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DEBYE CHARACTERISTIC TEMPERATURE OF CUBIC SOLIDS

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Elastic Debye temperature θ, for 81 cubic crystals (e.g. metals, semiconductors, alkali halides and alum salts) has been calculated by averaging the elastic constants. Nine different averaging procedures have been employed. It is demonstrated that the averaging process developed by us is found to give a better agreement for all the eighty-one cubic solids when compared with the results obtained by Numerical Integration and the experimental calorimetric values.

1. *Introduction*

The Debye characteristic temperature at absolute zero Kelvin, θ, has a great importance in the theoretical and experimental study of the various thermal, optical and electrical properties of crystalline solids. Quite recently it was suggested by Fedorov [1] that this parameter is also related to the atomic number of the constituent atoms of the solids. This demonstrates the universality of this parameter. A look at the literature may reveal that the calculation of θ depends a lot on the symmetry of the crystal concerned. This parameter is proportional to the mean sound wave velocity propagating in the crystal. The sound wave velocities, on the other hand, are related to the elastic constants of the crystal. The calculation of θ thus depends on an averaging of the elastic constants of the crystals alone.

There are two different methods adopted so far to calculate θ, and these are a rigorous approach and an approximate one. In the rigorous approach, emphasis is paid to describing the anisotropic dispersive model of the crystal and enormous arbitrary orientations of sound velocities are considered to estimate the mean sound wave velocity. These calculations are quite involved and are done only on the basis of numerical integration. In the recent past, several workers have carried out such calculations of θ for cubic crystals: Alers [2], Konti and Varshni [3a, b], and Wanner [4].

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The approximate calculation of θ replaces the anisotropic crystal by an ensemble of an aggregate (polycrystal) isotropic crystal. In such cases the averaging process becomes extremely simple and an algebraic expression emerges to calculate θ depending on only two parameters of the solid, the bulk modulus (B) and the rigidity modulus (G). The cubic symmetry implies that B does not depend on the crystal orientations. The dependence of G on crystal orientations gives rise to a different averaging process.

In the literature, more than a dozen averaging procedures have been developed, out of which nine successful ones have been selected here for the computation of θ for 81 cubic solids. While eight different averaging procedures are summarized by Ledbetter [5], the ninth one has been recently proposed by us (Shukla and Padial [6], and Padial and Shukla [7]). Ledbetter [5] has applied the eight different averaging procedures for 25 cubic crystals, while publishing the result for only six selected ones. Shukla and Padial [6] and Padial and Shukla [7] have calculated θ for 42 cubic crystals on their averaging procedure.

In the present paper we have considered the calculation of θ for a set of 81 cubic crystals for which necessary input data existed. For the completeness of the present paper we have also included our previous results (Shukla and Padial [6], Padial and Shukla [7]) here.

2. *Theory*

The Debye characteristic temperature θ is calculated on the basis of the formula

$$\theta = \frac{h}{k}\left[\frac{3n}{4\pi}\,\frac{N\varrho}{m}\right]^{1/3} u_m, \tag{1}$$

where h — Planck's constant; k — Boltzmann's constant; n — number of atoms in the molecule; N — Avogadro's number; ϱ — density of the atom; m — molecular weight of the solid; u_m — average sound wave velocity.

The explicit expression for u_m is given by

$$u_m = \left[\tfrac{1}{3}\sum_{i=1}^{3}\int\frac{d\Omega}{u_i^3 4\pi}\right]^{-1/3}, \tag{2}$$

where u_1 is the quasi-longitudinal wave velocity and (u_2, u_3) are the two quasitransversal wave velocity for each direction of propagation, $d\Omega$ is the increment of the solid angle.

In the rigorous approach, the integral appearing in (2) is solved by numerical integration. In the approximate solution, in which we are interested, u_m is given by

$$3u_m^3 = u_1^3 + 2u_2^3, \tag{3}$$

with

$$\varrho u_1^2 = B + \tfrac{4}{3}G, \tag{4}$$

$$\varrho u_2^2 = \varrho u_3^2 = G. \tag{5}$$

The orientation dependence of G has given rise to different averaging procedures which are given in Table I.

TABLE I

Summary of methods for averaging cubic-symmetry elastic coefficients

Method	Equation for shear modulus G	Key assumption
Voigt [9]	$G_V = \frac{1}{5}(C_{11}-C_{12}+C_{44})$	Uniform local strain, average C_{ij}
Reuss [10]	$G_R = \dfrac{5\,C_{44}(C_{11}-C_{12})}{3\,(C_{11}-C_{12})+4\,C_{44}}$	Uniform local stress, average C_{ij}
Hill arith. [11]	$G = \frac{1}{2}(G_V+G_R)$	Arithmetic average of the results of Voigt and Reuss
Hill geom. [11]	$G = (G_V G_R)^{1/2}$	Geometric average of the results of Voigt and Reuss
Hershey [12]	$G^3+\alpha G^2+\beta G+\gamma = 0$ $\alpha = (5\,C_{11}+4\,C_{12})/8$ $\beta = -C_{44}(7\,C_{11}-4\,C_{12})/8$ $\gamma = -C_{44}(C_{11}-C_{12})(C_{11}$ $+2\,C_{12})/8$	Elastic constants C^0_{ijkl} of an equivalent isotropic aggregate are unaltered by restoring the original elastic constants C_{ijkl} of one crystal in the aggregate.
Hashin, Shtrikman [13]	Lower bound: $(G_2 > G_1)$ $G_2 = G_1+3\left(\dfrac{5}{G_2-G_1}-4\,\beta_1\right)^{-1}$ Upper bound: $G = G_2+2\left(\dfrac{5}{G_1+G_2}-6\,\beta_2\right)^{-1}$ $G_1 = \frac{1}{2}(C_{11}-C_{12})$ $G_2 = C_{44}$ $\beta_1 = -\dfrac{3\,(B+2\,G_1)}{5\,G_1(3\,B+4\,C_1)}$ $\beta_2 = -\dfrac{B+2G_2}{5\,G_2(3\,B+4\,G_2)}$ $B = -\frac{1}{3}(C_{11}+2C_{12})$	Tensor $V_{ijkl}-C^0_{ijkl}$ is positive definite
Aleksandrov [14]	$G = {C_{44}}^{3/5}\left(\dfrac{C_{11}-C_{12}}{2}\right)^{2/5}$	Invariants of C_{ijkl}, written as 6×6 matrices, are equal.
Kroner [15]	$G = G_V\left\{1+\dfrac{5}{2\alpha}\left[1-\frac{1}{5}\times\left(\dfrac{5}{1-6\,\alpha\beta/25}+\dfrac{3}{1+4\,\alpha\beta/25}\right)\right]\right\}$ $\alpha = (B+2G_V)/(B+4\,G_V/3)$ $\beta = [C_{44}-\frac{1}{2}(C_{11}-C_{12})]/G_V$	Elastic moduli at adjacent points are uncorrelated; and $\sum_{j=1,3} \partial r_{ij}(r)/\partial r_j = 0$ that is mechanical equilibrium
Shukla et al. [16]	$G = \dfrac{2\,G_V G_R}{G_V+G_R}$	Harmonic average of the results of Voigt and Reuss.

3. *Numerical computations*

In Tables II and III are presented the input data to calculate θ. Table IV shows the computed θ for 81 cubic crystals by employing all the nine averaging procedures. We have also calculated the deviation of θ from the Numerical Integration value. To do that we have calculated $\frac{\Delta\theta}{\theta} = \frac{\theta - \theta_{\text{exact}}}{\theta}$ versus A $\left(\text{Zener parameter} = \frac{C_{11} - C_{12}}{C_{44}}\right)$ for several cubic crystals. These results are plotted in Figure 1.

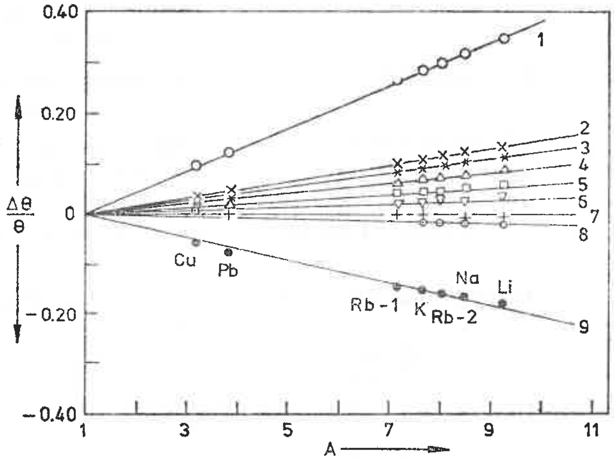

Fig. 1. Errors in elastic Debye temperatures for various averaging methods as a function of elastic anisotropy; *1* — Voigt, *2* — Hershey, *3* — Hill arith., *4* — Aleksandrov, *5* — Hill geom., *6* — Kröner, *7* — Padial et al., *8* — Hashin and Shtrikman, *9* — Reuss

4. *Discussion and conclusion*

A critical study of Table IV shows that the calculated θ by all the nine different averaging procedures are related by the following relation:

$$\theta_{\text{Voight}} > \theta_{\text{Kröner}} > \theta_{\text{Hershey}} > \theta_{\text{Hashin, Sht}} > \theta_{\text{Alek}} > \theta_{\text{Hill arith}} > \theta_{\text{Hill geom}}$$

$$> \theta_{\text{Padial et al.}} > \theta_{\text{exact}} > \theta_{\text{Reuss}} \tag{6}$$

In Table IV we could not show θ_{exact} for all the crystals. Such information was available for only 42 of them. An inspection of equation (6) shows that

$$\theta_{\text{Hill geom}} > \theta_{\text{Padial et al.}} > \theta_{\text{exact}} > \theta_{\text{Reuss}}.$$

This indicates that our averaging procedure predicts results very close to θ_{exact}.

In the earlier work of Ledbetter [5] also Eq. (6) was valid. But the work of Padial et al. [6, 7] was not known to him at that time. Kumazawa [8] had pointed out the need of a theory giving results close to that of Padial et al. [6, 7]. The study of Figure 1 indicates hat the deviation of calculated θ by averaging procedures, to those obtained from Numeri-

TABLE II

Crystal	Structure	Chemical formula	C_{11} (10^{11} dyn/cm^2)	C_{12} (10^{11} dyn/cm^2)	C_{44} (10^{11} dyn/cm^2)	a (10^{-8} cm)	M (a u)	T (K)	References
Copper	fcc	Cu	17.62	12.494	8.177	3.6029	63.54	0	[16]
Silver	fcc	Ag	13.149	9.733	5.109	4.0691	107.87	0	[17]
Gold	fcc	Au	20.163	16.967	4.544	4.0649	196.867	0	[17]
Palladium	fcc	Pd	23.41	17.61	7.12	3.8808	106.40	0	[18]
Nickel	fcc	Ni	26.12	15.08	13.17	3.5160	58.71	0	[19]
Lead	fcc	Pb	5.54	4.52	1.942	4.9146	207.19	0	[20]
Lithium-1	bcc	Li-1	1.481	1.248	1.077	3.50	6.939	78	[21]
Sodium	bcc	Na	0.815	0.679	0.578	4.2349	22.9898	78	[22]
Potassium	bcc	K	0.416	0.341	0.286	5.225	39.102	4.2	[23]
Rubidium-1	bcc	Rb-1	0.316 ± 0.017	0.257 ± 0.38	0.211 ± 0.20	5.585	85.470	0	[24]
Silicon	Diamond	Si	16.772	6.497	8.035	5.4294	28.086	77	[25]
Germanium	Diamond	Ge	13.11	4.923	6.816	5.6524	72.59	77	[27]
Vanadium	bcc	V	23.24	11.936	4.595	3.0352	50.942	0	[28]
Iron	bcc	Fe	23.7	13.5	11.95	2.8607	55.942	0	[29]

TABLE III

(Room temperature values)

Crystal	Chemical formula	C_{11} (10^{11} dyn/cm^2)	C_{12} (10^{11} dyn/cm^2)	C_{44} (10^{11} dyn/cm^2)	ν (g/cm^3)	v_a (10^{-21} cm^3)	References
Ammonium Chloride-1	NH_4Cl-1	3.79	0.97	0.83	1.526	0.02910	[30]
Ammonium Chloride-2	NH_4Cl-2	3.90	0.72	0.68	1.527	0.02908	[31]
Ammonium Bromide-1	NH_4Br-1	3.38	0.91	0.685	2.436	0.03338	[32]
Ammonium Bromide-2	NH_4Br-2	2.96	0.59	0.53	2.429	0.03348	[31]
Barium Nitrate	$Ba(NO_3)_2$	6.04	1.86	1.22	3.24	0.0446	[32]
Gallium Arsenide	GaAs	11.88	5.38	5.94	5.307	0.02263	[33]
Gallium Antimonide	GaSb	8.85	4.04	4.32	5.619	0.02829	[34]
Galena	PbS	10.2	3.8	2.5	7.5	0.026	[35]
Hexamethylenetetramine	$C_6H_{12}N_4$	1.643	0.433	0.515	1.339	0.1738	[30]
Calcium Fluoride	CaF_2	16.44	5.02	3.47	3.18	0.0136	[37]
Magnésia	MgO	28.9	8.8	15.5	3.58	0.0093	[36]
Sodium Chlorate	$NaClO_3$	4.99	1.41	1.17	2.49	0.0355	[38]
Pyrita	FeS_2	36.2	4.64	10.52	5.00	0.0199	[39]
Silver Chloride	AgCl	6.01	3.62	0.625	5.56	0.01214	[39]
Silver Bromide	AgBr	5.62	3.28	0.728	6.473	0.0241	[36]
Strontium Nitrate	$Sr(NO_3)_2$	4.73	2.18	1.46	2.986	0.03928	[43]
Thalium Bromide	TlBr	3.78	1.48	0.756	7.557	0.03090	[39]
Thalium Chloride	TlCl	4.01	1.53	0.760	7.00	0.028	[39]
Zinc Blende	ZnS	10.79	7.22	4.12	4.087	0.0198	[40]
Barium Fluoride	BaF_2	9.01	4.03	2.49	4.83	0.0180	[40]
Indium Antimonide	InSb	6.72	3.67	3.02	5.789	0.03393	[40]
Sodium Bromate	$NaBrO_3$	5.45	1.91	1.50	3.339	0.03752	[38]
Spinel	$MgAl_2O_4$	30.05	15.37	15.86	3.6	0.0094	[47]
Chromite	$FeCr_2O_4$	32.25	14.87	11.67	4.6	0.012	[48]
Alums:	K—Al—S	2.465	1.025	0.865	1.753	0.1123	[38]
	Rb—Al—S	2.535	1.033	0.844	1.884	0.1147	[36]
	Tl—Al—S	2.540	1.130	0.814	2.322	0.1143	[36]
	NH_4—Al—S	2.520	1.090	0.811	1.642	0.1146	[36]
	K—Ca—S	2.356	0.994	0.849	1.808	0.1131	[36]

	C_sCa—S	3.069	1.533	0.816	2.127	0.1192	[36]
	NH_4—Ca—S	2.395	1.029	0.805	1.784	0.1154	[36]
	Rb—In—S	2.366	0.954	0.826	2.107	0.1199	[36]
	C_s—In—S	2.957	1.407	0.816	2.212	0.1231	[36]
	CH_3NH_3—Al—S	2.971	1.782	0.584	1.589	0.1221	[36]
	CH_3—NH_3—Ca—S	2.898	1.686	0.562	1.717	0.1223	[36]
	CH_3—NH_3—Al—S_e	2.786	1.608	0.543	1.827	0.1275	[38]
	C_s—Al—S	3.115	1.539	0.839	1.999	0.1180	[38]
	K—Al—S_e	2.330	0.970	0.775	1.986	0.1187	[36]
	Rb—Al—Sb	2.246	0.995	0.778	2.113	0.1208	[36]
	NH_4—Al—A_e	2.384	1.040	0.752	1.888	0.1203	[38]
	C_s—Ca—S_e	2.530	1.140	0.766	2.342	0.1249	[38]
Magnesium	Mg	6.348	2.594	1.842	1.779	0.0227	[43]
Zinc-1	Zn-1	17.909	3.75	4.595	7.279	0.0149	[43]
Zinc-2	Zn-2	17.696	3.480	4.589	7.279	0.0149	[43]
Aluminum	Al	12.30	7.08	3.09	2.734	0.01637	[43]
Lithium Chloride	LiCl	4.94	2.26	2.49	2.063	0.01702	[51]
Lithium Bromide	LiBr	3.94	1.88	1.91	3.470	0.0208	[51]
Lithium Iodine	LiI	2.85	1.40	1.35	4.061	0.02739	[51]
Lithium Fluoride	LiF	12.46	4.24	6.49	2.646	0.0081	[53]
Sodium Fluoride	NaF	9.71	2.66	2.50	2.79	0.01250	[51]
Sodium Chloride	NaCl	5.750	0.986	1.327	2.241	0.02155	[53]
Sodium Bromide	NaBr	3.87	0.97	0.97	3.203	0.02697	[44]
Sodium Iodide	NaI	2.93	0.73	0.737	3.667	0.0339	[52]
Potassium Fluoride	KF	6.58	1.49	1.28	2.5257	0.01910	[51]
Potassium Chloride-1	KCl-1	4.032	0.66	0.628	1.981	0.03120	[44]
Potassium Chloride-2	KCl-2	4.83	0.54	0.663	2.038	0.0303	[52]
Potasium Iodide	KI	2.71	0.45	0.364	3.13	0.0440	[52]
Potassium Bromide	KBr	4.18	0.56	0.52	2.819	0.0350	[53]
Rubidium Fluoride	RbF	5.7	1.25	0.91	2.83	0.0301	[41]
Rubidium Chloride	RbCl	3.645	0.61	0.475	2.799	0.03587	[51]
Rubidium Bromide	RbBr	3.185	0.48	0.385	3.351	0.04097	[51]
Rubidium Iodide	RbI	2.585	0.375	0.281	3.545	0.04961	[51]
Cesium Bromide	CsBr	3.10	0.84	0.75	4.45	0.0397	[36]
Cesium Chloride	CsCl	3.64	0.92	0.80	3.99	0.0350	[36]
Cesium Iodide	CsI	2.45	0.71	0.62	4.52	0.0477	[36]

TABLE IV

Crystal	Chemical formula	Voight	Kroner	Hershey	Hashin and Shtrikman	Aleksandrov	Hill arith.	Hill geom.	Padial et al.	θ_{exact}	Reuss
Copper	Cu	376.9	346.0	354.0	347.1	351.9	352.0	350.0	348.0	344.0	325.0
Silver	Ag	245.3	228.1	232.5	228.1	230.6	230.6	229.5	228.5	226.2	214.7
Gold	Au	173.5	163.9	165.5	162.6	163.8	163.1	163.1	162.5	161.0	153.3
Palladium	Pd	291.5	277.9	280.9	277.9	279.2	279.1	278.5	277.9	275.6	266.0
Nickel	Ni	502.8	476.0	468.9	480.3	483.2	483.0	482.1	481.2	475.9	462.2
Lead	Pb	117.9	106.9	109.4	105.5	107.7	107.9	106.8	105.9	104.9	96.7
Lithium-1	Li-1	429.1	328.9	361.1	312.4	346.1	357.0	336.3	316.7	317.8	262.7
Sodium	Na	190.6	148.3	161.8	142.1	155.8	159.9	151.7	143.9	144.3	120.5
Potassium	K	114.7	91.0	98.6	88.1	95.3	97.3	93.1	89.1	89.1	75.5
Rubidium-1	Rb-1	69.1	55.5	59.8	54.0	58.0	59.0	56.8	54.6	54.5	46.5
Rubidium-2	Rb-2	70.5	56.1	60.4	53.4	58.1	59.5	56.7	54.0	54.2	45.4
Silicon	Si	659.7	648.8	652.7	651.9	652.5	652.3	652.3	652.2	648.9	644.9
Germanium	Ge	381.4	373.1	376.1	375.4	376.0	375.9	375.8	375.7	373.4	370.3
Vanadium	V	400.9	399.7	400.0	400.0	399.9	399.9	399.9	399.9	399.1	399.9
Iron	Fe	498.1	472.4	476.9	476.7	479.4	475.2	478.4	477.5	472.4	459.4
Ammonium Chloride-1	NH_4Cl-1	284.3	277.5	279.7	279.3	279.7	279.9	279.8	279.7		275.4
Ammonium Chloride-2	NH_4Cl-2	281.5	263.9	269.9	268.4	269.8	270.9	270.4	269.9		259.7
Ammonium Bromide-1	NH_4Br-1	211.4	199.8	203.6	202.6	203.5	204.1	203.8	203.6		196.6
Ammonium Bromide-2	NH_4Br-2	185.6	175.2	178.7	177.9	178.6	179.2	179.0	178.7		172.6
Barium Nitrate	$Ba(NO_3)_2$	206.3	201.4	202.9	202.6	202.8	203.0	202.9	202.9		199.6
Gallium Arsenide	GaAs	353.5	343.4	346.9	345.9	346.6	346.5	346.3	346.9		339.3
Gallium Antimonide	GaSb	272.7	265.5	268.0	267.2	267.7	267.6	267.5	267.4		262.4
Galena	PbS	216.3	215.2	215.5	215.5	215.5	215.5	215.5	215.5		214.8
Hexamethylenetetramine	$C_6H_{12}H_4$	120.0	119.7	119.8	119.8	119.8	119.8	119.8	119.8		119.6
Calcium Fluoride	CaF_2	516.0	505.5	508.7	508.3	508.5	508.9	508.7	508.6		501.6
Magnesia	MgO	951.0	935.3	891.0	940.2	941.2	941.1	941.0	940.1		931.0
Sodium Chlorate	$NaClO_3$	240.8	237.1	238.1	238.1	238.2	238.4	238.3	237.7		235.9
Pyrita	FeS_2	640.6	608.0	585.3	621.3	624.3	625.3	624.9	624.5		609.7
Silver Chloride	AgCl	150.7	146.6	147.3	146.9	146.9	147.2	147.1	147.0		143.6

Silver Bromide	AgBr	138.0	135.9	136.3	136.3	136.2	136.2	136.2	136.2		134.5
Strontium Nitrate	Ar(NO$_3$)$_2$	211.1	210.8	210.9	210.9	210.9	210.9	210.9	210.9		210.7
Thallium Bromide	TlBr	116.9	115.4	115.8	115.7	115.7	115.8	115.8	15.8		114.6
Thallium Chloride	TlCl	128.2	125.8	126.5	126.3	126.4	126.5	126.5	126.4		124.7
Zinc Blende	ZnS	345.0	329.5	333.7	330.9	332.4	332.2	331.7	332.0		318.8
Barium Fluoride	BaF$_2$	288.7	288.7	288.7	288.7	288.7	288.7	288.7	288.7		288.7
Indium Antimonide	InSb	209.8	202.7	204.9	204.0	204.6	204.5	204.3	204.2		199.0
Sodium Bromide	NaBrO$_2$	217.6	217.1	217.3	217.3	217.3	217.3	217.3	217.3		216.9
Spinel	MgAl$_2$O$_4$	918.4	874.4	728.6	882.9	887.4	886.9	885.7	884.5		854.2
Chromite	FeCr$_2$O$_4$	692.5	687.9	575.3	689.1	689.1	689.1	689.1	689.1		685.7
Alums:	K—Al—S	147.5	147.1	147.3	147.3	147.3	147.3	147.3	147.3		147.0
	Rb—Al—S	141.4	141.2	141.3	141.3	141.2	141.2	141.2	141.3		141.1
	Tl—Al—S	124.8	124.6	124.7	124.7	124.7	124.7	124.7	124.7		124.5
	NH$_4$—Al—S	148.4	148.3	148.3	148.3	148.3	148.3	148.3	148.3		148.3
	K—Ga—S	142.6	142.1	142.3	142.2	142.2	142.2	142.2	142.2		141.8
	Gs—Ga—S	131.4	131.3	131.6	131.4	131.4	131.4	131.4	131.4		131.3
	NH$_4$—Ga—S	140.5	140.2	140.3	140.2	140.2	140.2	140.2	140.2		140.0
	Rb—In—S	129.2	129.0	129.0	129.0	129.9	129.0	129.0	129.0		
	Cs—In	127.5	127.5	127.5	127.5	127.5	127.5	127.5	127.0		127.5
	CH$_3$NH$_3$—Al	130.4	130.4	130.4	130.4	130.4	130.4	130.4	130.4		130.4
	CH$_3$—NH$_3$—Ga—S	124.4	124.4	124.4	124.7	124.4	124.4	124.4	124.4		124.3
	CH$_3$NH$_3$—Al—Se	117.0	117.0	117.0	117.0	117.0	117.0	117.0	117.0		117.0
	Cs—Al—S	137.8	137.8	137.7	137.7	137.8	137.8	137.8	137.8		137.7
	K—Al—Se	130.1	130.0	130.0	130.0	130.0	130.0	130.0	130.0		129.9
	RbAl—Se	123.8	123.3	123.5	123.5	123.5	123.5	123.5	123.4		123.1
	NH$_4$—Al—Se	131.5	131.4	131.5	131.5	131.5	131.5	131.5	131.5		131.4
	Cs—Ga—Se	115.7	115.4	115.3	115.3	115.4	115.4	115.4	115.4		115.1
Magnesium	Mg	379.4	379.4	379.4	379.4	379.4	379.4	379.4	379.4		379.4
Zinc-1	Zn-1	371.7	365.5	367.7	367.4	367.7	367.8	367.8	367.8		363.9
Zinc-2	Zn-2	371.6	365.3	367.4	367.3	367.5	367.7	367.7	367.8		363.7
Aluminium	Al	429.8	428.9	429.2	429.1	429.1	429.1	429.1	429.1	430.5	428.4
Lithium-2	Li-2	442.8	337.5	371.5	319.9	355.7	367.4	345.3	324.4		268.3
Lithium Chloride	LiCl	402.8	390.7	394.9	393.6	394.5	394.4	394.2	394.0	425.92	385.8
Lithium Bromide	LiBr	254.9	247.4	219.9	249.1	249.7	249.6	249.4	249.3	274.07	244.1
Lithium Iodide	LiI	180.8	175.5	177.2	176.6	177.0	177.0	176.9	176.8		173.1
Lithium Fluoride	LiF	748.4	735.1	740.0	739.0	739.9	739.8	739.7	739.6	733.07	731.0

TABLE IV (continued)

Crystal	Chemical formula	Voight	Kroner	Hershey	Hashin and Shtrik-man	Alek-sandrov	Hill arith.	Hill geom.	Padial et al.	θ_{exact}	Reuss
Sodium Fluoride	NaF	460.8	456.2	457.7	457.5	457.6	457.7	457.7	457.7	491.85	454.6
Sodium Chloride	NaCl	331.1	320.9	324.6	324.0	324.6	324.8	324.8	324.7	322.43	318.6
Sodium Bromide	NaBr	210.1	207.2	208.2	208.2	208.2	208.2	208.2	208.2	224.36	206.3
Sodium Iodide	NaI	158.5	156.4	157.1	157.0	157.1	157.1	157.1	157.1	167.51	155.7
Potassium Fluoride	KF	329.7	316.4	320.8	319.8	320.7	321.3	321.1	320.6	327.58	312.6
Potassium Chloride-1	KCl-1	242.2	221.7	228.8	226.9	228.8	230.2	229.5	228.8		217.5
Potassium Chloride-2	KCl-2	263.1	230.8	242.6	239.3	242.7	245.5	244.1	242.6	236.10	226.4
Potassium Iodide-1	KI	137.4	122.4	127.5	125.9	127.5	128.8	128.1	127.4	130.77	119.4
Potassium Bromide	KBr	194.0	167.9	177.2	174.3	174.2	179.7	178.3	177.0	172.15	163.9
Rubidium Chloride	RbCl	179.5	158.9	166.0	163.7	165.8	167.7	166.7	165.0	168.80	154.9
Rubidium Bromide	RbBr	145.9	126.3	133.2	130.9	133.1	135.0	134.0	132.9	136.34	122.9
Rubidium Iodide	RbI	118.3	99.6	106.2	103.8	106.1	108.1	107.0	105.8	107.81	96.7
Cesium Bromide	CsBr	138.3	136.3	137.0	136.9	136.9	137.0	137.0	137.0	149.47	135.7
Rubidium Fluoride	RbF	240.4	224.2	229.5	228.0	229.3	230.4	229.9	229.4	211.70	219.9
Cesium Chloride	CsCl	162.3	158.4	159.7	159.5	159.7	159.8	159.7	159.7	159.39	157.2
Cesium Iodide	CsI	115.3	114.2	114.6	114.6	114.6	114.6	114.6	114.6	126.21	113.9

cal Integration, is quite insensitive for A below 3 and amounts to as much as 35% for $A = 9.2446$ (Lithium) by different averaging procedures; Voight (35%), Reuss (17%), Hill arith. (12%), Hill Geom. (5.8%), Aleksandrov (8.8%), Kröner (3.5%), Hashin (1.7%), Padial et al. (0.35%). The procedure employed by us gave the lowest deviation when compared to others.

Some comments which go against the physical reality of our averaging model are:

a) We have no theoretical justification for it. But the same is true for $\theta_{\text{Hill arith.}}$ and $\theta_{\text{Hill geom.}}$, which have been proclaimed successful in the literature.

b) We have assumed that the crystal is composed of isotropic Debye continuum. But similar comments can also be put forward for all the averaging procedures discussed above.

REFERENCES

[1] T. G. Bystrova, F. I. Fedorov, *Dokl. Akad. Nauk SSSR* **215**, 1336 (1974).
[2] A. Alers, *Physica Accoustics*, vol. IIIB, edited by W. P. Mason, Academic Press Inc., New York, pp. 1–42.
[3] A. Konti, Y. P. Varshni, a) *Can. J. Phys.* **47**, 2021 (1969), b) *Can. J. Phys.* **49**, 3115 (1971).
[4] R. Wanner, *Can. J. Phys.* **48**, 1270 (1970).
[5] H. M. Ledbetter, *J. Appl. Phys.* **44**, 1450 (1973).
[6] M. M. Shukla, N. T. Padial, *Rev. Bras. de Fisica* 39 (1973).
[7] N. T. Padial, M. M. Shukla, *Ciẽncia e Cultura* 977 (1975).
[8] M. Kumazawa, *S. Geophy. Rs.* **74**, 5311 (1969).
[9] W. Voigt, *Ann. Phys.* (*Leipzig*) **38**, 573 (1889).
[10] A. Reuss, *Z. Angew. Math. Phys.* **9**, 49 (1929).
[11] R. Hill, *Proc. Phys. Soc. London* **A65**, 349 (1952).
[12] A. V. Hershey, *J. Appl. Mech.* **21**, 2361 (1954).
[13] Z. Hashin, S. Shtrikman, *J. Mech. Phys. Solids* **10**, 343 (1962).
[14] K. S. Aleksandrov, *Sov. Phys. Dokl.* **10**, 893 (1966).
[15] E. Kröner, *J. Mech. Phys. Solids* **15**, 319 (1967).
[16] W. C. Overton Jr., J. Gaffney, *Phys. Rev.* **98**, 969 (1955).
[17] J. R. Neighbours, G. A. Alers, *Phys. Rev.* **111**, 107 (1958).
[18] J. A. Rayne, *Phys. Rev.* **118**, 1545 (1960).
[19] G. A. Alers, J. R. Neighbours, H. Sato, *Phys. Chem. Solids* **13**, 40 (1960).
[20] D. L. Waldorf, G. A. Alers, *Appl. Phys.* **33**, 3266 (1962).
[21] H. C. Nash, C. S. Smith, *Phys. Chem. Solids* **9**, 133 (1959).
[22] M. E. Diederich, J. Trivisonno, *J. Phys. Chem. Solids* **27**, 637 (1966).
[23] W. R. Marquardt, J. Trivisonno, *J. Phys. Chem. Solids* **26**, 273 (1965).
[24] C. A. Roberts, R. Meister, *Phys. Chem. Solids* **27**, 1401 (1966).
[25] E. J. Gutman, J. Trivisonno, *Phys. Chem. Solids* **28**, 805 (1967).
[26] H. J. McSkimin, P. Andreatch, *J. Appl. Phys.* **35**, 2161 (1964).
[27] H. J. McSkimin, P. Andreatch, *J. Appl. Phys.* **34**, 651 (1963).
[28] G. A. Alers, *Phys. Rev.* **119**, 1532 (1960).
[29] A. E. Lord Jr., D. N. Berthers, *J. Appl. Phys.* **36**, 1620 (1965).
[30] S. Haussuhl, *Acta Crystallogr.* **13**, 685 (1960).
[31] R. Sundarã Rao, T. Balakrishmann, *Proc. Natl. Inst. Sci. India* **16**, 235 (1950).
[32] S. Bhagavantam, R. Sundarã Rao, *Curr. Sci.* **17**, 296 (1948).
[33] E. Goens, J. Weerts, *Z. Phys.* **37**, 321 (1936).
[34] T. Bateman, H. McSkimin, J. Whelan, *J. Appl. Phys.* **30**, 544 (1959).

[35] B. Ramachamdra Rao, a) *Proc. Indian Acad. Sci.* **A22**, 194 (1954); b) *Curr. Sci.* **19**, 148 (1950).

[36] S. Haussuhl, a) *Z. Kristallogr.* **111**, 321 (1959); b) **110**, 1 (1958); c) *Forstschr. Mineva* **36**, 75 (1958).

[37] D. Huffman, M. Norwood, *Phys. Rev.* **117**, (1969).

[38] R. Bechmann, a) *Proc. Phys. Soc.* (London) **B63**, 577 (1950); b) **B64**, 323 (1951); c) **B65**, (1952); d) *Phys. Rev.* **110**, 1061 (1958).

[39] D. Arenberg, *J. Appl. Phys.* **21**, 941 (1950).

[40] S. Bhagavantam, *Proc. Indian Acad. Sci.* **A41**, 72 (1955).

[41] M. Durand, *Phys. Rev.* **50**, 449 (1936).

[42] D. Tannhauser, L. Brunnerand, A. Lawson, *Phys. Rev.* **102**, 1276 (1956).

[43] S. Bhimasenachar, T. Sechagiri Rao, *Proc. Natl. Inst. Sci. India* **16**, 235 (1950).

[44] C. Raman, D. Krishnamurti, *Proc. Indian Acad. Sci.* **A42**, 111 (1955).

[45] L. Bergmann, a) *Ultrasonics* Russian translation, IL, Moscow 1957; b) *Z. Naturforsch.* **a12**, 229 (1957).

[46] R. F. S. Hearmon, a) *Rev. Mod. Phys.* **18**, 409 (1946), b) *Adv. Phys.* **5**, 323 (1956).

[47] R. Verma. *J. Geophys. Res.* **65**, 2 (1960).

[48] M. Doraiswant, *Proc. Indian Acad. Sci.* **A25**, 413 (1947).

[49] R. Sundara Rao, a) *Proc. Indian Acad. Sci.* **A28**, 185 (1948); b) **A29**, 352 (1949); c) **A31**, 365 (1950); d) **A30**, 173 (1949); e) **A32**, 275 (1950); f) **A40**, 150 (1954); g) **A30** (1949); h) *Curr. Sci.* **18**, 204 (1949); i) **18**, 336 (1949); j) **17**, 50 (1948); k) **16**, 91 (1947).

[50] R. Potter, *Phys. Rev.* **103**, 47 (1956).

[51] A. V. Shubnikov, E. E. Flint, G. B. Boki, *Principles of Crystallography*, Kv. Akad. Nauk SSSR 1940, in Russian.

[52] N. Norwood, C. Briscoe, *Phys. Rev.* **112**, 45 (1958).

[53] G. A. Alers, J. R. Neighbours, *Rev. Mod. Phys.* **31**, 675 (1959).