icosahedra. The best estimate on the number of atoms in the unit-cell is not even an integer number, 320.1, originating from the introduction of partial occupancy of atomic sites in the X-ray structural analysis [1].

This work is the first attempt, using *ab initio* molecular dynamics, to study the stable configuration of the partially occupied sites (POS) in β-boron and to investigate POS impact on the electronic structure. We have found that the correlated POS configurations not only lower the total energy of the solid, but also widen the electronic band gap, giving consistent results with experiments.

The high pressure phases of boron[2,3] have also been studied with *ab initio* simulated annealing methods. We found that at around 120GPa, β-rhombohedral boron undergoes amorphization and that its electronic conductivity rises, due to delocalization of the electronics states near the Fermi level, consistent with experimental observations[2,3].

This work was performed under the auspices of the U. S. Dept. Energnergy at the University of California/LLNL under contract no. W-7450-Eng-48.

[1] Slack G. A., et al., *J. Solid State Chem*., 1988, **76**, 52. [2] Eremets M. I., et al., *Science*, 2001, **293**, 272. [3] Sanz D. N., et al., *Phys. Rev. Lett.* 2002, **89**, 245501.

Keywords: ab initio structural determination, high pressure structure, electronic structure

MS40.26.3

Acta Cryst. (2005). A**61**, C55

Oxides Under Pressure: from Densified Silica to the Rheology of the Earth's Mantle

Sandro Scandolo, *The Abdus Salam ICTP, Trieste, Italy*. E-mail: scandolo@ictp.trieste.it

The paper will describe recent advances in the atomistic simulation of oxides at extreme conditions of pressure. The simulations are carried out using interatomic force fields optimized by best fit on first-principles (density-functional theory) calculations. The paper will focus on two applications of the method: (a) the mechanisms of permanent densification in silica glass, and (b) the properties of dislocations in MgO, the second most abundant mineral in the Earth's lower mantle.

Keywords: simulation, DFT, high pressure

MS40.26.4

Acta Cryst. (2005). A**61**, C55

Novel High-pressure Phases: Theory and Experiment

Artem R. Oganov[a], Shigeaki Ono[b], Roman Martonak[c], Alessandro Laio[c], Paolo Raiteri[c], Michele Parrinello[c], *[a]Laboratory of Crystallography, Department of Materials ETH Hönggerberg, HCI G 515, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland. [b]Institute for Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology, 2-15 Natsushima-cho, Yokosuka-shi, Kanagawa 237-0061, Japan. [c]Computational Science,Department of Chemistry and Applied Biosciences ETH Zurich,LUI USI-Campus, Via G. Buffi 13, CH-6900 Lugano, Switzerland*. E-mail: a.oganov@mat.ethz.ch

Searching for new materials and new crystal structures at high pressures and temperatures is important for fundamental physics, for material sciences, and for understanding the structure and properties of planetary interiors. State-of-the-art computer simulations can fruitfully complement or even guide experimental efforts in this direction. Here, we present recent joint theoretical/experimental discoveries of new geophysically important phases of $MgSiO_3$ [1-3] and Al_2O_3[4] with implications for the structure, dynamics, electrical conductivity, rheology and seismic signatures of the Earth's lowermost mantle.

[1] Oganov A.R., Ono S., *Nature*, 2004, **430**, 445. [2] Murakami M., et al., *Science*, 2004, **304**, 855. [3] Oganov A.R., Martonak R., Laio A., Raiteri P., Parrinello M., 2005, *in preparation*. [4] Oganov A.R., Ono S., *Proc. Natl. Acad. Sci.*, 2005, *submitted*.

Keywords: high pressure, ab initio, Earth's mantle

MS40.26.5

Acta Cryst. (2005). A**61**, C55

$MgSiO_3$ Post-perovskite at D" Conditions

Renata M. Wentzcovitch, Taku Tsuchiya, Jun Tsuchiya, *Department of Chemical Engineering and Materials Science, Minnesota. Supercomputing Institute for Digital Technology and Advanced Computations, University of Minnesota, Minneapolis*. E-mail: wentzcov@cems.umn.edu

The thermoelastic properties of the newly found post-perovskite polymorph of MgSiO3, more stable than the Pbnm-perovskite phase at conditions close to those expected in Earth's D" region, has been investigated by first-principles and contrasted with those of the perovskite phase. We predict the major seismic trends such as velocity discontinuities, ratios of velocities and density anomalies, and anisotropy in aggregates with preferred orientation that should occur in the presence of this phase change. Consequences of this model mineralogy for the D" region will be discussed.

Research supported by JSPS, NSF/EAR 0135533 (COMPRES), 0230319, and NSF/ITR 0428774.

Keywords: phase transition, mantle mineralogy, thermoelasticity

MS41 COMPUTATIONAL SOLUTIONS FOR HIGH-THROUGHPUT CRYSTALLOGRAPHY

Chairpersons: Duncan E. McRee, James Holton

MS41.26.1

Acta Cryst. (2005). A**61**, C55

Crank - New Methods in Automated Structure Solution

Steven R. Ness, Rudolf A.G. de Graaff, Jan Pieter Abrahams, Navraj S. Pannu, *Department of Biophysical Structural Chemistry, Leiden University, Leiden, The Netherlands*. E-mail: s.ness@chem.leidenuniv.nl

We present Crank[1], a suite to help a user perform automated macromolecular structure solution. In this aim, it uses novel programs, including CRUNCH2 for substructure determination and BP3 for substructure refinement and phasing. In addition, Crank uses other commonly used crystallographic programs including SOLOMON, DM and various programs within the CCP4 suite. Crank uses the CCP4i package for its user interface, this allows for tight integration into the CCP4 suite and presents the user with a familiar interface. Crank uses the XML eXtensible Markup Language to store, manipulate and compare data, this XML can subsequently be used to assist in data deposition. We have tested Crank on a large number of datasets, including datasets from the Joint Center for Structural Genomics, our results show that Crank often outperforms existing automated substructure solution packages, and can lead to solutions where existing methods fail. For more information, please visit the Crank web site: http://www.bfsc.leidenuniv.nl/software/crank.

[1] Ness S. R., de Graaff R.A.G., Abrahams J. P., Pannu N.S., *Structure*, **12**, 1753-1761.

Keywords: automated macromolecular structure solution, BP3, crunch2

MS41.26.2

Acta Cryst. (2005). A**61**, C55-C56

Parallel Data Processing for High Throughput X-ray Structure Determination

Guenter Wolf, Herbert Axelrod, Henry van den Bedem, Hsiu-Ju Chiu, Mitchell D. Miller, Christopher L. Rife, Qingping Xu, Ashley M. Deacon, *Joint Center for Structural Genomics, Stanford University, Menlo Park, CA, USA*. E-mail: gwolf@slac.stanford.edu

The Structure Determination Core (SDC) of the Joint Center for the Structural Genomics (JCSG) has implemented a prototype system, Xsolve, which automates all of the processing steps needed to create an initial set of molecular coordinates from a dataset of diffraction images. The goal of Xsolve is to provide standardized, high quality data processing and automate the numerous time-consuming steps in the structure determination process. The current prototype produces a model that is over 95% complete in more than 80 % of the MAD cases