Electronic Transitions in Perovskite

Possible Nonconvecting Layers in the Lower Mantle

by

James Badro et al.

Heat Transport

- Conduction, Radiation or Convection
- Convection only occurs if the former two methods fail to transfer heat
- Changes in mineral conduction and radiation properties strongly affect mantle dynamics

Mantle Composition

- 80% perovskite
- (Mg,Fe)O undergoes a high-spin to low-spin transition between 60-70 GPa

Blue-shift

- Iron absorption bands shift to blue from IR and Red at high-pressure
- Badro et al. report two such shifts at 70 and 120 GPa
- This indicates to two regions of high IR and red transparency in the mantle…

K β-emission spectroscopy

- Originates from $3p \rightarrow 1s$ decay
- Interaction of X-rays with K-shell, the inner electron shell
- Characteristic peaks for high-spin and low-spin electrons
- HS and LS are properties defined by the interaction of *3p* and *3d* shells

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(Mg,Fe)-perovskite

Site and Spin

- 56% ferrous in dodecahedral (2+)
- 25% ferric in octahedral (3+)
- 19% ferrous in octahedral (2+)
- So 56% (ferrous) and 44% (ferric)
- Mixed state (HS and LS)
  55%HS, 45% LS
- Don't let the numbers fool you
- But an interesting point is introduced

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(Mg,Fe)-perovskite

Further Quantification Needed

- Of Al affect on compressibility
- Temperature effect (15-18 GPa?)

Post-perovskite

- “Conjecture” a connection with the HS-LS transition

- Propose that further theoretical modeling of mixed spin states of (Mg,Fe)O and (Mg,Fe)pv are needed

Light Absorption

- Radiative conductivity is hindered by IR light absorption in HS Fe-bearing lower-mantle phases
- In the LS state, IR absorption is hindered
- Indeed, even laser heating did not work above 120 GPa!

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The figure below shows the normalized blackbody thermal radiation as a function of wavelength at three different temperatures (2000, 2500, and 3000 K) that can be considered as bounds for the lower-mantle geotherm *(S7)*.

The absorption bands of (Mg0.9 Fe0.1)SiO3 perovskite are reported in the HS state (orange sticks) according to pressure-corrected measurements of Keppler et al. *(S8)* performed at room conditions, and in the LS state (blue sticks) according to the model proposed by Burns *(S9)*. In the HS state, the most intense absorption bands are in the near infrared (IR) region, where blackbody radiation is maximal at these temperatures (*S5*); this makes perovskite a very bad radiative thermal conductor. In the LS state, these same bands undergo a blue-shift to the visible region, where blackbody radiation is weaker. The total power throughput in perovskite therefore dramatically increases after the transition, since IR radiation travels with a larger mean free path. This contributes to an enhanced radiative thermal conductivity in this state (*S5*), and is characteristic of the mineral assemblages (see text) of Earth's lowermost mantle.

Correlation with the Mantle

- 70 GPa transition consistent with 1700 km depth consistent with transition pressure for Fe in (Mg,Fe)O
- 120 GPa consistent with D″ layer
- Increased radiative conductivity
- Rayleigh number is decreased, hindering convection, favoring layers