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High-pressure elasticity of alumina studied by first principles

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ABSTRACT

We investigate by first principles the elastic behavior of Al_2O_3-alumina under pressure (up to 300 GPa) in the corundum and Rh_2O_3 (II) phase. The results are in excellent agreement with available low pressure (<1 GPa) experimental data. The anisotropy in elasticity for corundum decreases up to 50 GPa and then increases slowly with pressure whereas for the Rh_2O_3 (II) phase the anisotropy increases monotonically with compression. Strong shear wave anisotropy in the Rh_2O_3 (II) phase is found to be associated with the relatively small c_{55} modulus, and its softening at high pressures. Unlike corundum, the directions of the fastest and slowest wave propagation, and the maximum polarization anisotropy of Rh_2O_3 (II) phase remain unchanged with pressure. At the corundum to Rh_2O_3 (II) phase transition pressure (78 GPa at 0 K), the anisotropy increases by more than 100% but the density and wave velocities increase only by 2%. The calculated (0 K) densities and wave velocities at lower mantle pressures are slightly larger (by 5%) than the corresponding seismic profiles. Our results suggest that the presence of free Al_2O_3 in small amounts in the lower mantle may not be detected in seismic density and velocity profile. However, its anisotropy may produce a detectable signal, particularly, at pressure conditions typical of the D" region.