

Keynote Lecture

KN32

Polymorphism and electronic transformations of deep Earth minerals

L. Dubrovinsky¹

¹*Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth, Germany*

While powder X-ray diffraction studies stepped over a megabar in pressure already in the 1970s, single crystal experiments remained much rarer and covered until recently a very limited pressure range barely reaching 15 GPa. Recent technological advances resulted in a revolutionary breakthrough in the high-pressure crystallography. The structure solution and the full refinement are now possible at pressures over 100 GPa. A comprehensive understanding of the iron- and aluminum-bearing magnesium silicate perovskite (Pv) and post-perovskite (PPv, CaIrO₃-type) crystal structures and their evolution under pressure and temperature is vital for evaluating seismic data of the Earth's lower mantle. We investigated materials with different compositions and iron oxidation states by means of single-crystal X-ray diffraction at pressures over 150 GPa and temperatures over 2500 K, and by Mössbauer spectroscopy. By structural studies of Pv at extreme conditions, we found (a) no spin state crossover in ferric iron occupying the bicapped trigonal prism ("A" crystallographic site), and (b) no crystal-chemically significant amount of ferric iron in the octahedral "B-site at any conditions of our experiments. We synthesized single crystals of PPv, refined their structure and distribution of iron between the structural sites. We demonstrated that incorporation of ferric iron and aluminum significantly increases the compressibility of magnesium silicate Pv and PPv. Based on experimental data we constrained the thermal equation of state for Pv and PPv with a variable content of iron (ferrous and ferric) and aluminum. We concluded that variation of $Fe^{3+}/\Sigma Fe$ can lead to significant changes of Pv bulk sound velocity (over 1%) demonstrating that the oxidation state of iron is a critical parameter for interpretation of seismic tomography data.

Keywords: pressure, single crystal, phase transitions