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A SIMPLIFIED METHOD FOR CALCULATING THE DEBYE TEMPERATURE FROM ELASTIC CONSTANTS

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Abstract—The Reuss–Voigt approximations are well known methods whereby the isotropic polycrystalline elastic constants can be calculated from the single crystal elastic constants. It is shown here that the Reuss and the Voigt approximations can be used to estimate, accurately, the mean sound velocity of a crystal. Using this method, the Debye Temperature, which is proportioned to the mean sound velocity, can be determined without recourse to the published tables or high speed computers. This approximation is valid for all crystal classes.

I. INTRODUCTION

THE Debye temperature is an important parameter of a solid. It is found in equations describing properties which arise from atomic vibrations, and in theories involving phonons.

One of the standard methods of calculating the Debye temperature is from elastic constant data, since θ is proportional to the sound velocity (averaged) v_m by the equation

$$\theta = \frac{h}{k}\left[\frac{3q}{4\pi}\frac{N\rho}{M}\right]^{1/3} v_m \tag{1}$$

and where h/k have the usual meanings of quantum mechanics, N is Avogadro's number, ρ is the density, M is the molecular weight of the solid and q is the number of atoms in the molecule ($q = 2$ for NaCl, 3 for CaF_2).

The use of equation (1) is often hindered by the problem of computing v_m. Since θ is a scalar, it follows that v_m must also be a scalar, and herein lies the difficulty of this method. The stress is a tensor quantity, and for each direction in a crystal, there are three velocities each of which is a complicated function of the stress components. The expression$^{(1)}$ for v_m is

$$v_m = \left(\frac{1}{3}\sum_{i=1}^{3}\int_V \frac{1}{v_i^3}\frac{d\Omega}{4\pi}\right)^{-1/3} \tag{2}$$

This integral is solved by numerical methods as follows: the three sound velocities, v_1, v_2, v_3 are found in an arbitrary direction and then stored; the process is repeated for a large sample of directions, throughout space; and a numerical summation using Simpson's rule made in place of the volume integral.

The equation shown above is the rigorous way to find the mean sound velocity, but it is impractical to use except by means of high speed computer methods. The solution of the equation requires knowledge of the elastic constants of the crystal.

This paper will be concerned with a substitute for equation (2) to determine the mean sound velocity. Only one class of symmetry—that of isotropy—lends itself to an easy calculation of v_m, for in that case equation (2) reduces to the simple form

$$v_m = \left(\frac{1}{3}\left[\frac{2}{v_s^3} + \frac{1}{v_l^3}\right]\right)^{-1/3} \tag{3}$$

In this case, isotropy includes truly isotropic materials like glass, and polycrystalline materials where the shear and longitudinal sound velocities, v_s and v_l are invariant with direction.

The idea presented in this paper is that the experimentally measured velocities v_s and v_l of the polycrystalline solid can be closely approximated by a simple, but well known, averaging scheme of the single crystal elastic constants, yielding $\bar{v}_s$ and $\bar{v}_l$. Further, it is proposed that the averaged velocities when used in equation (3) yield a value

$$\bar{v}_m = \left(\frac{1}{3}\left[\frac{2}{\bar{v}_s^3}+\frac{1}{\bar{v}_l^3}\right]\right)^{-1/3}, \tag{4}$$

which is little different from the value v_m calculated by the rigorous method, equation (2).

The particular averaging scheme used and recommended will be presented in Section II. A description of the detailed calculations involved in proving that $\bar{v}_m$ is a close approximation of v_m is presented in Section III. The results of several hundred crystals will be presented in Section IV. The implications and benefits to the materials scientist resulting from the use of $\bar{v}_m$ will be discussed in Section V. Numerous tables of the elastic constants used are collected in several appendices.

II. LITERATURE BACKGROUND FOR THE AVERAGING SCHEME

The recommended scheme for averaging the elastic constants and sound velocities is a synthesis of several ideas which have appeared in the literature. It will be called hereafter the VRHG approximation (VOIGT, REUSS, HILL and GILVARRY).

That part of the VRHG approximation due to VOIGT(1) is a simple linear relation between the isotropic shear and bulk moduli of a polycrystalline composite and the single crystal moduli (c_{ij}'s represent stiffness)

$$K_V = f_1(c_{ij}) \tag{5}$$

$$G_V = f_2(c_{ij}) \tag{6}$$

Equations (5) and (6) are expanded in Appendix I.

A different linear relation between the isotropic shear and bulk moduli and the single crystal elastic moduli was derived by REUSS(1) (s_{ij}'s represent compliance.)

$$K_R = f_3(s_{ij}) \tag{7}$$

$$G_R = f_4(s_{ij}) \tag{8}$$

Equations (7) and (8) are expanded in Appendix I.

Using energy considerations HILL(2) proved that the Voigt and Reuss equations represent upper and lower limits of the true polycrystalline constants, and he recommended that a practical estimate of the polycrystalline moduli were the arithmetic means of the extremes,

$$K_H = 1/2(K_R+K_V) \tag{9}$$

$$G_H = 1/2(G_R+G_V) \tag{10}$$

The probable values of the average sound velocities are computed from (9) and (10) as follows

$$\bar{v}_s = \sqrt{(G_H/\rho)} \tag{11}$$

$$\bar{v}_l = \sqrt{(K_H+4/3G_H)/\rho} \tag{12}$$

Finally the approximate sound velocity is found by using the values computed from (11) and (12) in (4), and the Debye temperature then is easily computed by (1). GILVARRY used virtually the same method to approximate the Debye temperature of sodium,(3) and deserves credit for insight to the method.

The point is that the VRHG approximation (equations (4) through (12)) for computing $\bar{v}_m$ requires only about ten minutes on the slide rule and is good for any symmetry, whereas the exact method using equation (1) requires numerical methods on a high speed computer, or access to tables such as have been published by DELAUNAY for some of the high symmetry solids.(4)

It is the purpose of this paper to demonstrate that the VRHG approximation is not only practical but quite accurate. In fact, the VRHG approximation was applied to the data of over 200 crystals of all classes. In all but a very few cases, which will be later discussed, the error of the approximation was less than the probable error of the experimental results themselves.

There are other approximations in the literature, but these, in the author's opinion, either lack generality or accuracy. For example, a number of "mathematical" approximations to equation (1) which have been explored by BLACKMAN(5) are sometimes accurate but cannot be applied generally—typically one technique is accurate for a certain class, but not for another. One approximation due to Post, is general to all crystal classes, but it yields results which are considerably more erroneous than the VRHG approximation.

The VRHG approximation as applied to the trigonal crystal alumina, is presented in detail in Appendix I.

III. PROVING THE VRHG APPROXIMATION

The proof consists of an analytical part and an experimental part. The analytical proof is that $\bar{v}_m$, equation (4), is close in value to v_m, equation (2), when the same elastic constant data are used in both calculations. The experimental proof is that the computed Young's modulus and Shear modulus, E_H and G_H from equations (9) and (10) which average the elastic constants of the single crystal, are close in value to the measured E and G of the highly dense polycrystalline phase which is hot pressed from the crystalline powder.

A. *Analytical proof*

A program for the IBM 7090 was written to solve equation (2) for v_m. The following is read into the computer program as input data: the elastic constants, c_{ij}, or the elastic compliances, s_{ij}; the density; the molecular weight of the crystal; the limits of integration shown in equation (1)—(for a cubic crystal the limits correspond to a one-fourth of the sphere); and the increment of angles in the numerical integration (usually 5°).

Given the elastic constants the elastic compliances are computed, or vice versa by a subroutine which inverts any reasonably sized $n \times n$ matrix.

Next the solution of the equations of motion of elastic waves is found. This involves solving the determinant for a particular direction of wave propagation. In the general case, each element of the determinant involves all elastic constants.(7) To get the velocities the eigenvalues of the determinant are obtained by a sub-routine which used double precision statistical methods.

The three velocities allow the integrand in equation (2) to be defined. The integrand is stored, and the program repeated for a new direction. The integration is replaced by a summation which sums the integrands according to Simpson's rule. The program is arranged so that any fraction of the sphere can be chosen for the integration (quadrant, octant, etc.) and the correct multiplication factor is retained. As a typical case, integrating one-fourth of a sphere at 5° intervals in the polar angles θ and ϕ takes about 10 sec on the IBM 7090.

If θ is the polar angle, and ϕ the azimuthal angle, the volume of integration is then $\sin \theta d\theta d\phi$. The limits on integration for θ is always 90°. The limits on ϕ are 30° for hexagonal crystals, 45° for tetragonal, 60° for trigonal, 90° for orthorhombic and 180° for monoclinic.

After v_m, equation (2), is computed; the Voigt and Reuss elastic moduli, equations (4) to (8), are computed and finally various sound velocities, including $\bar{v}_m$, equation (4).

The program was checked by comparing the Debye temperature θ from the computed v_m, with the Debye temperature given by others using various methods where in all cases the same elastic constants were used for the solid. (It was not always possible to ascertain whether the density was the same as that used by other authors.) This crosscheck is shown in Table 1.

Table 1. *Comparison of the value of the Debye temperature from this IBM program with values in the literature*

Element	Density	Mol. Wt.	θ (here)	θ (published)	Source of Information
Ag	10·635	107·88	226·5	226·4	Alers and Neighbors
Al	2·734	26·965	426·7	426·6	Huntington
Au	19·488	197·00	161·7	161·6	Alers and Neighbors
Cu	9·02	63·54	344·5	345·3	Overton and Gaffney
Li	0·545	6·94	326·0	335·9	Alers and Neighbors
Ni	8·968	58·71	476·2	476·2	Alers and Neighbors
Th	11·787	232·05	164·2	164·2	Armstrong Carlson, Smith
V	6·022	50·95	393·2	394·0	Bolef and Menes
Hexagonal					
Beryl	1·848	9·013	1463·5	1462.0	Smith
Cd	8·719	112·41	214·2	213·0	Garland and Silverman
Mg	1·779	24·32	386·0	385·8	Alers
Zn	7·134	65·38	328·3	328·1	Alers and Neighbors

The print out of the program is: (1) the basic information including crystal class, author and publication (source of elastic constant data), temperature of measurement, density, and instructions for the integration; (2) the elastic constants themselves in matrix form; (3) the Voigt, Reuss and Hill approximations for the isotropic moduli; (4) the final results, including the rigorous average sound velocity v_m, the approximate average sound velocity, the Debye temperature, and the approximation error.

$$\Delta = (\bar{v}_m - v_m)/v_m \tag{13}$$

The analytical proof is completed by showing that Δ is about the same order as the uncertainty in measuring elastic constants. This will be demonstrated in some detail in Section IV.

B. *Experimental proof*

When pure and finely divided crystalline powder is hot pressed, in the appropriate way, the result is a bar of the material which is uniform in density, and isotropic, which approaches the density of the single crystal, and which is large enough to make resonance measurements of the elastic moduli. If a sufficient number of these bars are prepared, with a variety of values of porosity all close to zero, the isotropic elastic constants of the polycrystalline materials at zero porosity can be obtained by extrapolation.

The experimental proof is completed by showing that the extrapolated values of the elastic moduli of the hot pressed solids (zero porosity) are close to the values obtained by the Hill mean, equations (9) and (10) from single crystal elastic constant data.

This proof has already been established for several polycrystalline metals by HILL.$^{(6)}$ Data on oxides are rarer. The polycrystalline elastic constants of hot pressed alumina were reported in the Master's thesis (1961) of DAE-HYUN CHUNG of Alfred University.$^{(7)}$ Chung's results are shown in Table 2. The values in the parenthesis are the writer's extrapolations. These results are plotted in Figs. 1 and 2. The results in the last line above are to be compared with the values predicted from the elastic constants of trigonal alumina, as shown in Appendix I.

Table 2. *Measured isotropic moduli of polycrystalline alumina*

Density	Porosity (%)	Young's modulus (kbars)	Shear modulus (kbars)
3·835	3·79	3571	1439
3·848	3·46	3607	1462
3·885	2·53	3702	1503
3·900	2·16	3764	1538
3·914	1·81	3784	1549
3·947	0·98	3928	1591
3·986	(0)	(4050)	(1650)

Table 3. *Predicted isotropic moduli of polycrystalline alumina*

	Young's modulus (kbars)	Shear modulus (kbars)
Max. (Voigt)	4083	1660
Mean (Hill)	4027	1634
Min. (Reuss)	3972	1607

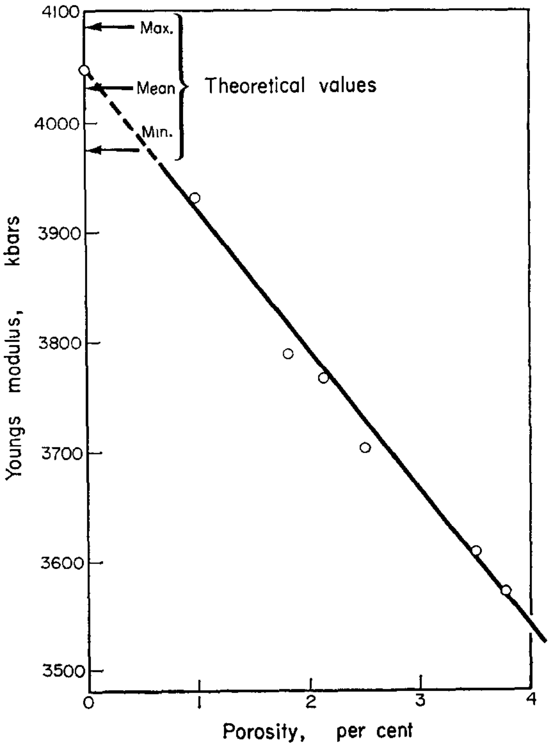

FIG. 1. Variation of Young's modulus with porosity for sintered alumina (after CHUNG$^{(8)}$).

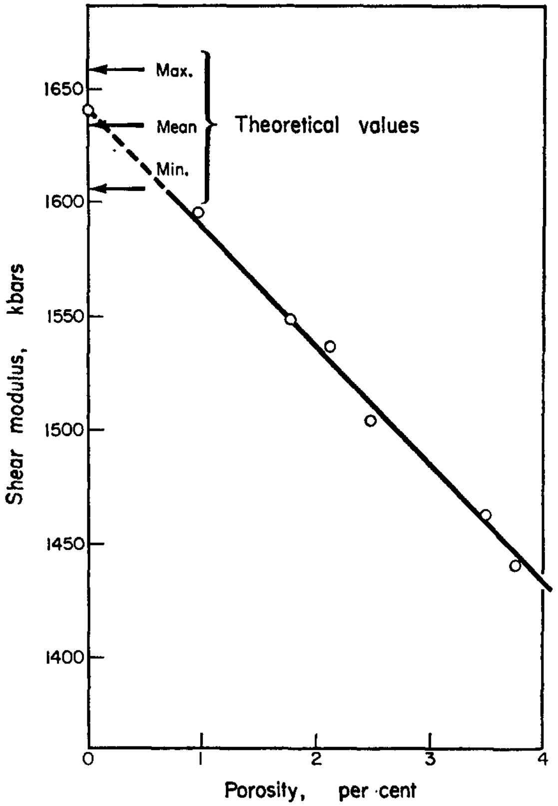

FIG. 2. Variation of shear modulus with porosity for sintered alumina (after CHUNG(8)).

The agreement between the mean values in Table 3 and the last row in Table 2 is remarkably good. Further work must, of course, be done on non-metallic polycrystalline solids, but the experimental proof can be considered as established, at least tentatively.

IV. THE VRHG APPROXIMATION FOR SIX CRYSTAL CLASSES

The IBM program for the calculation of v_m, $\bar{v}_m$, and Δ (equation (13)) was used for a number of sets of elastic constant data obtained by reading the literature, including 106 cubic crystals, 60 hexagonal crystals, 19 trigonal crystals, 18 tetragonal crystals, 19 orthorhombic crystals and one monoclinic crystal.*

A. *Cubic system*

Numerous approximations exist in the literature for the value of v_m for cubic symmetry. In the author's opinion none of the approximations are more accurate than the VRHG approximation.

It turns out that for most cubic crystals, the error Δ is less than 1 per cent. Those crystals in which it is more than 2 per cent are all highly anisotropic. A convenient method of defining anisotropy, following HILL,(2) is the spread of the computed shear modulus computed by the Reuss and Voigt limits, the degree of anisotropy is:

$$\delta = \frac{1}{2}\frac{G_v - G_R}{G_H} = \frac{G_v - G_R}{G_v + G_R} = \frac{3[2c_{44}-(c_{11}-c_{12})]^2}{12c_{44}^2+38c_{44}(c_{11}-c_{12})+3(c_{11}-c_{12})^2} \qquad (14)$$

It turns out that whenever δ is less than 20 per cent, Δ is less than 2 per cent This is illustrated in Fig. 3. Here it is shown that the results cluster around two simple curves, the upper composed mostly of the halide crystals, the lower being elements and other compounds besides halides. This relationship between Δ and δ permits a rather exact estimate of the Debye temperature from the elastic constants of a cubic crystal. The author recommends the following procedure. Compute $\bar{v}_m$ by the VRHG method. Compute δ by equation (14). If δ is less than 20 per cent, Δ is less than 2 per cent. If δ is more than 20 per cent, the value of Δ can be estimated, it being approximately 1/10 δ and positive.

B. *Hexagonal system*

In Appendix II, typical examples of the results obtained for 60 hexagonal crystals are presented. The maximum error in Δ is 3 per cent for ice. Cadmium and zinc are fairly anisotropic, and the value of Δ is about 2-1/2 per cent. But in general, the VRHG approximation is quite good for this class, and in most cases better than the probable accuracy in measuring elastic constants.

C. *Trigonal system*

In Appendix II, typical examples of the results obtained for 19 trigonal crystals are presented. Here the elastic constant data from one author compared with another are not always in agreement, and the value of Δ takes on a

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* The full tabular data can be obtained by writing the author.

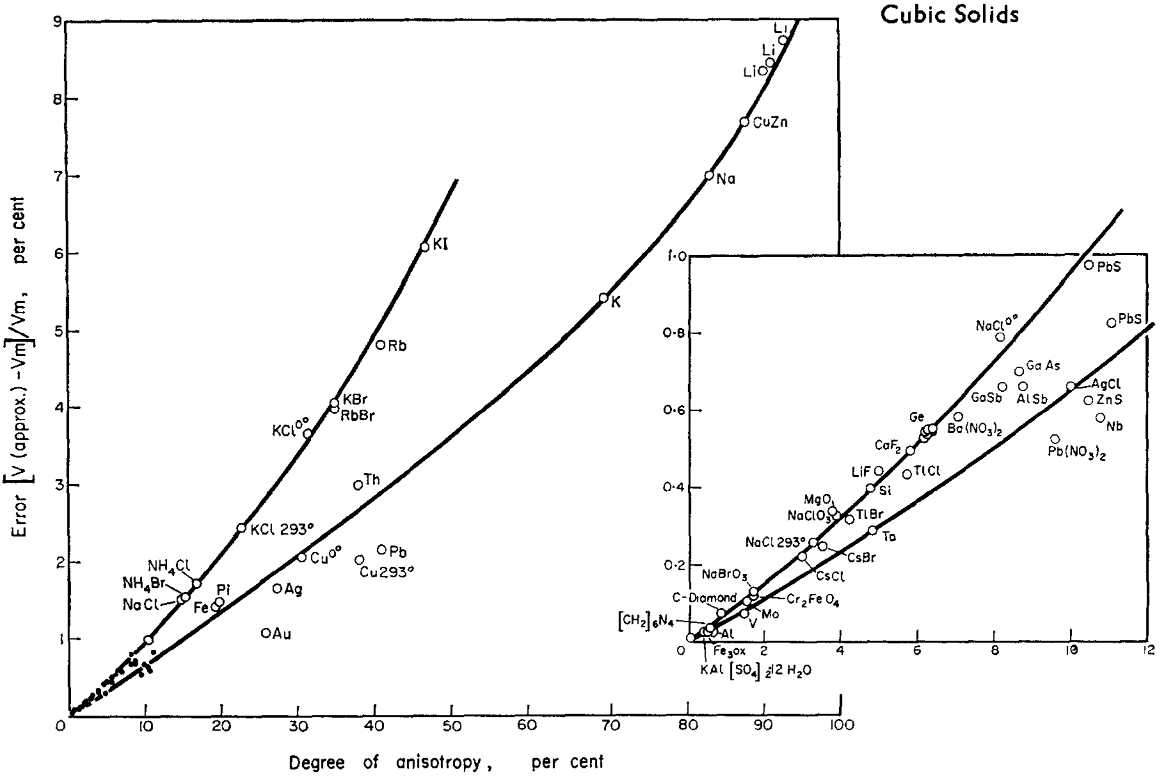

FIG. 3. Degree of anisotropy per cent.

number of values. Whenever, the elastic constant data are very good, the value of Δ is low. For instance, when the most recent measurements on alumina by Wachtmann and Teft in which the elastic constants were very carefully cross checked for internal consistency are used, Δ is only −1·36 per cent. Older data for alumina shows Δ to be as much as 8·5 per cent. The elastic constant data for Koga for α-quartz is very reliable, and in this case Δ is −2·2 per cent, whereas other data yields a higher error. The worst value calculated by the VRHG method is for mercury, where Δ is 25 per cent. However, these elastic constant data were reported in 1934, and should be rechecked. In the author's opinion, Δ is less than 2·5 per cent for this class whenever there has been careful cross checking of the elastic constant data by the experimenters.

D. *Tetragonal system*

In Appendix II, typical values obtained for 18 tetragonal crystals are presented. Again, whenever there is evidence of internal consistency of the elastic constants, the value of Δ is small. For instance, the values for v_m for Rutile are $5{\cdot}652\times10^5$ and $5{\cdot}557\times10^5$ from Birch, and from Joshi and Mutri respectively, revealing a discrepancy of about 2 per cent in the primary measurement data. Yet, the difference between the approximate and the rigorous values of v_m are 2 per cent, using the same data in both cases. Consequently, the approximation is about as accurate as the data itself. On the other hand, the values for the crystal KH_2PO_4 vary considerably from author to author, and correspondingly the value of Δ is somewhat higher. In the author's opinion, the VRHG approximation is reliable for this class.

E. *Orthorhombic system*

The results for the orthorhombic system are especially interesting as shown by the example in Appendix II. All values of Δ are low except for $KB_5O_8 \cdot 4H_2O$ which is 4·3 per cent. Especially interesting is the value for uranium in which Δ is below 1 per cent. The elastic constants for this solid were accurately determined and carefully checked for internal consistency. It would appear that the VRHG approximation is reliable for this class.

F. *Monoclinic system*

The data for one monoclinic crystal was found, which is presented in Appendix II.

G. *Temperature dependence of v_m*

The elastic constant data at absolute zero are needed for the determination of the Debye temperature. The elastic constant data at room temperature are more often available. There are a number of instances in the literature where the elastic constants at room temperature are accurately integrated by equation (2), to obtain a value of the Debye temperature, and this Debye temperature is then compared with the corresponding Debye temperature calculated from specific heat measurements. This value of θ thus obtained is meaningful only to the extent the v_m is independent of temperature. The temperature dependence of v_m was checked for three solids where the elastic constants were well determined from room temperature. In these three solids, Beryl, Cd, and Zn, the change of the rigorous value of v_m between room temperature and 0°, and the VRHG approximation is shown in Table 4, and in Fig. 4.

Table 4. Comparison of Δ with temperature extrapolation error (velocity in 10^5 cm/sec)

	Beryl	Cd	Zn
Absolute zero value of v_m	9·871	1·995	2·773
Room temp., value of v_m	9·752	1·812	2·551
Per cent change of v_m from R.T. to 0°K (in %)	1·0	0·93	0·63
Δ at absolute zero (in %)	0·088	0·248	0·22
Δ at room temp (in %)	0·082	0·254	0·241

It is evident that for most solids, especially where the anisotropy is not excessive, that the true value of the Debye temperature is off by as much when the room temperature values are used in equation (2), as when the VRHG approximation in place of equation (2).

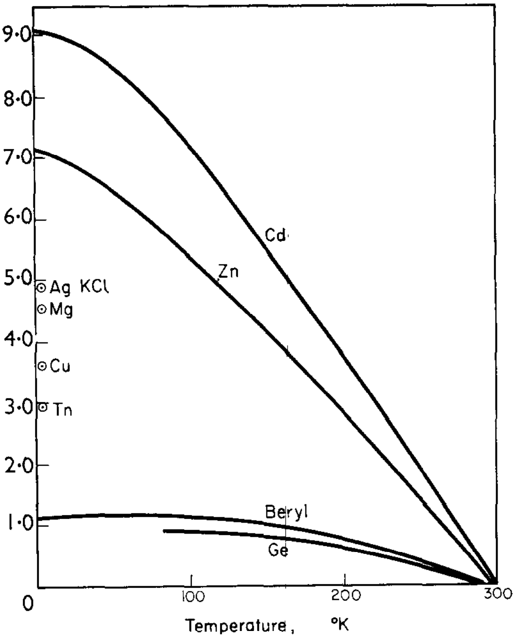

FIG. 4. Per cent change in value of mean sound velocity v_m from room temperature value.

V. DISCUSSION

It is concluded that the elastic constants of a well sintered solid can be predicted if the single crystal constants are known. The difference between predicted and observed values will result from the method of sintering.

It is also concluded that a solid does not have to be grown in the form of a single crystal in order to measure isotropic elastic parameters. The solid can be hot pressed from fine powder into a dense specimen and the appropriate experiments made. The values measured will be the integrated values of the single crystal and suitable for determining Debye θ.

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Note added in Proof: The VRHG approximation has been found accurately applicable to MgO at all temperatures, reported recently by Mr. D. H. Chung, (1963) *Phil. Mag.*, in press.

APPENDIX I

Computation of elastic constants of alumina

Equations for all crystal classes

Bulk Modulus (maximum) by the Voigt approximation:

$$K_V = 1/9(c_{11}+c_{22}+c_{33})+2/9(c_{12}+c_{23}+c_{13})$$

Shear Modulus (maximum) by the Voigt approximation:

$$G_V = 1/15(c_{11}+c_{22}+c_{33})- 1/15(c_{12}+c_{23}+c_{31}) + 1/5(c_{44}+c_{55}+c_{66})$$

Bulk Modulus (minimum) by the Reuss approximation:

$$1/K_R = (s_{11}+s_{22}+s_{33})+2(s_{12}+s_{23}+s_{13})$$

Shear Modulus (minimum) by the Reuss approximation:

$$15/G_R = 4(s_{11}+s_{22}+s_{33})-4(s_{12}+s_{23}-s_{13}) +3(s_{44}+s_{55})+s_{66})$$

Reduced equations for trigonal class:

$$K_V = 1/9(2c_{11}+c_{33})+2/9(c_{12}+2c_{13})$$

$$G_V = 1/15(2c_{11}+c_{33})-1/15(c_{12}+2c_{13}) +1/5(2c_{44}+c_{66})$$

$$1/K_R = (2s_{11}+s_{33})+2(s_{12}+2s_{13})$$

$$15/G_R = 4(2s_{11}+s_{33})-4(s_{12}+2s_{13}) +3(2s_{44}+s_{66})$$

Data for Al_2O_3, by WACHTMAN and TEFT, *J. Res. NBS*, **64A**, 3 (1960):

$$c_{11} = 4968 \text{ kbars} \qquad s_{11} = 0{\cdot}235\times 10^{-3}(\text{kbars})^{-1}$$

$$c_{33} = 4981 \qquad s_{33} = 0{\cdot}217$$

$$c_{44} = 1474 \qquad s_{44} = 0{\cdot}694$$

$$c_{66} = 1666 \qquad s_{66} = 0{\cdot}614$$

$$c_{12} = 1636 \qquad s_{12} = -0{\cdot}072$$

$$c_{13} = 1109 \qquad s_{13} = -0{\cdot}036$$

Bulk Modulus (kbars):

$$\text{Max: } K_V = 2514$$

$$K_R = 2509$$

$$\text{Mean: } K_H = 1/2(2514+2509) = 2512$$

Shear Modulus (kbars):

$$\text{Max: } G_V = 1660$$

$$\text{Min: } G_R = 1607$$

$$\text{Mean: } G_H = 1634$$

Young's Modulus (kbars):

$$\text{Max: } E_V = \frac{9K_V\times G_V}{3K_V+G_V} = 4083$$

$$\text{Min: } E_R = 3973$$

$$\text{Mean: } E_H = 4028$$

Longitudinal Modulus (kbars):

$$M_H = K_H+\tfrac{4}{3}G_H = 4692$$

Sound Velocity ($\rho = 3{\cdot}986$):

$$\bar{v}_s = 6{\cdot}41\times 10^5 \text{ cm/sec}$$

$$\bar{v}_l = 10{\cdot}91\times 10^5 \text{ cm/sec}$$

$$\bar{v}_m = 7{\cdot}09\times 10^5 \text{ cm/sec}$$

$$\theta = 1045^\circ\text{K}$$

APPENDIX II

Velocity units 10^5 cm/sec

Hexagonal system

Crystal	Accurate v_m	Approx. $\bar{v}_m$	Per cent Error
$BaTiO_2$	3·280	3·283	0·09
Beryl, 0°K	9·870	9·879	0·08
Beryl, 300°K	9·751	9·760	0·09
Beryl	9·360	9·314	0·09
Cd, 0°K	2·000	2·04	2·50
Cd, 300°K	1·813	1·859	2·46
CaBa	2·584	2·597	0·4
CdS	2·110	2·105	0·22
Co	3·392	3·412	0·59
ice	0·761	0·785	3·07
Mg, 0°K	3·67	3·672	0·03
Mg, 293°K	3·514	3·516	0·04
SiO_2	4·457	4·462	0·1
Y, 0°K	2·774	2·775	0·03
Y, 300°K	2·640	2·641	0·02
Zn, 4·2°K	2·732	2·795	2·29
ZnO	3·188	3·187	−0·02
Trigonal system			
Al_2O_3	7·190	7·093	−1·36
$AlPO_4$	3·644	3·531	−3·10
Bi	1·302	1·261	−3·16
$CaCO_3$	4·017	3·898	−2·94
Fe_2O_3	4·729	4·674	−1·17
Hg	0·559	0·698	24·96
$(NaBr)C_6H_{12}O_6$	2·243	2·254	0·50
$(NaCl)C_6H_{12}O_6$	2·280	2·270	0·50
$NaNO_2$	3·408	3·604	5·7

Trigonal system

Crystal	Accurate v_m	Appox. $\bar{v}_m$	Per cent Error
Sb	1·925	2·049	6·2
SiO_2	4·570	4·468	−2·22
Tourmaline	5·733	5·743	0·17
Tetragonal system			
$BaTiO_2(E)$	3·875	3·93	1·45
$BaTiO_3(D)$	3·439	3·523	2·42
In, 0°	1·12	1·03	8·7
In, 293°K	0·901	0·925	2·73
KH_2PO_4	2·758	2·860	3·73
$NH_4H_2PO_4$	2·664	2·788	4·62
$NiSO_46H_2O$	2·540	2·567	1·05
Sn	1·996	1·997	0·06
TiO_2	5·652	5·745	1·66
$ZrSiO_4$	2·216	2·267	2·29
Orthorhombic system			
$BaSO_4$	2·463	2·491	1·14
$CaCO_3$	3·942	3·991	1·26
$KB_5O_8 \cdot 4H_2O$	2·264	2·361	4·28
$MgSO_4 \cdot 7H_2O$	2·543	2·586	1·23
$SrSO_4$	1·979	2·080	5·10
S_8	1·978	2·019	2·11
Topaz	6·331	6·341	0·15
$ZnSo_4 \cdot 7H_2O$	2·758	2·794	1·33
U	7·286	7·349	0·86
Olivine	5·408	5·472	1·17
Monoclinic system			
$Li_2SO_4H_2O$	3·29	3·30	3·0