Elasticity of ZnO at High Pressure and High Temperatures

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The use of crystal chemical analogues such as ZnO to estimate the stability fields, crystal structures and mechanism by which four-coordinated structures transform to more close-packed forms is now well established, and has been proven useful in the study of high-pressure phases relevant to the Earth's mantle.

In 1967, experimental investigations of the sound velocity pressure dependence of polycrystal ZnO demonstrated a very singular behavior: isotropic shear velocity decreases with increasing density [1]. More recently, we report some results on the dependence of the single crystal elastic constants of wurtzite ZnO on pressure [2]. These data revealed that the shear moduli, C_{44} and C_{66}, decreases with pressure increasing. The deformations associated with this “anomalous” pressure behavior represent possible transformational strains from one structure to another (at pressure close to 9 Gpa, ZnO undergoes a structural phase transition from the wurtzite structure to the more dense NaCl, or B1 from, by shearing on certain crystallographic planes). These first results are significant to seismology and tectonophysics because a low value of dV_s/dP allows a low-velocity zone for shear waves to be compatible with a small thermal gradient. We determined experimentally the elastic and structural properties of ZnO at elevated pressures (up to 8 Gpa) and temperatures (up to 1273K). These new acoustic data exhibit anharmonic properties, which enable us to understand the high-pressure elasticity of oxide minerals.

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