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Multidisciplinary Impact of the Deep Mantle Phase Transition in Perovskite Structure

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A phase transition in (Mg, Fe) SiO_3 (magnesium silicate-perovskite) for pressure-temperature conditions near the base of Earth's mantle, first reported in May 2004, is stimulating strong multidisciplinary excitement and interactions. Experimentally and theoretically determined characteristics of this phase transition indicate that it may hold the key to understanding enigmatic seismological structures in the D″ region of the lowermost mantle, with important implications for heat transport, thermal instabilities, and chemical properties of the lower mantle.

All minerals undergo phase transitions with increasing depth into the Earth, reorganizing their crystal structures into denser-packed forms stable over a finite range of pressures and temperatures. The changes in material properties across such transitions often give rise to detectable contrasts in seismic velocities and density.

Such phase transitions in $(Mg, Fe)_2 SiO_4$ olivine occur near depths of 410 and 660 km, contributing to the corresponding major seismological discontinuities in the mantle transition zone. The 660-km transition involves a disassociative structural transition yielding two mineral forms: (Mg, Fe) SiO_3 magnesium silicate-perovskite (MgPv), and (Mg, Fe) O ferropericlase. Transitions in most other major upper mantle minerals, such as garnet, also yield MgPv below the transition zone.

Many mineral physics experiments and calculations have established remarkable stability of MgPv across a wide range of lower mantle conditions. This mineral is believed to be the most abundant inside the Earth, composing the bulk of a relatively homogeneous lower mantle layer.

Some early experimental work in the mid-1990s suggested that MgPv may destabilize in the lower mantle, transforming into constituent dense oxides; however, subsequent work in the last 8 years indicates stability of the phase to at least 120 Gigapascals (Gpa) (Figure 1).

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With improvement of experimental technology, indications of a transition in MgPv began to emerge, and in 2004 the dam suddenly broke as several groups working independently found experimental evidence for a post-perovskite phase transition in the $MgSiO_3$ end-member (Figure 1) under lowermost mantle conditions [e.g., *Murakami et al.*, 2004; *Oganov and Ono*, 2004; *Shim et al.*, 2004].

Theoretical calculations provided a structural interpretation (Figure 2) of this phase change (at T = 0K, absolute zero) [*Tsuchiya et al.*, 2004b], the phase boundary properties at finite T (Figure 3) [*Tsuchiya et al.*, 2004b; *Oganov and Ono*, 2004] and static elasticity [*Tsuchiya et al.*, 2004a; *Iitaka et al.*, 2004; *Oganov and Ono*, 2004], along with constraints on the phase boundary properties. Numerous groups are now exploring the effects of variable composition and high temperature on the elastic properties of the new post-perovskite phase (PPv). The importance of this discovery has been highlighted extensively in the popular scientific media.

A key parameter for the PPv transition is the Clapeyron slope, the slope of the phase transition boundary in P-T space. Initial theoretical work indicates a strong positive slope near 7–8 Megapascals/K. The transition should then occur at shallower mantle depths in lower temperature regions, and at greater depths in higher temperature regions (Figure 3), with the 1–1.2% density increase across the phase boundary favoring flow across the boundary.

A strong positive Clapeyron slope for an unspecified phase change had been proposed from geodynamical and seismological analysis (prior to identification of the post-perovskite phase), based on apparent topography of a seismic discontinuity in the D″ region in whole mantle convection models [e.g., *Sidorin et al.*, 1999]. However, the dynamic stability of such a transition was not explored until the recent discovery was announced.

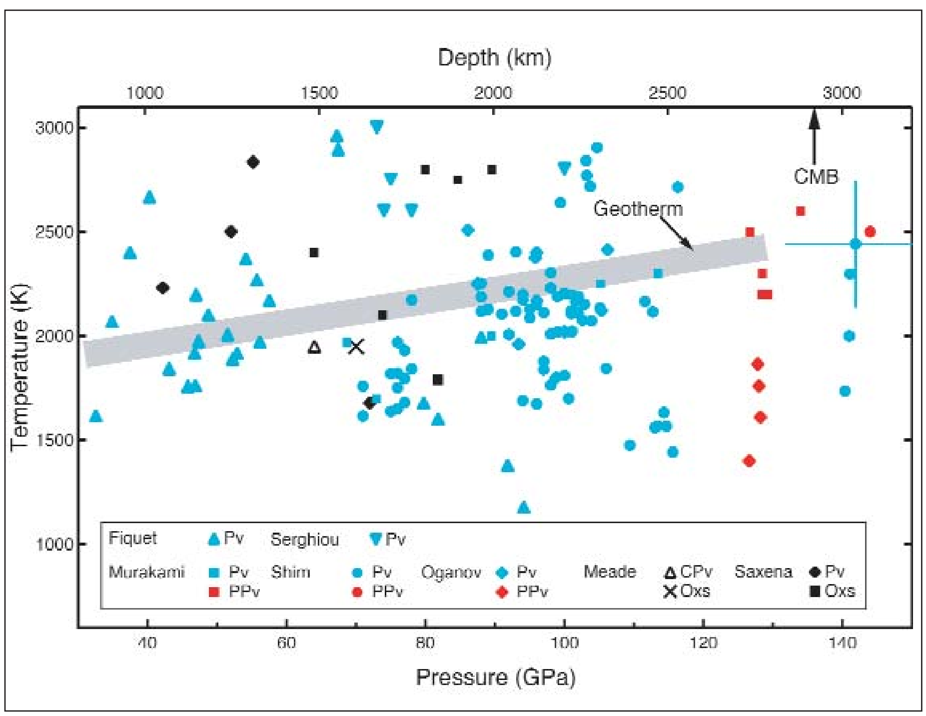

Fig. 1. A summary of high P-T experimental results on the stability of $MgSiO_3$ magnesium silicate-perovskite (Pv). An approximate geotherm is indicated by the shaded line. Experimental observations of possible decomposition of perovskite into dense oxides are indicated by the solid squares (Oxs). The red symbols indicate occurrence of the post-perovskite phase (PPv) transition from the recent X-ray diffraction studies mentioned in the text.

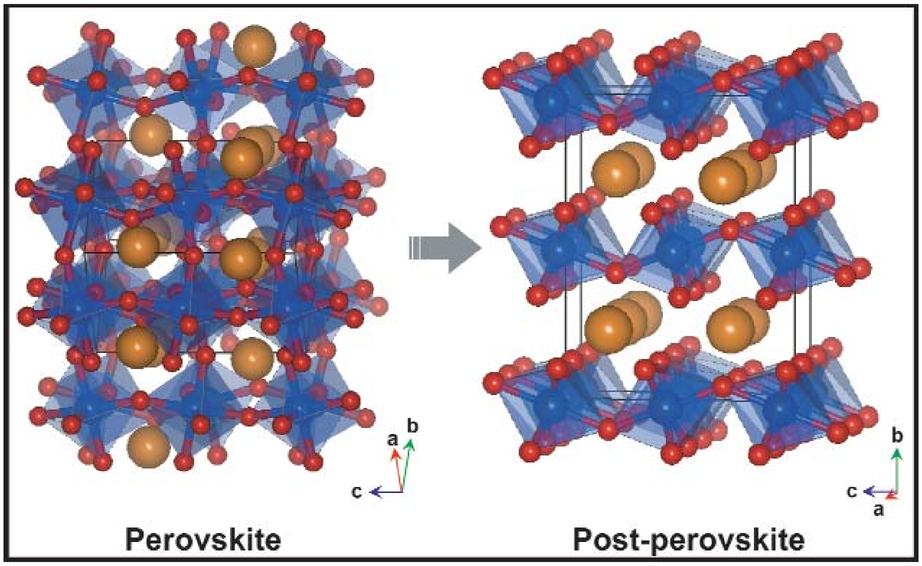

*Fig. 2. (left) The orthorhombic (space group Pbnm) structure of magnesium silicate perovskite and (right) the base-centered orthorhombic polymorph post-perovskite (space group Cmcm) structure ($CaIrO_3$-type). Orange spheres represent Mg ions, and octahedra represent SiO_6 units. The phase transition takes place near 125 GPa, with a 1.0–1.5% density increase from perovskite to post-perovskite. Elastic properties indicate about a 1.5% increase in shear velocity and about 1.0% in compressional velocity, and a small negative contrast in bulk sound velocity across the phase boundary [*Tsuchiya et al.*, *2004a, 2004b].*

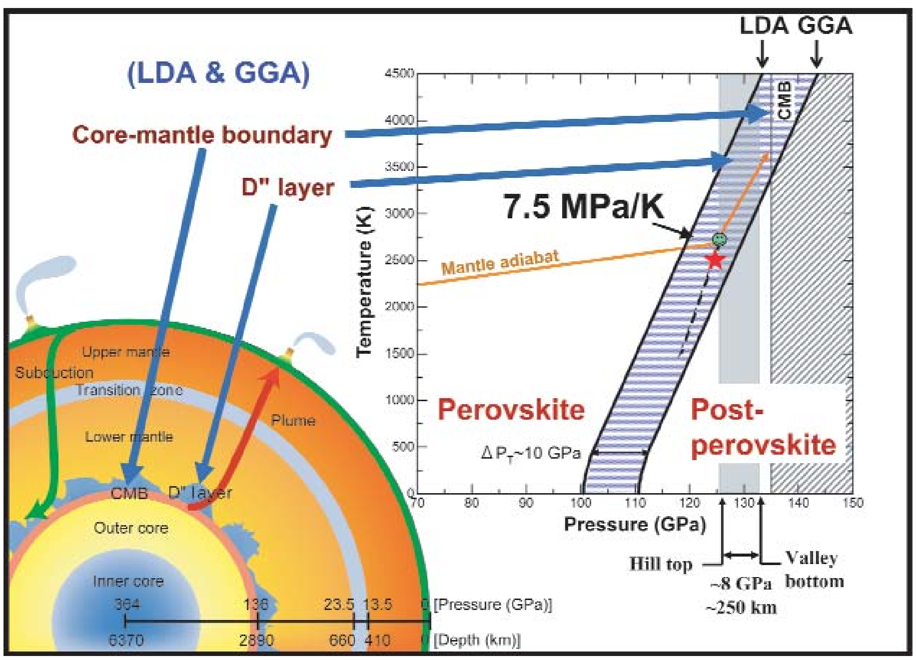

Fig. 3. High P-T phase diagram of $MgSiO_3$ predicted by first principles calculation based on the local density approximation (LDA) and generalized gradient approximation (GGA) [Tsuchiya et al., *2004b]. The lower and upper bounds were determined from LDA and GGA calculations, respectively. The calculated Clapeyron slope is about 7.5 MPa/K. The dashed line is the phase boundary proposed by combining data of the experimental transition condition (red star)* [Murakami et al., *2004] and the Clapeyron slope assumed to explain the D″ topography by solid-solid phase change [*Sidorin et al., *1999]. The vertical shaded bound is the pressure range across the D″ topography. The schematic Earth cross section demonstrates the correspondence of the Earth's structure and the post-perovskite phase transition.*

The implications are profound. Unmitigated, the phase transition should act to destabilize a hot thermal boundary layer at the base of the mantle, leading to numerous upwellings and increased heat transport [e.g., *Nakagawa and Tackley*, 2004; *Matyska and Yuen*, 2004].

Reconciling this tendency with the seismological observation of a predominance of large-scale length seismic velocity heterogeneities in D″ [e.g., *Lay et al.*, 2004] may require a fundamental reassessment of the importance of processes such as radiative transport in the deep mantle, for which there is otherwise little direct constraint [*Matyska and Yuen*, 2004; *Badro et al.*, 2004].

Multidisciplinary Issues

Many attributes of the post-perovskite phase transition are yet to be documented. Figure 1 indicates that there are some disagreements in the pressure-temperature bounds on the transition that need to be resolved, and that the theoretical calculation of the Clapeyron slope also needs to be experimentally confirmed. In addition, the effects of iron [e.g., *Mao et al.*, 2004], aluminum, and joint stability with $CaSiO_3$ calcium silicate-perovskite and ferro-periclase need to be assessed. The relationship of the PPv phase transition to possible changes in the spin state of iron in the deep mantle is another key issue [e.g., *Badro et al.*, 2004].

Seismologically, the major challenge presented by this discovery is the assessment of what features of the boundary layer at the base of the mantle [e.g., *Lay et al.*, 2004] may or may not be accounted for by the phase change boundary. While D″ discontinuities are one obvious focus for investigation, other features such as the large low-velocity provinces (sometimes called superplumes) in the deep mantle may need to be reevaluated in the context of the phase boundary behavior. Can lateral variations in iron content, for example, combine with thermal variations to explain the large shear velocity fluctuations in the D″ layer? Observations of seismic anisotropy in the lowermost mantle also can now be evaluated in the context of the PPv phase.

Geodynamical implications of the phase boundary are also wide open, especially given the likelihood that chemical heterogeneity exists in D″ and presumably would have complex interactions with the phase transition. The effects on heat transport through the D″ thermal boundary layer need to be assessed, along with corresponding implications for the heat flux boundary condition on the geodynamo and the thermal evolution of the inner core. Formulation of thermal-chemical convection with an appropriate multi-component system will need to be developed as well.

Geochemical aspects of the PPv transition also raise new challenges for sorting out not only chemical effects on the transition itself, but also the interaction of chemical heterogeneities with the deep mantle mixing regime. Provocative new observations such as the apparent 10% enrichment in iron relative to manganese for Hawaiian lavas compared to mid-ocean ridge basalts [e.g., *Humayun et al.*, 2004], suggest that significant chemical heterogeneities exist in the mantle. Iron-rich heterogeneities are likely to be concentrated in the D″ region as a consequence of core formation; thus, quantifying the role of iron enrichment on the phase transition is paramount.

The discovery of a phase transition in the Earth's most abundant mineral creates many challenges and opportunities for the mineral physics, seismological, geodynamical, and geochemical communities to work together to improve our understanding of the Earth.

With support from the U.S. National Science Foundation (NSF), a multidisciplinary workshop organized by the Cooperative Institute for Deep Earth Research (CIDER) was held at the Kavli Institute for Theoretical Physics of the University of California, Santa Barbara on 12 July–6 August 2004 (http://online.kitp.ucsb.edu/online/earth04/). Part of the workshop focused on the post-perovskite phase transition, and highlighted the emerging multidisciplinary challenges.

CIDER provides a promising community organization for communication and collaboration across the relevant disciplines, and the NSF Program for Cooperative Studies of the Earth's Deep Interior is a key source of research support. Special sessions recently held at the 2004 AGU Fall Meeting, and upcoming at the 2005 Joint Assembly, are another valuable means by which to inform and catalyze interactions across the community.

Acknowledgments

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References

Badro, J., J.-P. Ruef, G. Vankó, G. Monaco, G. Fiquet, and F. Guyot (2004), Electronic transitions in perovskite: Possible nonconvecting layers in the lower mantle, *Science, 305*, 383–386.

Humayun, M., L. Qin, and M. D. Norman (2004), Geochemical evidence for excess iron in the mantle beneath Hawaii, *Science, 306*, 91–94.

Iitaka, T., K. Hirose, K. Kawamura, and M. Murakami (2004), The elasticity of the $MgSiO_3$ post-perovskite phase in the Earth's lowermost mantle, *Nature, 430*, 442–445.

Lay, T., E. J. Garnero, and Q. Williams (2004), Partial melting in a thermo-chemical boundary layer at the base of the mantle, *Phys. Earth Planet. Inter., 146*, 441–467.

Mao, W. L., G. Shen, V. B. Prakapenka, Y. Meng, A. J. Campbell, D. L. Heinz, J. Shu, R. J. Hemley, and H.-K. Mao (2004), Ferromagnesian postperovskite silicates in the D″ layer, *Proc. Natl. Acad. Sci. U.S.A., 101*, 15,867–15,869.

Matyska, C., and D. A. Yuen (2004), The importance of radiative heat transfer for superplumes with a deep mantle phase transition, *Earth Planet. Sci. Lett., 125*, 255–266.

Murakami, M., K. Hirose, K. Kawamura, N. Sata, and Y. Ohishi (2004), Post-perovskite phase transition in $MgSiO_3$, *Science, 304*, 855–858.

Nakagawa, T., and P. J. Tackley (2004), Effects of a perovskite-post perovskite phase change near core-mantle boundary in compressible mantle convection, *Geophys. Res. Lett., 31*, L16611, doi:10.1029/2004GL020648.

Oganov, A. R., and S. Ono (2004), Theoretical and experimental evidence for a post-perovskite phase of $MgSiO_3$ in Earth's D″ layer, *Nature, 430*, 445–448.

Shim, S.-H., T. S. Duffy, R. Jeanloz, and G. Shen (2004), Stability and crystal structure of $MgSiO_3$ perovskite to the core-mantle boundary, *Geophys. Res. Lett., 31*, L10603, doi:10.1029/2004GL019639.

Sidorin, I., M. Gurnis, and D. V. Helmberger (1999), Dynamics of a phase change at the base of the mantle consistent with seismological observations, *J. Geophys. Res., 104*, 15,005–15,023.

Tsuchiya, T., J. Tsuchiya, K. Umemoto, and R. M. Wentzcovitch (2004a), Elasticity of post-perovskite $MgSiO_3$, *Geophys. Res. Lett., 31*, L14603, doi:10.1029/2004GL020278.

Tsuchiya, T., J. Tsuchiya, K. Umemoto, and R. M. Wentzcovitch (2004b), Phase transition in $MgSiO_3$ perovskite in the Earth's lower mantle, *Earth Planet. Sci. Lett., 224*, 241–248.

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New Approaches for Extending the Twentieth Century Climate Record

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Studying twentieth century climate is a key to understanding future climate change. Relatively little is still known, however, about climate variability in the first half of the century. Much could be learned from the relatively large climatic variations that occurred during that first half, including the decade-long "Dust Bowl" droughts of the 1930s and the warming of the Arctic from 1920 to 1945.

Poor digital data availability prior to around 1948 has hindered previous work to understand these important climatic variations.

Several projects now are focusing on digitizing earlier manuscript observations to create three-dimensional, gridded meteorological data sets for the first half of the twentieth century. These data sets are likely to provide further insights into processes governing interannual-to-interdecadal large-scale climate variability.

Meteorologists, geophysicists, navy pilots, ship crews, and numerous volunteer observers collected enormous amounts of atmospheric data in the first half of the twentieth century, sometimes under extreme and dangerous conditions. A large fraction of these data, especially upper air data, never made the transition to the "modern era" of climatology, which started after World War II. The reasons are manifold and include military secrecy; interrupted international collaboration; political and institutional changes during and following the war; and, sometimes, simply neglect.

Yet, these data can still be found today on paper in various meteorological archives. With new numerical and statistical techniques becoming available, these archives now could be fruitfully mined for climate research.

Data availability is comparably good for meteorological observations at the Earth's surface, which have been used continuously to study past climate variability. Several ongoing projects are increasing the data quality and quantity [e.g., *Worley et al.*, 2005]. Surface data, however, do not suffice to fully understand the mechanisms governing large-scale climate variability.

Upper air data are needed for accurate descriptions of important dynamical features such as the positions of the jet streams, the planetary wave structure, and the strength of the stratospheric polar vortex. Yet, gridded upper air data sets currently are available only for the second half of the twentieth century; they are based largely on radiosonde data, and since 1973, on radiosonde and satellite data (Figure 1).

Although the notion is widespread among climate scientists that there were no operational upper air measurements before about 1948, this is not the case (Figure 1). Radiosonde observations have been made since the mid-1930s. Prior to the radiosonde era, weather balloons with graphical registering devices were used. Even more common were kite soundings or aircraft measurements up to 4 or 5 km altitude. Pilot balloons have been launched routinely since the early twentieth century to obtain information on upper level winds. In addition to meteorological measurements, spectrographical total ozone observations reaching back to the 1920s can be used to derive indirect information on stratospheric dynamics.

The total amount of data is small by current standards, but it is non-negligible. It is estimated that several million pilot balloons were launched prior to 1948, and there were several hundred thousand radiosonde ascents and aircraft flights (Figure 1).

Significant fractions of these data are currently being digitized and processed by organizations such as the U.S. National Climate Data Center (NCDC), the National Center for Atmospheric Research (NCAR), and the World Data Center (WDC) for Meteorology in Obninsk, Russia. Additional work is done by scientists at the Swiss Federal Institute of Technology (ETH) Zürich in the framework of a Swiss National Science Foundation project led by the first author.

Re-evaluating historical upper air data is demanding work. After digitizing the numbers from paper, the data need to be corrected for various instrumental errors, a task made difficult by the lack of good background information.

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