Velocity contrast between perovskite and postperovskite in the (Mg,Fe,Al)(Si,Al)O3 system

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We calculated the acoustic velocity contrasts between perovskite and postperovskite in MgSiO3, FeSiO3 and Al2O3 compounds, using the ab initio planewave pseudopotential method in a pressure range of the Earth's lower mantle. Both FeSiO3 and Al2O3 pv and ppv have considerably smaller shear moduli than Mg-phases at deep mantle pressures, though the bulk moduli are comparable. The variations of Fe and Al contens will produce positive relative variations of shear to compressional velocities and bulk to shear velocities but negative variation of density to shear velocity at constant pressure. Both Fe and Al influence elasticity of ppv more than that of pv. Therefore velocity contrasts across the postperovskite phase change would decrease with increasing Fe and Al content. We find that positive velocity variations as observed are hardly produced by the phase change in pv with Fe,Al-rich composition.

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