MAR05-2004-000455

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Theoretical and experimental evidence for a post-perovskite phase of $MgSiO_3$ in Earth's D″ layer.

ARTEM R. OGANOV[1], 1Laboratory of Crystallography, Department of Materials ETH Hnggerberg, HCI G 515, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland

The Earth's lower mantle, the largest region within our planet (670-2890 km depths), is believed to contain ∼75 vol.% of (Mg,Fe)SiO_3 perovskite, ∼20% (Mg,Fe)O, and ∼5% $CaSiO_3$. This mineralogy was unable to explain many unusual properties of the D" layer, the lowermost ∼150 km of the mantle. Using *ab initio* simulations and high-pressure experiments we have demonstrated [1] that at pressures and temperatures of the D″ layer, $MgSiO_3$ transforms from perovskite into a layered $CaIrO_3$–type structure (space group *Cmcm*); this structure was also independently found in [2]. The elastic properties of the new phase and its stability field explain most of the previously puzzling properties of the D″ layer: its seismic anisotropy [3], strongly undulating shear-wave discontinuity at its top[4], and the anticorrelation between shear and bulk sound velocities [5]. This new phase is therefore likely to be a major Earth-forming mineral, and its discovery will change our understanding of the deep Earth's interior. Latest studies of the effects of impurities [6,7] on the stability of this phase, and similar phases of other compounds will be discussed.

REFERENCES:

1. Oganov A.R., Ono S. (2004). *Nature* **430**, 445-448.
2. Murakami M., et al. (2004). *Science* **304**, 855-858.
3. Panning M., Romanowicz B. (2004). *Science* **303**, 351-353.
4. Sidorin I., et al. D.V. (1999). *Science* **286**, 1326-1331.
5. Su W.J., Dziewonski A.M. (1997). *Phys. Earth Planet. Inter.* **100**, 135-156.
6. Mao W.L., et al. (2004). *Proc. Natl. Acad. Sci.* **101**, 15867-15869.
7. Ono S., Oganov A.R., Ohishi Y. (2004). *Submitted.*

[1]This work was done in collaboration with Dr. Shigeaki Ono (Japan)