

the VRH approximation, even for the anisotropic crystals like CdTe and ZnSe.

To examine a possible dependence of the VRH approximation on elastic anisotropy, we plotted the ratio of the measured modulus to the calculated VRH modulus as a function of percent elastic anisotropy in Figs. 1 and 2. The percent elastic anisotropy¹¹ referred here is

$$A^* (\text{in } \%) = [3(A-1)^2 / 3(A-1)^2 + 25A] \times 100, \quad (5)$$

where $A = 2c_{44} / (c_{11} - c_{12})$. Note that the limiting Voigt and Reuss moduli result in the wider spread as the elastic anisotropy of crystal becomes large. It is noteworthy, however, that the measured moduli lie within the spread for every crystals considered in the present program. As seen in Fig. 2, the ratio of shear moduli ($G_{\text{meas}}/G_{\text{VRH}}$) is smaller than unity in all cases and the deviation of this ratio from unity becomes large as the elastic anisotropy of crystal increases. Similar observation can be made also for the case of Young's modulus.

TABLE V. Mean velocity of sound for MgO, CaF₂, β-ZnS, CdTe, and ZnSe.^a

Materials and reference ^b		A* (%)	v _m [Eq. (6)]	v _m [*] [Eq. (7)]
MgO	Single-crystal (65C1)	2.28	6.617	6.654
	polycrystalline		...	6.626
CaF ₂	Single-crystal (60H1)	2.96	4.001	4.022
	polycrystalline		...	4.006
β-ZnS	Single-crystal (63E1)	8.49	3.122	3.135
	polycrystalline		...	3.127
CdTe	Single-crystal (62M1)	8.83	1.712	1.743
	polycrystalline		...	1.727
ZnSe	Single-crystal (63B1)	11.70	2.406	2.637
	polycrystalline		...	2.614

^a All values of the velocity are in units of 10⁵ cm/sec.
^b See Table II for the complete references.

The trend of this deviation with increasing elastic anisotropy suggests that, for highly anisotropic crystals like Li and RbI, the VRH approximation may not be the good procedure to follow. But, for the cubic crystals possessing low or moderate elastic anisotropies (i.e., A* < 10%), the VRH approximation is believed to be accurate in giving the probable isotropic elastic moduli and these VRH moduli are as good as ones we measure in the laboratory.

To provide an additional support to this conclusion, we take a numerical approach in which we calculate the mean velocity of sound in a given crystal and then compare this result with the corresponding quantities deduced from the Debye continuum relation. The mean velocity of sound in an anisotropic crystal is

$$v_m = \left[\frac{1}{3} \sum_{j=1}^3 \int_V \left(\frac{1}{v_j^3} \frac{d\Omega}{4\pi} \right)^{-1/3} \right], \quad (j=1, 2, 3), \quad (6)$$

where v_j represent three sound velocities that are the eigenvalues of the Christoffel equation involving the

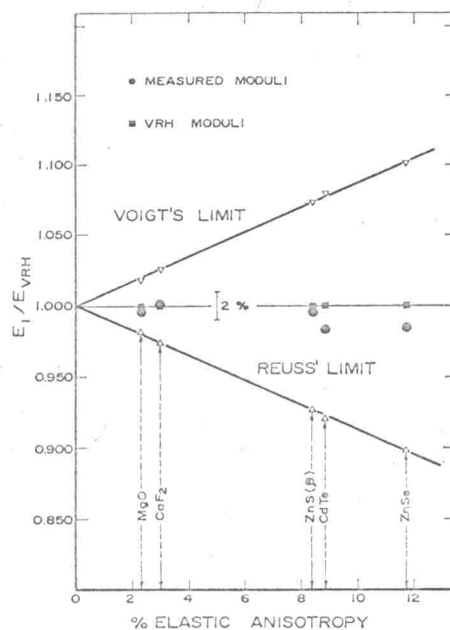


Fig. 1. Comparison between calculated and measured Young's moduli as a function of elastic anisotropy.

single-crystal elastic constants and $d\Omega$ is the element of a solid angle, i.e., $d\Omega = \sin\theta d\theta d\phi$. Since the integration of Eq. (6) is impractical to perform analytically, the integration is evaluated numerically as a procedure outlined by Alers.¹² Using the single-crystal elastic constants for the individual materials considered, values of the mean velocity of sound have been calculated by

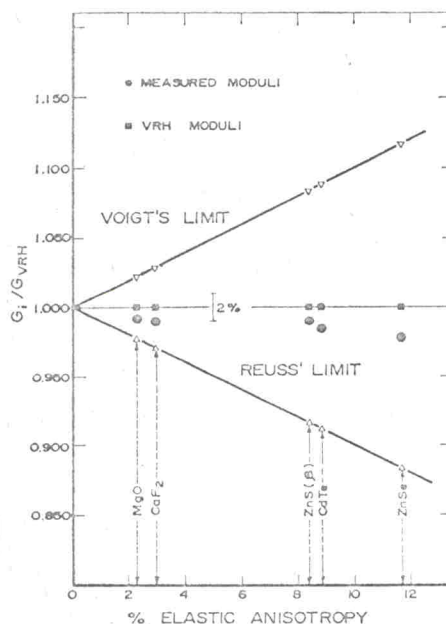


Fig. 2. Comparison between calculated and measured shear moduli as a function of elastic anisotropy.

¹² G. A. Alers, *Physical Acoustics*, W. P. Mason, Ed. (Academic Press Inc., New York, 1965), Vol. III-B, Chap. 1.