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ELASTICITY OF SINGLE-CRYSTAL MgF_2 (RUTILE STRUCTURE) UNDER PRESSURE

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The elastic moduli of single-crystal MgF_2 (rutile structure) have been measured ultrasonically to 7 kbars. Zero-pressure moduli are in good agreement with the results of others. The pressure derivative of the shear modulus $c_s = (c_{11} - c_{12})/2$ is -0.7 ± 0.1 which is consistent with the negative values also found in rutile-structure oxides. Estimates of the isotropic aggregate modulus derivatives are in good agreement with derivatives measured on polycrystalline aggregates by Rai and Manghnani. The calculated isotropic aggregate bulk modulus derivative is $K' = 5.1 \pm 0.2$, which is lower than for the rutile-structure oxides, and comparable to that for other fluorides. More covalent bonding may increase the value of K', and hence the value for stishovite (SiO_2, rutile) may be quite high.

1. Introduction

The elastic properties of materials with the rutile crystal structure are of particular interest in geophysics because of the existence of stishovite, the high-pressure rutile-structure phase of SiO_2 [1]. Stishovite may exist as a stable phase in all or part of the lower mantle [2,3]. In any case, its density and elastic properties are important reference data for estimating the properties of possible mantle mineral assemblages and for interpreting the density and elastic velocity profiles of the mantle [4,5]. Because of the difficulty of making or collecting sufficient quantities of stishovite, even its zero-pressure eleastic properties are still quite uncertain [6–9], and shock wave data for silica do not provide very strong constraints [10,11].

To date, the single-crystal elastic properties of three other rutile-structure oxides have been measured under pressure (Table 1); rutile itself (TiO_2), GeO_2, and cassiterite (SnO_2). Two notable features of the results are the unusually large-pressure derivatives of the bulk modulus, K' (compared with "usual" values of 4–5), and the negative pressure derivatives of one shear mode, c_s'. In trying to infer from these results the likely properties of stishovite, it would be useful to know to what extent the properties are intrinsic characteristics of the crystal structure, and to what extent they depend on the character of the interatomic bonding (ionic vs. covalent) or the character of the metals (transition vs. group IV). The pattern of relative magnitudes of the elastic moduli of rutile is in fact slightly different than that of the other two, indicating that the transition character of Ti has some influence. Transition metals are also associated with anomalous elastic properties in other compounds [5].

An indication of the influence of bond character on the elastic properties can be obtained from a comparison of the oxides with fluorides which crystallize in the rutile structure, since the latter should be more ionic. Zero-pressure single-crystal elastic moduli have been measured for MgF_2, MnF_2 and CoF_2 (see Table 1), but no measurements of single-crystal properties under pressure have been reported to date. Recently the pressure dependence of the elastic moduli of polycrystalline MgF_2 have been reported by Rai and Manghnani [12]. Measurements of the single-crystal moduli under pressure are still desirable because they

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