mantle. Here we report equation of state (EoS) and Rietveld refinement data of MgGeO3-ppv phase (CaIrO3-type, Cmcm) together with EoS data of silicate-ppv phase experimentally determined for the first time.

Germanate and silicate ppv phases were synthesized from MgGeO3 and Mg0.9Fe0.1SiO3 orthopyroxene at 86 GPa, ~1600 K and 103 GPa, ~1900 K, respectively, using laser-heated diamond cells with Ar or NaCl pressure medium. Angle-dispersive X-ray diffraction experiments were conducted at 13-ID-D, Advanced Photon Source. EoS data (bulk modulus, its pressure derivative, and room pressure unit cell volume) were obtained using Birch-Murnaghan EoS to be 203(6) GPa, 4.4, 179.7(9) A^3 for MgGeO3-ppv and 219(5) GPa, 4.4, 164.9(6) A^3 for silicate-ppv. Rietveld refinement of MgGeO3-ppv was performed using GSAS/EXPGUI. A change in compression mechanism was found at ~45 GPa. Although b-axis is the most compressible axis in the pressure range investigated, it is significantly more compressible at the lower pressure range. The reason is explained by decrease of distortion of GeO6 octahedron in the lower pressure range, and by both increase of distortion of GeO6 octahedron and shortening of Mg-O distances in the higher pressure range.

**Keywords: high-pressure phases, X-ray powder diffraction, Rietveld refinement**

**MS54.27.3**

*Acta Cryst*. (2005). A**61**, C71

**Refinement of High Pressure Metrology to 150 GPa**

Agnès Dewaele[a], Paul Loubeyre[a], Mohamed Mézouar[b], *[a]DPTA, Commissariat à l'Energie Atomique, France. [b]ESRF, Grenoble, France.* E-mail: agnes.dewaele@cea.fr

In static high pressure experiments, the pressure cannot be directly measured. Therefore, secondary pressure scales must be used, such as luminescence gauges (like ruby) and x-ray gauges (gold, platinum, MgO, etc.). The calibration of these gauges is a critical issue: for instance, geophysical studies of the Earth's mantle transition zone minerals under high pressure and temperature have revealed to be inconsistent because of the use of incompatible pressure gauges [1]. We have measured ambient temperature equations of state of 13 metals (Be, Al, Fe, Co, Ni, Cu, Zn, Mo, Ag, Ta, W, Pt, Au) under quasi-hydrostatic conditions in a diamond anvil cell, up to at least 65 GPa and at a maximum pressure of 153 GPa. The use of state of the art pressurizing and x-ray diffraction techniques [2] allowed us to obtain standard synchrotron x-ray diffraction accuracy in the volume determination to the maximum pressure. This data set can been used to re-calibrate the static pressure scale based on the ruby luminescence wavelength measurement [3]. The accuracy of various forms of luminescence wavelength vs. pressure in different pressure ranges will be discussed. In particular, this recalibration confirms recent suggestions of an underestimation of pressure by [3] at ultra-high pressure.

[1] Bina C.R., *Nature*, 2001, **411**, 536. [2] Dewaele A., et al., *Phys. Rev. B*, 2004, **70**, 94112. [3] Mao H.K., et al., *J. Geophys. Res.*, 1986, **91**, 4673.

**Keywords: diamond anvil cells, high-pressure physics, X-ray diffraction**

**MS54.27.4**

*Acta Cryst*. (2005). A**61**, C71

**Shock-Induced Superheating-Melting and Geophysical Implications**

Sheng-Nian Luo, *Plasma Physics, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA.* E-mail: sluo@lanl.gov

Superheating is a metastable state with the long-range order of a solid sustained above the equilibrium melting temperature, and a rare phenomenon. The limit of superheating was attempted realistically by assuming an arbitrary critical nucleation rate [1]. Based on classical nucleation theory and supercooling experiments, we developed the systematics relating materials properties to the maximum superheating (supercooling) and heating (cooling) rates, consistent with shock wave experiments, molecular dynamics simulations and Landau-type models [2-5]. Superheating is more achievable under ultrafast heating rate. There are strong indications of superheating in shock experiments on translucent solids using optical pyrometry [6-8] and on single crystal Al during dynamic spallation [9].

High strain- and heating-rates experiments such as shock wave loading are an essential complement to diamond-anvil cell techniques for investigating translucent minerals and opaque metals [10]. We present an exhaustive survey on superheating-melting behavior of alkali halides, silicates and metals, and their geophysical implications.

[1] Lu K., Li Y., *Phys. Rev. Lett*., 1998, **80**, 4474. [2] Luo S.N., Ahrens T.J., *Appl. Phys. Lett.*, 2003, **82**, 1836. [3] Luo S.N., Ahrens T.J., Cagin T., Strachan A., Goddard W.A., Swift D.C., *Phys. Rev.* B, 2003, **68**, 134206. [4] Luo S.N., Strachan A., Swift D.C., *J. Chem. Phys.*, 2004, **120**, 11640. [5] Luo S.N., Swift D.C., *J. Chem. Phys.*, 2004, **121**, 7387. [6] Luo S.N., Akins J.A., Ahrens T.J., Asimow P.D., *J. Geophys. Res.*, 2004, **109**, B05205. [7] Boness D.A., Brown J.M., *Phys. Rev. Lett.*, 1993, **71**, 2931. [8] Lyzenga G.A., Ahrens T.J., Mitchell A.C., *J. Geophys. Res.*, 1983, **88**, 2431. [9] Kanel G.I., Razorenov S.V., Baumung K., Singer J., *J. Appl. Phys.*, 2001, **90**, 136. [10] Luo S.N., Ahrens T.J., *Phys. Earth Planet. Int*., 2004, **143-144**, 369.

**Keywords: superheating-melting, shock, molecular dynamics**

**MS54.27.5**

*Acta Cryst*. (2005). A**61**, C71

**Predicting Crystal Structures of New High-pressure Mineral Phases**

Colin W. Glass[a], Artem R. Oganov[a], Nikolaus Hansen[b], *[a]Laboratory of Crystallography, Department of Materials ETH Hönggerberg, HCI G 515, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland. [b]Institute of Computational Science, ETH-Zentrum, HRS H 03, Hirschengraben 84, 8092 Zürich, Switzerland.* E-mail: coglass@student.ethz.ch

We approached the problem of predicting crystal structures using three different methods: CMAES [1], Metadynamics [2,3] and Evolutionary Algorithms [4].

The different methods and their results for the high-pressure structures of $MgSiO_3$ and $MgCO_3$ will be presented and discussed. On the methodological side, we will focus on our implementation of an Evolutionary Algorithm based on spatial heredity and combined with local optimization. This algorithm proved to be an efficient way to tackle high dimensional problems such as crystal structure prediction and hence has a promising future in predicting, on a fully theoretical basis, new crystal structures under pressure.

[1] Hansen N., Ostermeier A., *Evol. Comp*. , 2001, **9**, 159. [2] Martonak R., Laio A., Parrinello M., *Phys. Rev. Lett*. , 2003, **90**, 075503. [3] Oganov A.R., Martonak R., Laio A., Raiteri P., Parrinello M., 2005, *in preparation*. [4] Michalewicz Z., Fogel D.B., *How to Solve It: Modern Heuristics*., Springer, Berlin, 2004.

**Keywords: structure prediction, global optimization, evolutionary algorithm**

## MS55 TIME RESOLVED DIFFRACTION

***Chairpersons:*** Jianming Cao, Hervé Cailleau

**MS55.27.1**

*Acta Cryst*. (2005). A**61**, C71-C72

**Laser-Plasma X-ray Sources and Their Applications**

Davide Boschetto, Kim Ta Phuoc, Antoine Rousse, *Laboratoire d'Optique Appliquée ENSTA/Ecole Polytechnique, 91761 Palaiseau cedex, France.* E-mail: davide.boschetto@ensta.fr

A single atomic vibrational motion is on the order of 100 fs (1 fs=$10^{-15}$ s), which sets the fundamental timescale of material in response to an external excitation. Using pump-probe approach and initiating the dynamics with an ultra-short laser pulse, the new tool of femtosecond X-ray diffraction provides a direct means of monitoring the atomic positions during photo-induced transition in materials on this fundamental timescale and with sufficient spatial resolution.

In this talk we will show on one side the first type of femtosecond X-ray source, based on the laser-plasma interaction on solid target [1], together with its applications in the study of non-thermal melting in semiconductor [2] and the direct measurement of coherent optical phonons [3].