American Mineralogist, Volume 92, pages 174–178, 2007

Effect of cation ordering and pressure on spinel elasticity by ab initio simulation

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Abstract

We present here a first principle computational study of the effect of cation disorder on the elasticity of spinel. Our calculated elastic moduli and structural parameters are comparable with reported experimental and theoretical results. We find that bulk modulus for $MgAl_2O_4$ spinel does not soften at pressure as high as 27 GPa, while shear modulus c_s [$\frac{1}{2}(c_{11} - c_{12})$] decreases with pressure. Disorder increases both the bulk modulus and shear modulus in aluminate spinel, but decreases both for the silicate spinel. The elastic properties of ringwoodite are significantly affected by Si-Mg disorder; a 10% disorder decreases the seismic velocities by 3–5%. Thus, a small amount of disorder will significantly affect seismic observations.

Keywords: Spinel, first principle model, elastic anisotropy, cation disorder