

**FA2-MS15-T01**

**Shear deformation and phase transitions in mantle minerals studied by atomic scale simulations.** Sandro Jahn. *GFZ German Research Centre for Geosciences, Telegrafenberg 14473 Potsdam, Germany.*  
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Investigations of the physical properties of silicates and their thermodynamic stability under extreme conditions of pressure and temperature are indispensable to obtain a better understanding of the structure and dynamics of the Earth. In recent years, substantial progress has been made in this field through the development of new methods in high pressure mineral physics using both experimental and atomic scale modeling approaches. The latter are especially powerful when they are used to predict properties or phase behavior at conditions where experiments are difficult to perform or to reveal some of the underlying principles of measured properties or processes. Here, we use a combined approach of atomic scale modeling techniques to shed light on the mechanisms of non-elastic deformation and polymorphic phase transitions of mantle silicates. While first-principles calculations in the framework of density-functional theory provide the most accurate information on the crystal structures and their thermodynamic stabilities, a combination of classical molecular dynamics and metadynamics is employed to study the actual deformation or transformation process. Examples include phase transformations between various polymorphs of MgSiO<sub>3</sub> pyroxenes [1-3] and between the Mg<sub>2</sub>SiO<sub>4</sub> polymorphs olivine and ringwoodite. Shear deformations observed in the metadynamics simulations will be related to rheological properties of the corresponding silicates. For Mg<sub>2</sub>SiO<sub>4</sub> olivine, a change of slip system is predicted towards high pressure and/or high temperature.

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**Keywords: High-pressure minerals, Molecular dynamics, Phase transitions**

**FA2-MS15-T02**

**Interplay Between Structural and Electronic Behavior in Iron Bearing Earth Lower Mantle Minerals.** L. Dubrovinsky<sup>a</sup>, C. McCammon<sup>a</sup>, K. Glazyrin<sup>a</sup>, O. Narygina<sup>a</sup>, M. Merlini<sup>b</sup>, I. Kantor<sup>c</sup>, M. Hanfland<sup>c</sup>, A. Chumakov<sup>c</sup>. <sup>a</sup>*Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany.*  
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A major goal in the geosciences is to understand (and predict) how the Earth works, which requires a detailed knowledge of how the mineral phases which make up the Earth behave under high pressure and high temperature conditions. Much attention has been focused on the silicate perovskite and magnesium-iron oxide phases, since they make up major part of the Earth's interior. Special attention has been focused on possible phase transformations of the materials due to their

significant implications for mantle behavior. The majority of measurements have been made on *pure* MgSiO<sub>3</sub> perovskite, however, and almost exclusively using X-ray powder diffraction. Although the importance of Fe and Al as minor components of the silicate perovskite phase has been well documented in the past decade in numerous papers including many published in *Science* and *Nature*, the few studies using methods sensitive to these elements (e.g., X-ray emission spectroscopy and nuclear forward scattering) were not sufficiently systematic and/or sensitive to recognize any significant changes in the pressure range below 100 GPa. We studied silicate perovskites (Mg<sub>0.88</sub>Fe<sub>0.12</sub>)SiO<sub>3</sub> and (Mg<sub>0.9</sub>Fe<sub>0.1</sub>)(Si<sub>0.975</sub>Al<sub>0.025</sub>)O<sub>3</sub> and series of magnesiowustites by means of high resolution X-ray single crystal and powder diffraction in laser-heated diamond anvil cells, Mossbauer spectroscopy, and nuclear forward scattering at pressure up to 120 GPa and temperature above 2000 K. We will discuss effects of changes in iron electronic state on structure of mantle minerals.

**Keywords: mantle mineralogy, laser-heating, DACs, single crystals, structure**

**FA2-MS15-T03**

**P<sub>2</sub>/c to C<sub>2</sub>/c phase transition in clinopyroxenes and the geodynamic implications.** Matteo Alvaro<sup>a</sup>, Fabrizio Nestola<sup>b</sup>, Fernando Camara<sup>c</sup>, Chiara M. Domeneghetti<sup>d</sup>, Vittorio Tazzoli<sup>d</sup>, Ross J. Angel<sup>a</sup>. <sup>a</sup>*Crystallogr. Lab., Virginia Tech, Blacksburg, U.S.A.* <sup>b</sup>*Dip. di Geoscienze, Università di Padova, PD, Italy.* <sup>c</sup>*C.N.R. – IGG – Unita' di Pavia, PV, Italy.* <sup>d</sup>*Dip. di Scienze della Terra, Univ. di Pavia, PV, Italy.*  
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Clinopyroxenes are chain silicate minerals, in which there are two chains, made up by corner-sharing SiO<sub>4</sub> - tetrahedra running parallel to the *c* - axis. The two chains are crosslinked by M1 (containing Mg, Fe<sup>2+</sup>, Fe<sup>3+</sup>, and Al) and M2 (containing Ca, Fe<sup>2+</sup>, Mg and Na) polyhedra. There are three polymorphs (HT-C<sub>2</sub>/c, P<sub>2</sub>/c, HP-C<sub>2</sub>/c) stable at different pressure and temperature conditions. At ambient conditions the space group is P<sub>2</sub>/c, which transforms to HT-C<sub>2</sub>/c and HP-C<sub>2</sub>/c at high-temperature and high-pressure conditions respectively. The HP and HT C<sub>2</sub>/c structures have the same Wyckoff positions as one another but different geometries. Moreover both the high-pressure and high-temperature phase transitions are strongly dependent upon composition. Clinopyroxenes represent about 12% of the upper mantle of the Earth, and are involved in many geodynamic processes. Therefore the knowledge of their structural, physical-chemical and thermodynamic properties will be crucial in interpreting the structure and dynamics of the upper mantle.

Pure clinoenstatite MgSiO<sub>3</sub> is stable at least up to 8-8.5 GPa (240-255 km depth) and it undergoes a phase transformation from P<sub>2</sub>/c to C<sub>2</sub>/c at about 6.2 GPa accompanied by a strong and discontinuous change in density. Such a density change would cause a sudden jump in the seismic velocity waves at the upper mantle close to 180-190 km depth. But a more realistic composition for upper-mantle P<sub>2</sub>/c clinopyroxene would include a small but significant amount of both Ca and Fe in its structure. Both Ca and Fe separately strongly decrease the pressure of the transformation. The average M2 ionic radius is of course the only parameter which allowed us to evaluate the effect of Ca and Fe together. We have