JOURNAL OF MATERIALS SCIENCE 28 (1993) 6050–6057

The technical constants of some cubic and non-cubic materials

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The elastic constants (technical constants) for some polycrystalline materials of cubic and non-cubic (hexagonal, tetragonal, trigonal and orthorhombic) symmetry have been computed by a new averaging scheme involving the squared reciprocal sound velocities. The computed values are compared with those from the averaging scheme of Hill. An examination of the data reveals that the predictions for the shear modulus and Young's modulus of cubic materials agree with those of Hill within 0.01% and 0.5%, respectively, while the new scheme overestimates the values of the bulk modulus for cubic materials by 3.8% on average. For the non-cubic materials, the predicted values of shear modulus, Young's modulus and bulk modulus are within 2.7%, 0.3% and 13.5%, respectively, of Hill's values.

1. Introduction

The elastic coefficients relating stress and strain for polycrystalline materials and single crystals have wide-ranging uses in science and engineering. For example, they are of fundamental importance in characterizing many mechanical, physical, optical, piezoelectric and thermal properties. For polycrystalline materials, the elastic coefficients can be specified either by Lame's constants or by any two of the following parameters: shear modulus, G, Young's modulus, E, bulk modulus, B, and Poisson's ratio. Standard elasticity procedures are used to relate the two chosen parameters. For single crystals, the stiffnesses, C_{ij}, or the compliances, S_{ij}, specify the elastic coefficients. In the present context, we refer to elastic constants for single crystals and to technical constants for polycrystalline materials.

Recently, a new method was presented [1] for using sound velocity measurements to determine the Debye temperature. It deals with an evaluation of the Debye temperature by direct integration and the adoption of the Debye theory of lattice vibration as an averaging scheme to predict the Debye temperature from sound velocity measurements. The scheme also has the advantage of being able to predict the technical constants. Moreover, it involves the averaging of the squared reciprocal velocities on which the technical constants actually depend. In contrast, Middya *et al.* [2] and Ledbetter and Naimon [3] used averaging schemes that involved the average velocity and cubed reciprocal velocity, respectively. Voigt [4] and Reuss [5] used classical averaging schemes to calculate G, E and B, and Hill [6] used their geometric average values. We have made [1] a comparison of the results of their computational scheme to predict the Debye temperature with the results from schemes by Alers [7] and Wanner [8] and with experimental data for cubic and non-cubic materials. It was concluded that the advantage of our computational procedure comes from the fast rate of convergence and the ability of the code to compute the Debye temperature for all crystal symmetries. It was noted that Alers' code is only capable of computing the Debye temperature for cubic, hexagonal and tetragonal symmetries, while Wanners' code is suitable only for cubic symmetries.

In this paper, we examine the values of the technical constants (G, E and B) computed by the new averaging scheme for some materials of cubic and non-cubic (i.e. of hexagonal, tetragonal, trigonal and orthorhombic) symmetry. The computed values are compared with those from the averaging scheme of Hill [6] (geometric mean value of the Voigt and Reuss values) and with the experimental data where available.

2. Computational procedures

The procedures perform the numerical integration of the phase velocities over the quadrant bounded by the crystallographic directions [1 0 0], [0 1 0] and [0 0 1]. By summing up the values of the integrands using the well-known Simpson's one-third rule [9] with two nested loops, the following equations are evaluated

$$(1/V^3)^{-1/3} = [\int(V_L^{-3}(\theta,\psi) + V_{t1}^{-3}(\theta,\psi) + V_{t2}^{-3}(\theta,\psi))\sin\psi\,d\psi\,d\theta/4\pi]^{-1/3} \quad (1)$$

$$1/\rho V_L^2 = (\rho)^{-1/2}\int V_L^{-2}(\theta,\psi)\sin\psi\,d\psi\,d\theta/4\pi \quad (2)$$

$$1/\rho V_t^2 = (\rho)^{-1/2}\int[V_{t1}^{-2}(\theta,\psi) + V_{t2}^{-2}(\theta,\psi)]\sin\theta\,d\psi\,d\theta/4\pi \quad (3)$$

where V is the velocity of sound, V_L is the quasi-longitudinal velocity of sound, V_{t1} and V_{t2} are the

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quasi-transverse velocities of sound, ρ is the mass density, θ is the polar angle, and ψ is the angle between the z-axis (in the Cartesian system) and the propagating wave.

The inner loop performs the integration at constant ψ, while the outer loop finishes the integration. After this, the average phase velocities are calculated with the mean value theorem. The values of G, E and B are calculated from

$$G = [(1/\rho V_{\mathrm{t}}^2)^{-1}]/2 \quad (4)$$

$$E = [3(1/\rho V_{\mathrm{L}}^2)^{-1} - 4G]/[\{(1/\rho V_{\mathrm{L}}^2)^{-1}\}/G - 1] \quad (5)$$

$$B = (1/\rho V_{\mathrm{L}}^2)^{-1} - 4G/3 \quad (6)$$

The input elastic constants are values of C_{ij} taken from the data compiled by Simmons and Wang [10], Alexandrov and Ryzhova [11], Meissner and coworkers [12, 13], and Hearmon [14, 15]. Full details of the averaging scheme are given elsewhere [1].

3. Results and discussion

3.1. Technical constants for some cubic materials

To assess how the results of the present averaging scheme rate with other methods and how well they compare with experiment, the same input stiffnesses listed by Middya *et al.* [2] and Ledbetter and Naimon [3] are used. Table I lists the experimental values of shear modulus, G, and the values calculated by Middya *et al.* [2] Ledbetter and Naimon [3], Hill [6] and the present method, and the percentage difference between the present method and that of Hill. The corresponding information pertinent to Young's modulus and the bulk modulus is presented in Tables II and III.

Several major observations can be made from these tables. First, the method of Ledbetter and Naimon is insufficient to predict the technical constants, even though the invariance relation of the bulk modulus is preserved. This fact is clearly demonstrated in Table I, where the predicted shear moduli deviate substantially from the experimental values for most of the materials under consideration. The data marked by the letter b seem to suggest otherwise. However, the bulk of these materials possess significant isotropy. The experimental value of 45.1 GPa for G for copper, which compares well with the calculated value, appears to be in definite error, because it differs substantially from the other two values listed by Middya *et al.* (48.3 and 47.7 GPa). Further illustration of the shortcoming of the method of Ledbetter and Naimon is obtained by noting that the calculated value of G for silver deviates approximately 3% from the experimental value. The deviation of their calculated values from the experimental ones becomes greater as the degree of anisotropy increases. For example, the method of Ledbetter and Naimon predicts a value of 7.4 GPa for the shear modulus of lead, which is approximately 14% lower than the experimental value. The underlying assumption for the averaging method of Ledbetter and Naimon is that the average reciprocal cubed velocities are equal for single crystals and polycrystals of the same materials. That is

$$V^{-3} = (1/3)[(B + 4G/3)^{-1.5} + 2G^{-1.5}]\rho^{1.5} \quad (7)$$

for polycrystals and

$$V^{-3} = (1/3)(V_{\mathrm{L}}^{-3} + V_{\mathrm{t1}}^{-3} + V_{\mathrm{t2}}^{-3}) \quad (8)$$

for single crystals.

Anderson [18] attempted unsuccessfully to use Equation 7 in lieu of Equation 8 using values for B and G calculated from the arithmetic mean values of Voigt and Reuss as suggested by Hill, to compute V and, therefore, the Debye temperature. He showed that the margin of error between the mean velocity values computed from Equations 7 and 8 may be as big as 10% and is additive. Clearly then, the assumption of equal mean reciprocal cubed velocities for single crystals and polycrystals of the same materials does not hold with respect to experimental or calculated values for the technical constants. The reason why the two equations are not equivalent may be deduced from their origin. Equation 7 assumes the existence of one longitudinal mode and two equal transverse modes in a solid material made up of aggregates regarded as grains oriented randomly. By contrast, Equation 8 assumes the existence of three vibrational modes, one longitudinal and two different transverse ones, in a solid crystal regarded as a solid continuum. Therefore, the equations are not equivalent because they describe waves propagating in two basically different solids.

Second, neither the current averaging scheme nor that of Middya *et al.* is capable of predicting entirely satisfactory results for the bulk modulus. This is clearly demonstrated in Table III, where it is shown that the difference between the calculated and experimental values for B may differ by more than 10%. Generally, the Hill method (in which B is taken to be a scalar which is rotationally invariant and may be calculated either from the Voigt or Reuss averaging schemes) seems to yield results which agree with the experimental values far better than those of the current method and that of Middya *et al.* The occasional lack of success of the Hill method (i.e. Voigt or Reuss) appears to be due to experimental error. The bulk modulus is usually determined via C_{11} and C_{12} and it is widely understood that the determination of C_{12} is subject to relatively large experimental error, because it has to be determined indirectly. This is especially true when the elastic moduli are determined from the elastic compliances (see Hearmon [14]).

At first, one might be inclined to suggest that the lack of success of the present method in calculating the bulk modulus is due to computing the mean value for the longitudinal velocity. One might also question the validity of the assumptions made in the present averaging scheme. To explore these thoughts, we rewrite the expressions for the longitudinal velocity in terms of the technical constants

$$\rho V_{\mathrm{L}}^2 = (B + 4G/3) \quad (9)$$

$$\rho V_{\mathrm{L}}^2 = G[(4G - E)/(3\mathrm{G} - E)] \quad (10)$$

TABLE I Comparison of the experimental and calculated values for shear modulus, G, for some cubic materials

Material	G (10^{11} Pa)					Difference[g] (%)
	Experimental	Midya *et al.* [2]	Ledbetter and Naimon [3]	Hill [6]	Present	
Cu[a]	0.477[c] 0.451[d] 0.455[e]	0.4826	0.4559	0.461	0.4659	+ 1.1
Cu[b]	0.483[c]	0.483	0.4557	0.465	0.4657	+ 0.2
Ag[b]	0.294[c]	0.3045	0.2858	0.2847	0.2858	+ 0.4
Ag[a]	0.291[c] 0.288[d] 0.286[e]	0.2911	0.2735	0.2825	0.2836	+ 0.4
Au[a, b]	0.2817[c] 0.278[c] 0.276[d] 0.277[e]	0.282	0.2643	0.2706	0.2743	+ 1.4
Ni[a]	0.785[c] 0.75[d] 0.77[e]	0.7844	0.7637	0.7768	0.7737	− 0.4
Pb[a]	0.086[c]	0.088	0.074	0.082	0.084	+ 2.4
V[a]	0.474[c]	0.4754	0.4647	0.475	0.4747	− 0.1
Nb[a]	0.376[c] 0.375[d] 0.366[e]	0.3791	0.3647	0.3761	0.3747	− 0.4
Ta[a]	0.700[c] 0.687[d]	0.6931	0.6795	0.6904	0.6895	− 0.1
Mo[a]	1.18[c] 1.158[d] 1.197[e]	1.228	1.2141	1.2271	1.2241	− 0.2
W[a]	1.526[c] 1.514[c] 1.53[d] 1.485[e]	1.5217	1.5117	1.5217	1.5217	0
Pt[a]	0.637[c] 0.622[c] 0.61[e]	0.6383	0.6247	0.6344	0.6347	+ 0.1
MgO[b]	1.306[c]	1.3092	1.2924	1.3101	1.3024	− 0.6
MgO[a]	1.292[f]	1.3017	1.2852	1.3029	1.2952	− 0.6
CaF_2[b]	0.409[c]	0.4256	0.4119	0.4252	0.4219	− 0.8
CaF_2[a]	0.411[f]	0.4123	0.3996	0.4118	0.4096	− 0.5
β-ZnS[b]	0.317[c]	0.3311	0.3148	0.3263	0.3248	− 0.5
β-ZnS[a]	0.318[f]	0.3158	0.2979	0.3094	0.3076	− 0.6
ZnSe[a, b]	0.289[c] 0.285[f]	0.2977	0.2799	0.2925	0.2899	− 0.9
CdTe[a, b]	0.138[c] 0.139[f]	0.1428	0.138	0.1404	0.1401	− 0.1
						Average = 0 (+ 0.01)

[a] Data used by Ledbetter and Naimon [3].
[b] Data used by Middya *et al.* [2].
[c] See [2].
[d] See [16].
[e] See [17].
[f] See [3].
[g] Diff. = 100 (present value − Hill's value)/(Hill's value).

Table II lists the values of Young's modulus calculated from Equation 10 using the current averaging scheme, and the methods of Middya *et al.* and Hill. The table also lists the experimental values of Young's modulus from the equation

$$E = 9BG/(3B + G) \quad (11)$$

where the values of G and B represent the experimental values listed in Tables I and III, respectively. When there is more than one value listed for G or B, the arithmetic mean value is used.

Close examination of the results in Table II shows that the agreement between the experimental values of Young's modulus, E, and the current calculated values, is excellent. Because the same longitudinal velocity is used to calculate E and B, the apparent discrepancy may not be attributed to the method of computing V_L, nor to the underlying assumption of the existence of quasi-longitudinal waves which travel with their own velocity. Assuming there is agreement with this notion, then the source of the discrepancy for the calculated values of bulk modulus in Table III

TABLE II Comparison of the experimental and calculated values for Young's modulus for some cubic materials. Young's modulus, E, is calculated from $E = 9BG/(3B + G)$

Material	E (10^{11} Pa)				Difference[c] (%)
	Experimental	Middya *et al.* [2]	Hill [6]	Present	
Cu[a]	1.2668	1.3047	1.2521	1.2665	+ 1.2
Cu[b]		1.3084	1.2501	1.2639	+ 1.1
Ag[b]	0.7959	0.8336	0.8054	0.8125	+ 0.9
Ag[a]		0.7989	0.7744	0.7805	+ 0.8
Au[a, b]	0.7924	0.8034	0.7714	0.7827	+ 1.5
Ni[a]	2.0699	2.0704	2.0433	2.0468	+ 0.2
Pb[a]	0.2422	0.2466	0.2312	0.2372	+ 2.6
V[a]	1.2956	1.2948	1.2934	1.2931	0
Fe[a]	2.1269	2.1099	2.0704	2.0769	+ 0.3
Nb[a]	1.0507	1.0605	1.0514	1.0491	− 0.2
Ta[a]	1.8844	1.8623	1.8536	1.8540	0
Mo[a]	3.1011	3.2006	3.1942	3.1924	− 0.1
W[a]	3.9062	3.9028	3.9029	3.9029	0
Pt[a]	1.7585	1.7817	1.7707	1.7724	+ 0.1
MgO[b]	3.0904	3.1184	3.0980	3.1080	+ 0.3
MgO[a]		3.0734	3.0527	3.0639	+ 0.4
CaF_2[b]	1.0779	1.0977	1.0919	1.0901	− 0.2
CaF_2[a]		1.0761	1.0719	1.0704	− 0.1
ZnSe[a, b]	0.7434	0.7735	0.7526	0.7570	+ 0.6
CdTe[a, b]	0.3747	0.3865	0.3784	0.3799	+ 0.4
					Average = + 0.5

[a, b] See Table I.

[c] Difference = 100 (present value − Hill's value)/(Hill's value).

TABLE III Comparison of the experimental and calculated values for bulk modulus for some cubic materials. For the sources of the experimental values, [2]

Material	B (10^{11} Pa)				Difference[c] (%)
	Experimental	Middya *et al.* [2]	Hill [6]	Present	
Cu[a]	1.376 1.3974	1.4667	1.370	1.4583	+ 6.5
Ag[a]	1.027	1.0438	1.0027	1.0523	+ 5.0
Au[a, b]	1.766	1.7715	1.735	1.7808	+ 2.6
Ni[a]	1.90	1.914	1.8467	1.9254	+ 4.3
Pb[a]	0.438	0.447	0.4274	0.4516	+ 5.7
V[a]	1.537	1.5601	1.5857	1.5909	+ 0.3
Fe[a]	1.795	1.8807	1.7833	1.8969	+ 6.4
Nb[a]	1.736	1.7444	1.7183	1.7494	+ 1.8
Ta[a]	2.04	1.9824	1.9610	1.9863	+ 1.3
Mo[a]	2.779	2.7105	2.6827	2.7144	+ 1.2
W[a]	3.055 2.963 3.296	2.9895	2.9895	2.9895	0
Pt[a]	2.838	2.8459	2.8270	2.8501	+ 0.8
MgO[a]	1.641 1.663	1.5037	1.549	1.6097	+ 3.9
CaF_2[a]	0.999	0.9198	0.90	0.9224	+ 2.5
	0.438	0.447	0.4274	0.4516	+ 5.7
β-ZnS[a]	0.775 0.766	0.7302	0.6927	0.7364	+ 6.3
ZnSe[a]	0.598	0.6475	0.5953	0.6557	+ 10.2
CdTe[a]	0.424	0.4985	0.4238	0.4429	+ 4.5
					Average = + 3.8

[a, b] See footnotes b and c in Table I.

[c] Difference = 100 (present value − Hill's value)/(Hill's value).

must come from error propagation in Equation 9. We can demonstrate this by rearranging Equation 11 for B in terms of E and G

$$B = EG/[3(3G - E)] \tag{12}$$

and pursuing an example. The current calculated values of G and E for copper are 46.59 and 126.68 GPa, respectively. Insertion of these values in Equation 12 yields a value of 150.29 GPa for B. Suppose that we allow a + 1% error in computing G. The value of G would then be 47.05 GPa and the resulting value for B would be 137.13 GPa. Such a value agrees quite well with the experimental value and also with that predicted by the Voigt method and, consequently, by the Hill method. With this value of G and the original value for B in Equation 11, on the other hand, the resulting value for E would be 125.55 GPa. This value differs from the current calculated value by less than 1%. The foregoing suggest that the nature of the equations employed to calculate B leads to error propagation.

The trend in Table III is that the current averaging scheme always yields values for B that are higher than the experimental values. It is suggested, therefore, that B could be computed from Equation 12 after E and G are computed from their respective velocities with G increased by 1%. Of course, such calculation is not without its dangers. Therefore, B is best calculated as an invariant scalar either by the Voigt or Reuss method.

Third, the agreement between the experimental values and the calculated current values of G and E (Tables I and II) is excellent and by far better than that of Middya *et al.* For some of the materials marked by the letter a, the averaging scheme of Middya *et al.* appears to yield calculated values that agree better with the experimental values than with those of the present scheme. This is a misleading appearance because some of the elastic moduli listed by them seem to be questionable. For example, of all the data listed by Simmons and Wang [10] for silver, they chose the set of data that differs greatly from the rest of the data listed. When the elastic moduli for silver listed by Ledbetter and Naimon (also from Simmons and Wang) are used, the resulting calculated values for E and G for silver are about 2.5% and 3%, respectively, higher than those predicted by the current method. These values do not compare well with the experimental data: the values of E and G are about 4.7% and 4.8% higher than the arithmetic average of the experimental values. This trend exists throughout Tables II and III. Thus, the method of Middya *et al.* suffers in two main ways: (1) from disagreement of their results with those of the present averaging scheme and the experimental data, and (2) their method uses the average of the reciprocal phase velocities while the technical constants are actually proportional to the squared velocities.

Fourth, the agreement in results for G and E of the present averaging scheme and the geometric mean values of Hill is rather remarkable, despite the fact that the starting premises of the two schemes are entirely different. The maximum disagreement between the two approaches is less than 1.5%, excluding the results for lead, where the disagreement is about 2.5%. It must be emphasized, however, that the present method predicts values for G and E that agree better with experimental observations than those of the Hill method.

The results of this research show that averaging methods derived from sound velocity measurements follow the scheme of the averaging methods based on static deformation of materials. That is, averaging the reciprocal velocity tends to yield results representing an upper bound for the technical constants similar to that of Voigt's classical work. Averaging the cubed reciprocal velocity, on the other hand, tends to yield results representing a lower bound for the technical constants similar to that of Reuss' classical work. However, the results of the upper and lower bounds predicted from sound velocity measurements are closer to observations than those of Voigt and Reuss.

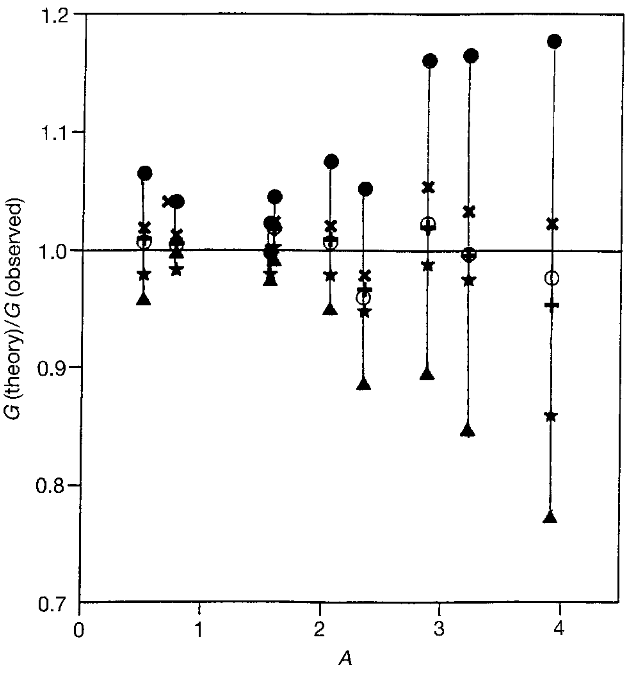

Figure 1 Values of the ratio shear modulus (theory) to shear modulus (observed) as a function of the Zener elastic anisotropy factor A ($= 2C_{44}/(C_{11} - C_{12})$) for some cubic materials. (●) [4], (▲) [5], (×) (2), (★) [3], (+) [6], (○) present work, (——) ideal value.

As expected, this work has shown that averaging the squared reciprocal velocity on which the technical constants actually depend appears to be superior to previous averaging schemes, not only in terms of agreement with observation, but also in terms of simplicity. Moreover, the current averaging scheme is self-consistent because it applies to all crystal symmetries. This finding is depicted in Fig. 1 where the ratio of G (theoretical) to G(observed) is plotted versus the Zener anisotropy factor A ($= 2C_{44}/(C_{11} - C_{12})$. As can be seen in the figure, the present method yields ratios falling between those of Middya *et al.* and Ledbetter and Naimon, and closer to observation than either of theirs. The concordance between the present method and Hill's is also illustrated in the figure.

3.2. Technical constants for some non-cubic materials

The results for the calculation of the shear modulus G are presented in Table IV. The table lists the experimental values of G (column 2), the computed values using Hill's method (column 3), the computed values using the new averaging scheme (column 4), and the percentage deviation (column 5) between the present

TABLE IV Comparison of the values of shear modulus obtained by Hill's method and by the present method with experimental data for some hexagonal, trigonal, tetragonal and orthorhombic materials

Material	G (10^{11} Pa)			Difference[a] (%)	Reference
	Experimental	Hill [6]	Present		
Cd	0.241	0.2392	0.2308	– 3.5	[17]
Co	0.764	0.8233	0.8172	– 0.7	[17]
	0.750	0.570	0.5735	+ 0.6	[16]
Mg	0.1736	0.1721	0.1720	– 0.1	[17]
	0.174	0.1737	0.1736	– 0.1	[16]
Zn	0.372	0.3893	0.3805	– 2.3	[16]
Zr	0.341	0.3602	0.3594	– 0.2	[16]
Hf	0.53	0.5581	0.5577	– 0.1	[17]
Ti	0.3934	0.4335	0.4328	– 0.2	[17]
Sb	0.2	0.2264	0.2194	– 3.1	[17]
		0.2698	0.2524	– 6.5	
Bi	0.1285	0.1173	0.1158	– 1.3	[17]
	0.1290	0.1249	0.1209	– 3.2	[16]
Se	0.217	0.1086	0.0947	– 14.7	[16]
		0.0659	0.0584	– 12.8	
Te	0.154	0.1444	0.1293	– 11.7	[16]
In	0.0373	0.469	0.480	+ 2.4	[17]
Sn	0.204	0.2287	0.2281	– 0.3	[17]
	0.1844	0.1775	0.1831	+ 3.2	[16]
α-U	0.7044	0.7921	0.7814	– 1.4	[17]
	0.7360				[16]
Ga	0.43	0.3684	0.3666	– 0.5	[17]
	0.346				[16]
				Average: – 2.7	

[a] Difference (%) = 100 (present value – Hill's value)/(Hill's value).

TABLE V Comparison of the values of Young's modulus obtained by Hill's method and by the present method with experimental data for some hexagonal, trigonal, tetragonal and orthorhombic materials

Material	E (10^{11} Pa)			Difference[a] (%)	Reference
	Experimental	Hill [6]	Present		
Cd	0.623	0.6244	0.6141	– 1.6	[17]
	0.5528	0.5693	0.5588	– 1.8	[19]
Co	2.001	2.1586	2.1503	– 0.4	[16]
	2.073	1.5597	1.5583	– 0.1	[19]
Mg	0.444	0.4445	0.4445	0	[16]
	0.435	0.4465	0.4465	0	[19]
Zn	0.9259	1.0758	1.0927	+ 1.6	[19]
	0.922	0.9746	0.9825	+ 0.8	[17]
Zr	0.9467	0.9598	0.9587	– 0.1	[19]
	0.9560				[16]
Hf	1.370	1.4294	1.4292	0	[17]
	1.382				[19]
Ti	1.161	1.1461	1.1457	0	[19]
	1.06				[17]
Sb	0.5494	0.5660	0.5645	– 0.3	[17]
	0.780	0.6661	0.6624	– 0.6	[19]
Bi	0.318	0.3165	0.3141	– 0.8	[19]
	0.340	0.333	0.3276	– 1.6	[16]
Se	0.580	0.2618	0.2548	– 2.7	[16]
		0.1688	0.1639	– 3.0	
Te	0.412	0.3601	0.3508	– 2.7	[16]
In	0.1105	0.1356	0.1388	+ 2.4	[19]
	0.105				[16]
Sn	0.55	0.5976	0.5974	0	[17]
	0.4146	0.4804	0.4968	+ 3.4	[19]
α-U	1.766	1.9217	1.9259	+ 0.2	[17]
	1.864				[16]
Ga	1.20	0.9108	0.911	0	[17]
	0.965				[16]
				Average: – 0.3	

[a] Difference (%) = 100 (present value – Hill's value)/(Hill's value).

results and those of Hill. Similar information is listed in Tables V and VI for Young's modulus, E, and the bulk modulus, B, respectively. An examination of these tables reveals that the concordance of the values of shear modulus and Young's modulus between the present scheme and that of Hill's is rather good. The average deviations for the values of G and E are -2.7% and -0.3%, respectively. Complete comparison between the experimental values and the computed values for either averaging scheme seems to be unobtainable because of the discrepancies among the experimental values. Broadly speaking, the agreement between the calculated values and the experimental values is satisfactory. The fact that the calculated values are in agreement with observation for most of the materials considered suggests that the apparent discrepancies between theory and observation may be due to metallurgical effects (mainly texture) in polycrystalline materials and/or experimental error in measuring the elastic constants. As was the case for cubic symmetry, the present averaging scheme yields theoretical values for the bulk modulus, B, that are higher than the observed values (by 34.9% on the grand average) as well as higher than the theoretical values of Hill (by 13.5% on the grand average), and his method yields theoretical results in better agreement with observations than the present method.

Again, it may be argued that some of the discrepancy between the present theoretical and observed values of B may be an artefact and is largely due to error propagation because of the nature of the equation used to compute B. This is especially true in the cases of antimony, selenium and tellurium. For these materials, the stiffnesses producing the large percentage deviations appear to be questionable because the margins of difference between Hill's theoretical values and the observed values are objectionably large in comparison with the results of the other data sets for these materials and for the other materials considered here. Additionally, the discrepancy between the theoretical values of B and the experimental values may reflect the experimental difficulties connected with measuring the bulk modulus. For example, the experimental value of B quoted for selenium dates back to 1915. While the age of a datum does not *per se* permit questions of precision of measurement, the following quotients of the Young's modulus, E, shear modulus, G, and bulk modulus, B, for selenium, tellurium and antimony do cast some doubt on the reliability of the experimental value of B for selenium:

TABLE VI Comparison of the results of bulk modulus obtained by Hill's method and by the present method with experimental data for some hexagonal, trigonal, tetragonal and orthorhombic materials

Material	B (10^{11} Pa)			Difference 1[a] (%)	Difference 2[b] (%)	Reference
	Experimental	Hill [6]	Present			
Cd	0.468	0.5278	0.5948	+ 12.7	+ 27.1	[16]
	0.476	0.5261	0.6447	+ 22.5	+ 35.3	[17]
Co	1.920	1.9033	1.9435	+ 2.1	+ 1.2	[17]
	1.915	1.8278	1.8365	+ 0.5	− 4.1	[16]
Mg	0.289	0.3555	0.3566	+ 0.3	+ 23.4	[17]
	0.354	0.3460	0.3471	+ 0.3	− 1.9	[16]
Zn	0.599	0.7561	0.8831	+ 16.8	+ 47.4	[16]
	0.605	0.6547	0.7840	+ 19.7	+ 29.6	[17]
Zr	0.833	0.953	0.96	+ 0.7	+ 15.2	[16]
	0.898					[17]
Hf	1.09	1.0865	1.0892	+ 0.3	− 0.1	[16]
	1.098					[17]
Ti	1.052	1.0727	1.0831	+ 1.0	+ 3.0	[16]
	1.236					[17]
Sb	0.3924	0.3781	0.4405	+ 16.5	+ 12.3	[17]
	0.3828	0.4204	0.5868	+ 39.6	+ 53.3	[16]
Bi	0.315	0.3483	0.3655	+ 4.9	+ 16.0	[16]
	0.353	0.3361	0.3759	+ 11.8	+ 6.5	[17]
Se	0.091	0.1496	0.2744	+ 45.5	+ 201.5	[16]
		0.1332	0.2819	+ 52.7	+ 209.8	
Te	0.230	0.2407	0.4068	+ 40.8	+ 76.9	[16]
In	0.410	0.4159	0.4314	+ 3.7	+ 5.2	[16]
	0.436					[17]
Sn	0.51	0.5145	0.5237	+ 1.8	+ 2.7	[17]
	0.542	0.5494	0.5790	+ 5.4	+ 6.8	[16]
α-U	1.02	1.1166	1.1993	+ 7.4	+ 17.6	[17]
	0.988					[16]
Ga	0.5	0.5744	0.5897	+ 2.7	17.9	[17]
	0.569					[16]
				Average: + 13.5 Average excl. Se and Te: + 8.5	Average: + 34.9 Average excl. Se and Te: 15.7	

[a] Difference 1 (%) = 100 (present value − Hill's value)/(Hill's value).

[b] Difference 2 (%) = 100 (present value − experimental value)/(experimental value).

$E(\mathrm{Se})/E(\mathrm{Te}) = 1.41$, $G(\mathrm{Se})/G(\mathrm{Te}) = 1.41$, $B(\mathrm{Se})/B(\mathrm{Te}) = 0.4$ (low?); $E(\mathrm{Sb})/E(\mathrm{Te}) = 1.3$ or 1.9, $G(\mathrm{Sb})/G(\mathrm{Te}) = 1.3$, $B(\mathrm{Sb})/B(\mathrm{Te}) = 1.7$. Interestingly, the elements selenium and tellurium lie in column 6A of the periodic table and are considered as metalloids. Hence, at the bottom of Table VI we have presented average values with and without the data for selenium and tellurium. Thus, excluding the data for selenium and tellurium, the average difference between the values of B predicted by the present scheme and the experimental value is 15.7%, while the average difference between the values predicted by our scheme and by Hill's is 8.5%. Nevertheless, one should be discouraged from using the present averaging scheme to compute B. It appears that it is best to use the Voigt averaging method for B.

4. Conclusion

The new averaging scheme [1], involving the averaging of the squared reciprocal sound velocities computed from input values of C_{ij}, has been used to calculate the technical constants G, E and B for several materials of cubic and non-cubic (hexagonal, tetragonal, trigonal and orthorhombic) symmetry. The results have been compared with those from the averaging scheme of Hill [6]. For the calculated values of G and E, agreement between the two schemes was within 2.7% and 0.5%, respectively. However, the values computed by the new scheme tended to overestimate the values of bulk modulus computed by Hill's scheme by 13.5% on average. This study has confirmed that the new averaging scheme is an efficient computational method for calculating the technical constants of both cubic and non-cubic materials from input of C_{ij} data.

Acknowledgements

The authors are grateful to NASA Lewis Research Center for the provision of a research grant and to Dr J. D. Whittenberger (Program Manager) for stimulating discussions.

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Received 19 June 1992
and accepted 20 April 1993