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Structure and elasticity of MgO at high pressure

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ABSTRACT

The structural and elastic properties of MgO periclase were studied up to 150 GPa with the first-principles pseudopotential method within the local density approximation. The calculated lattice constant of the B1 phase over the pressure range studied is within 1% of experimental values. The observed B1 phase of MgO was found to be stable up to 450 GPa, precluding the B1-B2 phase transition within the lower mantle. The calculated transition pressure is less than one-half of the previous pseudopotential prediction but is very close to the linearized augmented plane-wave result. All three independent elastic constants, c_{11}, c_{12}, and c_{44}, for the B1 phase are calculated from direct computation of stresses generated by small strains. The calculated zero-pressure values of the elastic moduli and wave velocities and their initial pressure dependence are in excellent agreement with experiments. MgO was found to be highly anisotropic in its elastic properties, with the magnitude of the anisotropy first decreasing between 0 and 15 GPa and then increasing from 15 to 150 GPa. Longitudinal and shear-wave velocities were found to vary by 23 and 59%, respectively, with propagation direction at 150 GPa. The character of the anisotropy changes qualitatively with pressure. At zero pressure longitudinal and shear-wave propagations are fastest along [111] and [100], respectively, whereas above 15 GPa, the corresponding fast directions are [100] and [110]. The Cauchy condition was found to be strongly violated in MgO, reflecting the importance of noncentral many-body forces.