The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO$_3$

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Ab Initio Calculations

• Explore material properties at P-T regime inaccessible to experiments

• Determine:
  – Single crystal structure
  – Stress response to strain
  – Elastic constants
  – P & S wave velocity

• It is important to calculate these properties at mantle temperatures (not 0 K)
Perovskite Elastic Moduli

Table 1
Calculated elastic moduli of MgSiO$_3$ perovskite (GPa), at selected pressures and temperatures.

- Average difference between O°K & 3500°K is ~14 %

- Some constants are more effected by temperature than others ($C_{13} \sim 2\%$, $C_{66} \sim 40\%$)
Perovskite – 90 GPa

S Wave Speed

Directional Dependence

Table 3
Shear wave splitting \(((V_{S1} - V_{S2})/\langle V_S \rangle) \times 100\) for MgSiO₃ perovskite in various propagation directions at various pressure and temperatures.

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No Directional Dependence
Post Perovskite

Table 4
Calculated elastic moduli of post-perovskite phase (GPa), at selected pressures and temperatures

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- Average difference 0 - 4000K ~ 16 %
Post Perovskite – 136 GPa

S Wave Speed

P Wave Speed

• Temp. Independent
• Greater than Pv.

Table 6
Shear wave splitting \( \left( \frac{V_{S1} - V_{S2}}{<V_S>} \right) \times 100 \) for post-perovskite in various propagation directions at various pressure and temperatures.

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Transversely Isotopic Aggregate

Perovskite Post Perovskite

Isotropic in x & y, anisotropic in z

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Bulk & Shear Modulus

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Table 7
Temperature dependence of bulk (K) and shear (G) moduli for MgSiO₃ perovskite at approximately 90 GPa and post-perovskite phase at approximately 136 GPa
Seismic Wave Velocity

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Seismically observed $R_{s/p}$ ranges from 1.5 – 2.5
Elegant Retreat

• “Taken at face, this low value of $R_{s/p}$ is totally incompatible … with the existence of post-perovskite in D”

• This “may make it possible to map out regions of post-perovskite in the lowermost mantle”
MgSiO₃ Perovskite

Table 1
Calculated elastic moduli of MgSiO₃ perovskite (GPa), at selected pressures and temperatures.

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Table 2
Calculated unit cell parameters of MgSiO₃ perovskite at selected pressures and temperatures.

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Table 3
Shear wave splitting \((V_{S1} - V_{S2})/\langle V_{S}\rangle \times 100\) for MgSiO₃ perovskite in various propagation directions at various pressure and temperatures.

Fig. 1. Variation of compressional wave velocities of MgSiO₃ perovskite with propagation direction at approximately 90 GPa and 0 K—light grey, 1500 K—dark grey, and 3500 K—black.

Fig. 2. Variation of shear wave velocities of MgSiO₃ perovskite with propagation direction at approximately 90 GPa and 0 K—light grey, 1500 K—dark grey, and 3500 K—black.
MgSiO3 Post-Perovskite

Table 5
Calculated unit cell parameters of post-perovskite at selected pressures and temperatures.

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Table 6
Shear wave splitting \((\langle F_{31} \rangle - \langle F_{32} \rangle)/\langle F_3 \rangle)^*100\) for post-perovskite in various propagation directions at various pressure and temperatures.

Fig. 3. Variation of compressional wave velocities of post-perovskite phase with propagation direction at approximately 136 GPa and 0 K—light grey, 3000 K—dark grey, and 4000 K—black.

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Table 4
Calculated elastic moduli of post-perovskite phase (GPa), at selected pressures and temperatures.

Fig. 4. Variation of shear wave velocities of post-perovskite phase with propagation direction at approximately 136 GPa and 0 K—light grey, 3000 K—dark grey, and 4000 K—black.