The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of $MgSiO_3$

Stephen Stackhouse[a,*], John P. Brodholt[a], J. Wookey[b], J.-M. Kendall[b], G. David Price[a]

[a] *Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, UK*
[b] *School of Earth Sciences, University of Leeds, Leeds, LS2 9JT, UK*

Received 8 August 2004; received in revised form 25 October 2004; accepted 23 November 2004
Available online 4 January 2005
Editor: B. Wood

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

Image removed due to copyright considerations.

- Average difference between O°K & 3500°K is ~14 %
- Some constants are more effected by temperature than others (C_{13} ~2% C_{66} ~ 40%)

Perovskite – 90 GPa

S Wave Speed

Directional Dependence

Table 3
Shear wave splitting $((V_{S1}-V_{S2})/<V_S>)*100$ for $MgSiO_3$ perovskite in various propagation directions at various pressure and temperatures[a]

Images removed due to copyright considerations.

No Directional Dependence

Post Perovskite

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

Image removed due to copyright considerations.

- Average difference 0 - 4000K ~ 16 %

Post Perovskite – 136 GPa

S Wave Speed

Table 6

Shear wave splitting $((V_{S1}-V_{S2})/<V_S>)*100$ for post-perovskite in various propagation directions at various pressure and temperatures[a]

Images removed due to copyright considerations.

P Wave Speed

- Temp. Independent
- Greater than Pv.

Transversely Isotopic Aggregate

Perovskite

Post Perovskite

Image removed due to copyright considerations.

Isotropic in x & y , anisotropic in z

Bulk & Shear Modulus

Images removed due to copyright considerations.

Table 7
Temperature dependence of bulk (K) and shear (G) moduli for $MgSiO_3$ perovskite at approximately 90 GPa and post-perovskite phase at approximately 136 GPa

Seismic Wave Velocity

Images removed due to copyright considerations.

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 $MgSiO_3$ perovskite (GPa), at selected pressures and temperatures

Images removed due to copyright considerations.

Fig. 2. Variation of shear wave velocities of $MgSiO_3$ perovskite with propagation direction at approximately 90 GPa and 0 K—light grey, 1500 K—dark grey, and 3500 K—black.

Table 2
Calculated unit cell parameters of $MgSiO_3$ perovskite at selected pressures and temperatures

Images removed due to copyright considerations.

Table 3
Shear wave splitting $((V_{S1}-V_{S2})/<V_S>)*100$ for $MgSiO_3$ perovskite in various propagation directions at various pressure and temperatures[a]

Fig. 1. Variation of compressional wave velocities of $MgSiO_3$ 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

Images removed due to copyright considerations.

Table 6
Shear wave splitting $((V_{S1}-V_{S2})/<V_S>)*100$ for post-perovskite in various propagation directions at various pressure and temperatures[a]

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.

Images removed due to copyright considerations.

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.