	2045	1547
CaO	8193	4890	6544	4930	8161	4917
Tl_3TaS_4	2689	686	2218	1668	2037	1419
FeS_2	8724	4670	7935	5913	7653	5530
KCl	4477	1772	3871	2864	3647	2552
NH_4Cl	5055	2111	4427	3226	4196	2904
NH_4Br	3175	1475	3076	2205	2927	1992
ZrC	7975	4658	7518	5363	7360	5139
$Bi_{12}SiO_{20}$	1179	551	1058	737	1014	673
PbS	4115	1818	3709	2546	3564	2339
KF	5111	2248	4619	3137	4443	2871
RbF	3934	1611	3517	2388	3366	2160

Cr	6975	3743	6561	4429	6417	4213
$SrCl_2$	4857	1801	4299	2890	4096	2579
CsCl	3020	1416	2778	1846	2693	1715
UC	4845	2177	4423	2942	4272	2711
Tl_3TaSe_4	2399	750	2098	1384	2168	1210
CsF	3086	1232	2774	1830	2662	1655
$Bi_{12}GeO_{20}$	1153	632	1098	724	1303	695
TiC	10315	6058	9991	6577	9881	6408
$Bi_4(SiO_4)_3$	1413	873	1388	912	1709	899

Continuation of the table 2

UO_2	6042	2434	5456	3538	5246	3227
CsBr	2639	1298	2472	1593	2414	1202
CsI	2323	1184	2192	1412	2146	1340
NaF	5885	3160	5624	3603	5535	3462
NaCl	4727	2429	4480	2859	4395	2723
$NaClO_3$	4454	2177	4189	2651	4097	2503
NaBr	3517	1762	3324	2103	3257	1996
CaF_2	7183	3256	6688	4178	6515	3895
NaI	2867	1419	2713	1695	2659	1608
$Bi_4(GeO_4)_3$	1278	784	1273	791	1272	789
SrO	6152	3463	6007	3709	5958	3629
$NaBrO_3$	4087	2126	3934	2398	3882	2311
SrF_2	7114	3582	6852	4062	6762	3908
TlCl	2393	1042	2246	1331	2194	1242
TlBr	2257	987	2123	1249	2076	1169
Mo	6716	3284	6478	3731	6396	3588
W	5236	2858	5232	2864	5231	2862
$Y_3Fe_5O_{12}$	7215	3865	7187	3917	7178	3900
PbF_2	3361	1598	3294	1731	3278	1688
V	6167	2697	6000	3049	5944	2937
NaCN	3997	507	3611	1787	3473	1489
RbCN	2739	842	2587	1232	2534	1117
AgBr	2949	1055	2830	1334	2789	1253
KCN	3573	993	3354	1581	3278	1413

AgCl	3288	1064	3129	1466	3075	1345
$N_2H_6Cl_2$	4964	2204	4925	2252	4917	2236
CsCN	2316	577	2180	972	2132	860
NaO_2	4546	1164	4439	1522	4403	1413

Note: *,** (see table 3)

Table 3

Elastic anisotropy factor, Koshi correlation and orientational Grüneisen parameters in cubic monocrystals

Substance	A	Δ	$\gamma_{[100]}$	$\gamma_{1[110]}$	$\gamma_{2[110]}$	$\gamma_{[111]}$	References on c_{ij} and density
1	2	3	4	5	6	7	8
Li (78 K)	9.391	0.864	0.049	0.982	3.855	2.700	[11]
CuZn	8.495	0.751	0.295	1.129	3.842	2.778	[11]
BN	1.524	2.526	0.455	0.798	1.574	1.382	[19]
Na	7.000	0.677	0.513	1.252	3.763	2.791	[4]
K (83 K)	5.778	0.703	0.519	1.236	3.619	2.714	[4]
LiF	1.939	1.323	0.547	0.963	2.008	1.715	[5]
C (diamond)	1.211	4.606	0.623	0.790	1.147	1.073	[4]
MgO	1.570	1.589	0.657	0.984	1.801	1.587	[4]
Ge	1.663	1.386	0.678	1.030	1.942	1.702	[4]
LiCl	1.858	1.102	0.696	1.054	1.993	1.734	[5]
Ne (24.3 K)	2.727	0.822	0.704	1.228	2.840	2.307	[4]

Continuation of the table 3

Ni (4 K)	2.384	0.874	0.735	1.213	2.651	2.192	[4]
α-Fe	2.322	0.883	0.744	1.213	2.614	2.170	[4]
GaAs	1.828	1.104	0.749	1.131	2.186	1.883	[4]
GaP	1.707	1.170	0.775	1.122	2.067	1.803	[20]
LiBr	1.854	1.016	0.823	1.196	2.268	2.226	[5]
Si	1.564	1.246	0.825	1.123	1.922	1.708	[4]
Kr (77 K)	2.853	0.723	0.825	1.330	2.968	2.419	[4]
InAs	2.082	0.875	0.845	1.221	2.462	2.111	[4]
LiI	1.862	0.964	0.852	1.221	2.292	1.978	[11]
$(CH_2)_6N_4$	1.167	2.333	0.879	0.999	1.285	1.224	[11]

AlSb	1.836	0.939	0.889	1.246	2.291	1.985	[11]
LSAT*	1.512	1.115	0.944	1.209	1.944	1.748	[21]
InSb	1.980	0.823	0.950	1.322	2.327	2.556	[4]
ZnSe	2.253	0.748	0.950	1.362	2.684	2.266	[20]
Cu	3.209	0.621	0.956	1.453	3.181	2.583	[11]
C_{60}	2.164	0.750	0.978	1.372	2.637	2.240	[22]
$Ba(NO_3)_2$**	2.970	0.618	1.004	1.473	3.108	2.550	[4]
$Mg(BrO_3)_2 \cdot 6H_2O$	1.702	0.808	1.019	1.315	2.203	1.951	[23]
$Zn(BrO_3)_2 \cdot 6H_2O$	1.568	0.843	1.137	1.390	2.167	1.951	[23]
$SrTiO_3$	1.161	1.204	1.206	1.303	1.574	1.507	[4]
$Co(BrO_3)_2 \cdot 6H_2O$	1.537	0.785	1.222	1.448	2.186	1.992	[23]
$Cu(BrO_3)_2 \cdot 6H_2O$	1.501	0.801	1.226	1.449	2.147	1.954	[23]
$LaGaO_3$	1.326	0.893	1.258	1.421	1.919	1.789	[21]
$LiBaF_3$	1.169	1.049	1.281	1.378	1.660	1.593	[21]
$Ni(BrO_3)_2 \cdot 6H_2O$	1.462	0.769	1.286	1.490	2.143	1.960	[23]
$Sr(NO_3)_2$	2.384	0.544	1.293	1.647	2.963	2.533	[24]
Ag	3.013	0.494	1.303	1.701	3.263	2.726	[11]
Cr_2FeO_4	1.305	0.812	1.351	1.498	1.963	1.842	[4]
Fe_3O_4	1.162	0.915	1.382	1.470	1.739	1.674	[4]
MnO	1.534	0.658	1.391	1.600	2.315	2.112	[25]
Cu_3Au	2.532	0.479	1.424	1.764	3.112	2.665	[4]
$Y_3Al_5O_{12}$	1.033	1.035	1.440	1.460	1.519	1.506	[20]
ZnS (sphalerite)	1.934	0.526	1.459	1.730	2.760	2.441	[11]
Re	1.016	0.995	1.484	1.493	1.522	1.516	[4]
$KAl(SO_4)_2$	1.143	0.785	1.514	1.587	1.822	1.762	[4]
$Y_3Ga_5O_{12}$	1.104	0.814	1.524	1.578	1.753	1.711	[20]
Pd	2.782	0.408	1.598	1.918	3.310	2.838	[4]
Ta	1.568	0.523	1.609	1.798	2.517	2.307	[4]
Pb	3.892	0.367	1.636	1.991	3.641	3.054	[4]
CuBr	2.545	0.400	1.663	1.956	1.956	2.811	[4]
CuCl	3.400	0.368	1.674	2.006	2.006	3.004	[4]
Nb	1.959	0.424	1.711	1.944	2.934	2.622	[4]
$Pb(NO_3)_2$	1.890	0.425	1.727	1.949	2.892	2.598	[4]

$Mg_3Al_2(SO_4)_3$	1.065	0.633	1.751	1.781	1.890	1.863	[4]
BaF_2	1.026	0.615	1.811	1.823	1.865	1.855	[24]
Al	1.220	0.465	1.910	1.988	2.308	2.222	[4]

Continuation of the table 3

Au (0 K)	2.846	0.268	2.171	2.386	3.592	3.178	[11]
$AgPO_3$	1.004	0.3805	2.234	2.236	2.242	2.240	[26]
$CeRu_2$	6.657	1.151	2.807	2.870	4.202	3.770	[27]
$Ni(NH_3)_6(NO_3)_2$	2.649	0.115	3.192	3.259	3.977	3.736	[24]
PbSe	0.262	1.688	3.034	2.476	0.110	0.275	[4]
KI	0.329	0.809	2.912	2.434	0.393	0.597	[5]
NH_4I	0.238	0.561	3.270	2.832	0.405	0.641	[28]
RbBr	0.288	0.813	3.050	2.585	0.405	0.624	[5]
RbCl	0.316	0.787	3.159	2.519	0.443	0.117	[5]
KBr	0.351	0.879	2.803	2.336	0.445	0.647	[5]
RbI	0.253	0.737	3.181	2.815	0.449	0.497	[5]
CaO	0.984	1.292	1.380	0.543	0.513	1.345	[4]
Tl_3TaS_4	0.169	0.283	3.636	3.296	0.519	0.806	[20]
FeS_2	0.624	3.529	1.768	1.431	0.554	0.669	[4]
KCl	0.378	0.928	2.711	2.285	0.580	0.789	[5]
NH_4Cl	0.428	0.944	2.561	2.155	0.637	0.831	[4]
NH_4Br	0.447	0.898	2.239	2.137	0.699	0.893	[4]
ZrC	0.754	3.578	1.458	1.243	0.717	0.797	[4]
$Bi_{12}SiO_{20}$	0.500	0.893	2.220	1.862	0.806	0.987	[20]
PbS	0.510	0.832	2.394	2.066	0.861	1.029	[4]
KF	0.503	0.859	2.408	2.089	0.901	1.087	[5]
RbF	0.409	0.728	2.616	2.283	0.902	1.113	[5]
Cr	0.714	1.487	1.759	1.543	0.924	1.028	[4]
$SrCl_2$	0.388	0.471	2.882	2.551	0.939	1.183	[4]
CsCl	0.588	0.870	2.209	1.935	0.983	1.141	[4]
UC	0.598	0.769	2.343	2.052	0.979	1.154	[4]
Tl_3TaSe_4	0.294	0.293	3.274	2.973	1.010	1.621	[20]

CsF	0.454	0.537	2.687	2.378	1.010	1.230	[28]
$Bi_{12}GeO_{20}$	0.763	1.423	1.685	1.511	1.012	1.780	[20]
TiC	0.428	1.846	1.438	1.322	1.018	1.074	[4]
$Bi_4(SiO_4)_3$	0.917	2.282	1.253	1.187	1.025	1.828	[20]
UO_2	0.468	0.530	2.662	2.365	1.074	1.269	[4]
CsBr	0.664	0.893	2.054	1.834	1.097	2.014	[4]
CsI	0.704	0.984	1.936	1.736	1.099	1.214	[5]
NaF	0.769	1.152	1.757	1.597	1.119	1.208	[5]
NaCl	0.731	0.985	1.908	1.723	1.133	1.243	[5]
$NaClO_3$	0.674	0.819	2.075	1.870	1.164	1.294	[5]
NaBr	0.673	0.925	1.993	1.802	1.165	1.283	[5]
CaF_2	0.607	0.636	2.316	2.088	1.212	1.374	[4]
NaI	0.748	1.026	2.034	1.848	1.212	1.332	[5]
$Bi_4(GeO_4)_3$	0.982	1.615	1.279	1.265	1.232	1.238	[20]
SrO	0.872	1.160	1.591	1.505	1.255	1.305	[4]
$NaBrO_3$	0.786	0.868	1.866	1.735	1.303	1.389	[5]
SrF_2	0.778	0.728	1.977	1.849	1.404	1.496	[4]
TlCl	0.613	0.497	2.438	2.243	1.406	1.571	[4]
TlBr	0.625	0.495	2.425	2.236	1.432	1.589	[4]

Continuation of the table 3

Mo	0.775	0.625	2.074	1.954	1.509	1.603	[4]
W	0.995	0.742	1.700	1.697	1.690	1.691	[4]
$Y_3Fe_5O_{12}$	0.974	0.699	1.765	1.752	1.705	1.716	[20]
PbF_2	0.854	0.481	2.165	2.100	1.832	1.901	[4]
V	0.782	0.374	2.425	2.342	1.946	2.039	[4]
NaCN	0.076	0.027	4.266	4.216	2.034	2.484	[29]
RbCN	0.467	0.159	3.308	3.189	2.160	2.401	[30]
AgBr	0.618	0.218	2.971	2.869	2.192	2.343	[11]
KCN	0.395	0.127	3.496	3.381	2.192	2.468	[31]
AgCl	0.527	0.174	3.201	3.091	2.212	2.424	[11]
$N_2H_6Cl_2$	0.957	0.339	2.379	2.355	2.289	2.306	[24]
CsCN	0.347	0.096	3.672	3.578	2.366	2.659	[32]
NaO_2	0.292	0.084	3.631	3.593	3.072	3.219	[33]

Notes:

* LSAT – a complex metallic oxide with an ideal perovskite structure $La_{0,294}Sr_{0,706}Al_{0,647}Ta_{0,353}O_3$

** barium nitrate gets into the second group of crystals of the given table with $\gamma_{[100]} = 2.35$; $\gamma_{1[110]} = 2.10$; $\gamma_{2[110]} = 1.15$; $\gamma_{[111]} = 1.32$ according to the data on c_{ij} received by Huntington. [11].

Two Grüneisen parameters in the crystallographic direction [110] are conditioned by differently polarized transversal waves of this direction of – $\upsilon_{t1[110]}$ и $\upsilon_{t2[110]}$ with the velocity of the first one being equal to the velocity of transversal wave transmission in the cube direction ($\upsilon_{t1[110]} = \upsilon_{t[100]}$). Both tables are divided into two approximately equal groups of substances (this relation was received spontaneously) if we use two types of inequality between $\gamma_{[hkl]}$. The first group includes substances with values of orientational Grüneisen parameter have the following correlation $\gamma_{[100]} < \gamma_{1[110]} < \gamma_{[111]} < \gamma_{2[110]}$. The second group includes substances with $\gamma_{2[110]} < \gamma_{[111]} < \gamma_{1[110]} < \gamma_{[100]}$.

The criterion of dividing substances according to their anharmonic anisotropy can be put in a slightly different way: the first group includes crystals with the smallest and the second one with the largest values of Grüneisen parameter along the direction [100] as compared with γ along two other directions. If we take a closer look at the values of elastic anisotropy factor and Koshi correlation in table 3 we can see that the most significant general criterion for including the substance into one or another group is value A deviation from one (when A = 1 the crystal is elastically isotropic): $\gamma_{[100]}$ is the smallest among orientational Grüneisen parameters when A > 1 and the largest when A < 1. At the same time the classification of substances according to their chemical bond type, type of crystal lattice or their chemical formula (elementary or complex substances) is not determinative. Although, at a more detailed consideration of the table one can notice some filling-in preferences.

For example, crystals of alkali metals, inert gasses, “classical” semiconductors (Ge, Si, GaAs, InSb), fullerene (C_{60}), LSAT show a minimal interatomic interaction anharmonicity in the cubic plane. Within every part of the table the substances are placed in the order of anharmonicity ascending either along the direction [100] ($\gamma_{[100]}$) or along [110] ($\gamma_{2[110]}$). Among the first ones the most harmonic interatomic interaction in the cubic plane is shown by the lithium crystals ($\gamma_{[100]} \sim 0{,}05$ at liquid nitrogen temperature), among the second ones – the crystals of plumbum selenide in the plane of rhombic dodecahedron ($\gamma_{2[110]} \sim 0{,}11$). On the other end of the anharmonicity scale in the first group are the crystals of nickel nitrate hexaammine. Here the Grüneisen parameters exceed 3 along all the three directions. According to S. Haussühl’s investigations [24] this crystal is characterized by anomalous thermoelastic properties. The second group of crystals is closed by alkali metal cyanides, silver halogenide and sodium superoxide, the last also having $\gamma > 3$ like $Ni(NH_3)_6(NO_3)_2$.. The record anharmonicity values among the given crystals are shown by sodium cyanide ($\gamma_{[100]} = 4.27$, $\gamma_{1[110]} = 4.22$) and $CeRu_2$ ($\gamma_{2[110]} = 4.20$). Two substances – metallic tungsten and superionic phosphate glass ($AgPO_3$) – have an equal anharmonicity value of interatomic interaction along all directions. The results provided by the given tables bring us to the following conclusions. Depending on the elastic anisotropy factor two types of anharmonicity anisotropy are realized in the cubic crystals $A = 2c_{44} / c_{11} - c_{12}$: with A>1 $\gamma_{[100]} < \gamma_{1[110]} < \gamma_{[111]} < \gamma_{2[110]}$ and $\gamma_{2[110]} < \gamma_{[111]} < \gamma_{1[110]} < \gamma_{[100]}$ with A<1. This distribution of cubic crystals in relation to anharmonicity anisotropy does not depend on type of chemical bond or on type of lattice structure.

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