

For aggregates of more than two components, the Hashin-Shtrikman bounds can be generalized, but here the two-phase bounds were simply applied successively, using the arithmetic mean of the bounds for the two-phase aggregates. In these cases, the results are not strict bounds, but they should still be good estimates of the elastic velocities, with uncertainties of no more than a few percent. Anisotropies within individual components have not been considered, since in most cases the variations in moduli due to anisotropies are much less than the contrast in moduli between phases.

Fig. 1 shows some calculated oxide-mixture properties in relation to the isochemical phases — specifically, some olivine (α -), β - and spinel (γ -) phases. The relevant simple oxides and the polymorphs of SiO_2 and GeO_2 are included for reference. In all cases discussed in this paper, the rutile-structure phases of SiO_2 and GeO_2 were used in the oxide-mixture calculations. Compounds and polymorphs and/or their oxide mixtures are joined by the straight lines. Fig. 1 includes the data compiled by Liebermann and Ringwood [9] for these AB_2O_4 phases. It is evident from Fig. 1 that the oxide-mixture properties are quite systematically related to the properties of the other phases. If the oxide mixtures are considered as polymorphs, then the observation by Liebermann and Ringwood [9] of considerable variation in the velocity-density trends joining polymorphs is even more noticeable here, most notably in the nearly horizontal spinel-oxides trends. D. Anderson [11] has previously noted that spinels commonly have v_b 's comparable to their isochemical oxide mixtures. It was also noted by Liebermann and Ringwood [9] that the v - ρ slopes decreased with increasing mean atomic weight. This trend is also evident in Fig. 1.

3. Elasticity and crystal structure

In Figs. 2 and 3, the velocity ratios v_p/v_p^o , v_b/v_b^o and v_s/v_s^o , where superscript "o" denotes the oxide-mixture property, are plotted against the density ratio ρ/ρ^o for some AB_2O_4 - and ABO_3 -type compounds (the latter including some garnets). The straight lines join polymorphs. The cases in Fig. 1 are included in Fig. 2. It can be seen in Figs. 2 and 3 that in many cases compounds with the same crys-

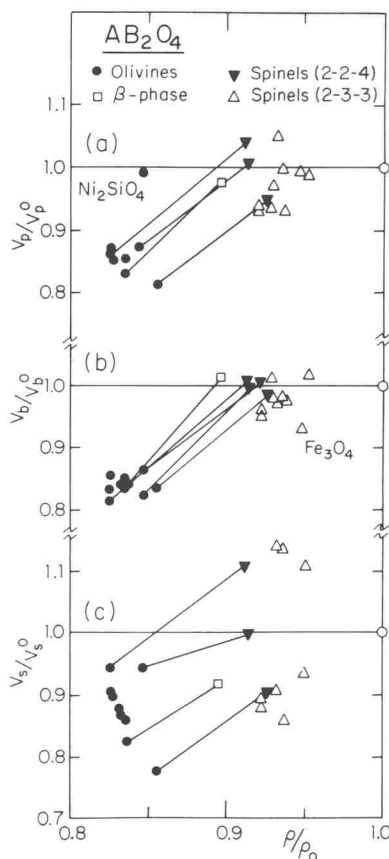


Fig. 2. Relative velocity vs. relative density for AB_2O_4 -type compounds. Compressional velocity, v_p , bulk velocity, v_b , shear velocity, v_s , and density, ρ , are normalized to those of the isochemical oxide mixtures, denoted by superscript "o". Straight lines join polymorphs. Data are those of Fig. 1, with additions from [32, 33, 40, 41].

tal structure cluster into a narrow range of the velocity and density ratios. The tendency is stronger for v_b than for v_p or v_s . The most notable exceptions are the shear velocities (and hence the v_p 's, to a lesser extent) of the spinels and olivines relative to the oxides. Note, however, that there is more regularity between the olivine-spinel pairs than between either of these and the oxides.

In Fig. 4, the polymorphs of SiO_2 and GeO_2 are plotted, in this case with the properties normalized to those of the rutile structure phase. For the α -quartz phases, the v_b ratios are similar, but the densities are quite discordant — note the change in scale from Figs. 2 and 3. The data in parentheses are the velocities for stishovite measured by Chung [12] relative to those of Mizutani et al. [5].

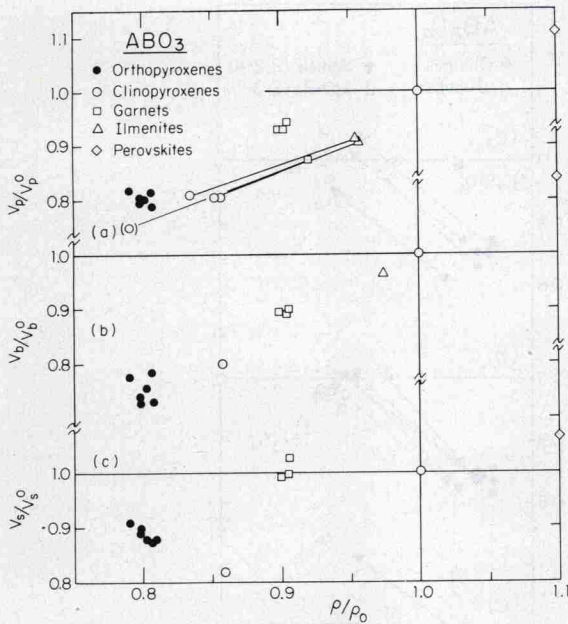


Fig. 3. Relative velocity vs. relative density for some ABO_3 -type compounds (including some garnets), analogous to Fig. 2. Data are from [9, 32, 33, 42–44].

The normalization to the oxide-mixture properties has evidently not removed compositional effects from the shear velocities of the olivines, spinels and α -quartz's. On the other hand, no compositional effects are evident in the v_s ratios for the orthopyroxenes and garnets, whereas crystal structural effects are quite evident (Fig. 3c). The commonly remarked irregularity of shear properties (e.g., [13]) thus seems to arise from both compositional and structural effects. Compositional effects on the v_b ratios cannot be resolved, except possibly for one or two spinels (e.g., Fe_3O_4 , Fig. 2b). Since v_p is not independent of v_b and v_s , it reflects the variations of v_s .

On the basis of the data for the olivine, spinel, orthopyroxene and garnet structures shown in Figs. 2 and 3, one would expect to be able to predict ρ , v_b and, for the ABO_3 compounds, v_s for an unmeasured phase to within 2–3% relative to the properties of a measured phase. The availability of data for many simple oxides makes the oxide mixture a convenient reference "phase" for this purpose, although spinel phases would probably be better referred to olivine phases. (The oxide mixture density as a reference for estimating the density of unmeasured phases has of

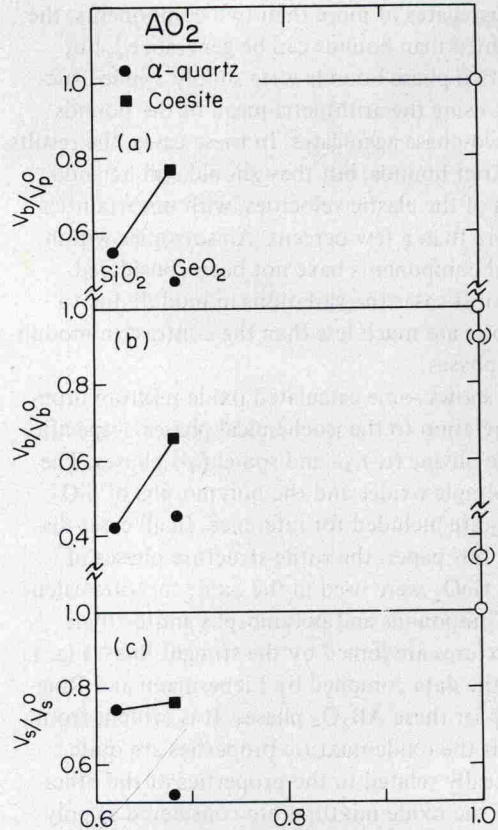


Fig. 4. Relative velocity vs. relative density for AO_2 -type compounds, normalized to the properties of the rutile-structure polymorph. Circles in parentheses are v_b and v_s of stishovite (SiO_2 -rutile) from Chung [12] relative to those of Mizutani et al. [5]. Data are from [4, 5, 12, 32, 33, 45].

course been frequently used before: e.g. [14].) In addition, the normalization to the oxide mixtures has defined relationships between structure pairs which are not represented, such as garnet–perovskite or ilmenite–perovskite.

A wide range of slopes is defined in Figs. 2–4 by the possible transitions between the structures represented. It is interesting that the slopes tend to be lower for transitions in which the silicon (or its analogue in non-silicates) changes from 4- to 6-coordination. Silicon is in 4-coordination in olivine, spinel, pyroxene, α -quartz and coesite structures, and in 6-coordination in the ilmenite, perovskite and rutile structures (note that rutile-structure phases were assumed in the oxide mixtures). The garnet structure is intermediate – for example, the high-pressure garnet form of $MnSiO_3$ has one-quarter of the silicon ions in 6-coordination [14].