

Report on the AGU fall meeting 2007 9th-14th December, San Francisco, USA

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Conference summary :

The AGU fall meeting gathers each year more than 14,000 persons and presents an overview of all topics in Earth's science. During the week, I attended a lot of interesting sessions and the list of which is given below (a description of the whole sessions is available at :

<http://www.agu.org/meetings/fm07/?content=program>) :

- Advances in computational studies of Earth materials. This session broadly covered the application of computational methods to mineral physics and material properties that complement experimental work, and provide a theoretical framework for understanding geomaterials.
- Diffusion and transport properties in geomaterials. The presentations dealt with many topics as conductivity, diffusion of defects and electronic properties of minerals.
- « Quantification of rock fabrics » session treated of microstructures of geomaterials.
- Behaviour of iron in the deep Earth and new views of the mantle core. This session was focused on the spin transition and the changes of materials behaviour in the core and in perovskite.
- Frontiers in the chemistry and physics of the Earth's mantle. This session covered a lot of subjects as partitioning of iron in mantle materials and spin transition.
- Plasticity of minerals at high pressure and temperatures and implications for Deep-Earth rheology and anisotropy.
- « Structures and properties of Earth's interior probed using advanced radiation laboratory tools, and seismic waves » dealt with using the synchrotron to establish the properties of geomaterials.

All these sessions were split into 2 parts : one was reserved to the talks and the other to the posters.

My poster 'Are CaIrO_3 and MgGeO_3 isomechanical to MgSiO_3 -post-perovskite ?' was presented in the 'Plasticity of minerals at high pressures and temperatures and implications for deep Earth rheology and anisotropy' session. It was well-received and stimulated interesting discussions with people in the field of plastic deformation and computing science.

This AGU fall meeting was a great success for future development of my scientist career and I would like to thank the ESF-EUROCORES-EuroMinSci program for the funding of this travel by a dissemination grant.

Presented abstract :

Are CaIrO_3 and MgGeO_3 isomechanical to MgSiO_3 -post-perovskite ?

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The recent discovery of MgSiO_3 post-perovskite (pPv) and prediction of its elastic properties using atomistic modelling has major implications for the interpretation of seismic anisotropy of the D" layer. Because they don't take into account lattice preferred orientations induced by convective flow, the elastic properties are not sufficient to interpret seismic anisotropy and it is necessary to investigate the plasticity of this mineral. However, it is well known that pressure and temperature near the core-mantle boundary make experimental studies extremely difficult. To circumvent this difficulty, experimental studies are often carried out on analogous phases (stable at lower pressures) which are supposed to exhibit the same mechanical properties as the high-pressure phase.

In this work, we calculate the dislocation properties of MgGeO_3 pPv at 120GPa and CaIrO_3 pPv at ambient pressure using the Peierls-Nabarro (PN) model. The so-called PN model is a fundamental concept of the dislocation theory which describes the resistance of the lattice to dislocation motion, a very important factor for the plasticity of silicates. The PN model also provides an analytical description of the dislocation core and of its potential spreading in the glide plane. Known for several decades, the PN model has triggered a renewed interest when Christian and Vitek (1970) showed that realistic models of dislocations could be built by incorporating generalized stacking faults (GSF) into the PN model. Here, we use the *ab initio* total-energy package VASP to calculate GSF, which are incorporated in the PN model. In that way, we obtain a model of the dislocation core profile and the value of the stress required to move a dislocation (the so-called Peierls stress) for ten slip systems of each compound. These results are compared to those recently published on MgSiO_3 post-perovskite to assess the potential relevance of the analogue approach in studying the rheology of the D" layer.

We show that, besides the crystal structure, atomic bonding is an important feature in constraining plastic strain anisotropy. The greatest contrast between Ca-O and Ir-O bond strengths compared to Mg-O and Ge-O or Si-O makes CaIrO_3 behave very distinctly from MgSiO_3 . Although still present, differences are smaller between MgGeO_3 and MgSiO_3 .