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

with data to 2.5 Å or better.

Xsolve, a Java Message Service (JMS) based control system, can run on a Linux cluster different processing strategies in parallel, e.g. the data can be processed in several different space groups or MAD/SAD structure determination can be attempted using various wavelength combinations.

Xsolve supports a wide range of crystallography software programs, which can be used in parallel: data reduction with Mosflm, Denzo/HKL2000, XDS and Scala; heavy atom solution and phase determination with Solve, SHELXD/E and Sharp; phase improvement with Resolve and model building with Resolve and ARP/wARP.

The JCSG is supported by NIGMS/PSI (P50-GM 62411). SSRL operations are funded by DOE BES, and the SSRL Structural Molecular Biology program by DOE BER, NIH NCRR BTP and NIH NIGMS.

**Keywords: automatic structure solution, MAD, software**

**MS41.26.3**

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

**Iterative Model Building and Evaluation with Statistical Density Modification**

Thomas Terwilliger, *Bioscience Division, Los Alamos National Laboratory, Mail Stop M888, Los Alamos, NM 87545 USA.* E-mail: JMHolton@lbl.gov

Automated model-building beginning with an FFT-based search for helices and sheets and followed by chain extension using tripeptide fragments from high-resolution structures and pattern-based probabilistic identification of side chains has been successful in automated model building for maps with resolution as low as 3 A. Model-building can be combined with refinement and statistical density modification to improve the quality and completeness of atomic models of macromolecules and to evaluate the quality of atomic models. A useful tool in removing model bias is prime-and-switch phasing. In this technique a substantially correct model containing some atoms in incorrect positions is used to estimate ("prime" initial phases, and a second source of phase information such as a flat solvent region is used without reference to the original phase probabilities in density modification. After prime-and-switch phasing the density at incorrect atomic positions is often considerably decreased compared to that at correct positions. This technique has been incorporated as an integral part of iterative model-building and refinement in the PHENIX software (http:www.phenix-online.org).

**Keywords: model building, PHENIX, atomic models**

**MS41.26.4**

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

**Automated Operation of Protein Crystallography Beamlines at the SPring-8**

Masaki Yamamoto[a], Go Ueno[a], Raita Hirose[b], Koh Ida[a], Takashi Kumasaka[a,c], [a]*SPring-8/RIKEN.* [b]*PharmAxess Inc.* [c]*Tokyo Institute of Technology*. E-mail: yamamoto@postman.riken.go.jp

RIKEN Structural Genomics Beamlines (BL26B1&B2) at the SPring-8 have been constructed for high throughput protein crystallography. The beamline operation is automated cooperating with the sample changer robot named SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger) [1].

Since April 2004, BL26B2 has been continuously operated with the sample changer. More than twenty-five crystals a day have been constantly delivered by sample-tray to the beamline. The crystal screening at the beamline can be finished within ten minutes per a sample. For qualified crystals, unattended data collections have been perpetually performed. The sample-tray is portable with a Dewar and experimental conditions are uploaded to the web site, which have been developed considering the mail-in data collection.

The operation software BSS (Beamline Scheduling Software) provides the intuitive GUI and unified control of beamline instruments with the networked client-server architecture. The software structure has flexibility to be implemented at other protein crystallography beamlines. Other than BL26B1 and B2, three other beamlines have already adopted BSS. Further application to other beamlines is progressing to achieve the unified and user-friendly environment among all beamlines at the SPring-8.

[1] Ueno G., Hirose R., Ida K., Kumasaka T., Yamamoto M., *J. Appl. Cryst*.,2004, **37**, 867-873.

**Keywords: automated data collection, high-throughput protein crystallography, mail-in data collection**

**MS41.26.5**

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

**Automated Protein Structure Determination with *BnP***

William Furey[a], L. Pasupulati[a] , S. A. Potter[b], H. Xu[b], R. Miller[b,c], C. M. Weeks[b], [a]*VA Med. Center, Pittsburgh PA & Dept. Pharmacol., U. Pittsburgh.* [b]*Hauptman-Woodward Institute, Buffalo NY.* [c]*Center for Comp. Res., SUNY at Buffalo.* E-mail: fureyw@pitt.edu

*BnP*[1] is a protein structure determination package with a graphical user interface suitable for both manual and automated operation. *BnP*'s main function is to couple the direct-methods program *SnB*, used to determine heavy atom/anomalous scatterer substructures, with the protein-phasing package *PHASES*, used for heavy atom refinement, protein phasing, density modification, and skeletonization. It also creates data and scripts for external programs required for automated chain tracing, graphical visualization, and refinement. In addition to seamlessly interfacing the various packages, near total automation is implemented such that one needs only to specify a few parameters, and the entire phasing process starting with diffraction data and resulting in interpretable electron-density maps is carried out by clicking a single button. With a couple of additional button clicks external programs for automated chain tracing or chain tracing/refinement can then be launched. The overall strategies and methodology employed will be described, with emphasis on those aspects required to facilitate automation and recent developments simplifying user input. Extensive test results verify the package's effectiveness. This work was supported by NIH grant EB002057.

[1] C. M. Weeks et. al., *Z. Kristallogr*., 2002, **217**, 686-693.

**Keywords: automated structure determination, high-throughput, phasing methods**

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**MS42 COMPLEMENTARITIES OF NEUTRON AND X-RAYS METHODS IN MATERIAL SCIENCE**

***Chairpersons:*** Andreas Schreyer, Mark R. Daymond

**MS42.26.1**

*Acta Cryst*. (2005). A**61**, C56-C57

**Integrated Use of Synchrotron and Neutron Diffraction to Monitor Residual Stress Evolution in Welded Aerospace Structures**

Lyndon Edwards, *Department of Materials Engineering, Open University, Milton Keynes, UK MK7 6A.* E-mail: l.edwards@open.ac.uk

The factors controlling fatigue initiation and crack growth in welds are reasonably well understood and the importance of residual stress, HAZ hardness and microstructure is well known. However, previous access to reliable, spatially accurate residual stress field data has been limited. Recent advances in neutron and synchrotron diffraction allow a far more detailed picture of weld residual stress fields to be obtained which permits the development and use of predictive models that can be used for accurate design against fatigue in aircraft structures. This paper describes a fully integrated study of the 3D residual stress distribution accompanying state-of-the-art fusion welds in 2024 and 7150 aluminium aerospace alloys, and how they are affected by subsequent machining and service loading. A particular feature of this work has been the development of integrated neutron and synchrotron techniques allowing the non-destructive evaluation of the residual stress field in the full range of specimens used to provide the design data required for welded aircraft structures. This has included small bend specimens used to study initiation and short fatigue crack growth, centre-cracked panels used to study long fatigue crack growth, and large integral welded double stringer/skin mock-ups used to investigate the likely failure mode of welded wing-