field (TMF). Indeed, by properly selecting the phase shift between the signals sent to three or more heaters around the crucible, the magnetic field may be made "travelling" along the crucible. In this way the normal growth parameters of the melt growth (pulling/solidification rate, temperature gradient, rotations) are enriched with new degrees of freedom, namely intensity, frequency and direction of the non-stationary magnetic field. By choosing the right field parameters, the crystal grower has the possibility of either stimulating or damping the melt convection, acquiring in this way a good control over transport phenomena in the liquid phase. This in turn provides an efficient control of the solid-liquid interface shape.

In this presentation the concept of travelling magnetic field and the necessary hardware modification will be presented. The results of TMF applied to Czochralski growth of silicon and Vertical Gradient Freeze of germanium and silicon will also be reported. These examples also show that the use of this magnet-heater ensemble provides bulk crystals of superior quality.

[1] P. Rudolph, *J. Crystal Growth* **2009** 310 1298
[2] Ch. Frank-Rotsch, P. Rudolph, *J. Crystal Growth* **2009** 311 2294
[3] P. Rudolph, M. Czupalla, B. Lux, *J. Crystal Growth* **2009** 311 4543

Keywords: Semiconductor, Crystallization, Czochralski

KN09

Acta Cryst. (2011) A**67**, C8

Discovery of post-Perovskite at high pressure and its geophysical implications

Kei Hirose, *Department of Earth and Planetary Sciences, Tokyo Institute of Technology (Japan)*. E-mail: kei@geo.titech.ac.jp

Recent developments in X-ray diffraction (XRD) measurements at the synchrotron radiation source, combined with laser-heated diamond-anvil cell (LH-DAC) techniques, enables the crystal structure determinations at ultrahigh-pressure and -temperature (*P-T*) conditions expected for the deep Earth. MgSiO$_3$ perovskite is known to be a primary mineral in the Earth's lower mantle below 660-km depth and the most abundant mineral inside the Earth, but its stability and possible phase transition to a denser structure in the lowermost mantle has long been a matter of debate because large seismic anomalies found in this region are not reconciled with the known properties of perovskite. Recently we discovered a novel phase transition from MgSiO$_3$ perovskite to post-perovskite through a drastic change in the XRD pattern at high *P-T* conditions near the base of the mantle around 2600-km depth [1, 2]. Crystal structure of post-perovskite was determined with the aid of computer simulations of atomic positions using the XRD pattern. Unlike perovskite, MgSiO$_3$ post-perovskite is a strongly anisotropic crystal; it has an orthorhombic symmetry (space group: *Cmcm*) with a SiO$_6$-octahedral sheet-stacking structure along the *b*-axis. It is isostructural with UFeS$_3$ and CaIrO$_3$, which are stable at ambient condition. The Mg^{2+} site in post-perovskite is smaller than in perovskite, resulting in a volume reduction of 1.0-1.5%. The calculated [3, 4] and measured elastic properties [5] of post-perovskite now explain the seismic-wave velocity structure in the lowermost mantle. The high positive pressure/temperature slope (Clapeyron slope) of the perovskite/post-perovskite transition boundary destabilizes the thermal boundary layer at the bottom of the mantle and remarkably enhances the mantle convection. Recent measurements of transport properties demonstrated that both electrical and thermal conductivities of post-perovskite are much higher than those of perovskite. The electronically highly conductive post-perovskite layer in the lowermost mantle enhances the electromagnetic coupling between solid mantle and liquid core, which possibly changes the Earth's rotation speed [6].

In addition, we are now able to perform XRD measurements up to 377 GPa and 5700 K, corresponding to the center of the Earth [7]. With such techniques, hcp (hexagonal-close-packed) structure has been found to a stable form of iron in the Earth's solid inner core (5100 to 6400-km depth). While the effect of impurities such as nickel and some light alloying element(s) remains to be examined, the knowledge of crystal structure of inner core material helps to predict physical properties and interpret seismic structures.

[1] M. Murakami et al. *Science* **2004**, *304*, 855-858. [2] K. Hirose *Rev. Geophys.* **2006,** *44*, RG3001. [3] T. Iitaka et al. *Nature* **2004**, *430*, 442-445. [4] A. Oganov and S. Ono *Nature* **2004**, *430*, 445-448. [5] M. Murakami et al. *Earth Planet. Sci. Lett.* **2007**, *259*, 18-23. [6] K. Ohta et al. *Science* **2008**, *320*, 89-91. [7] S. Tateno et al. *Science* **2010**, *330*, 359-361.

Keywords: post-perovskite, perovskite, high-pressure

KN10

Acta Cryst. (2011) A**67**, C8-C9

Exploration of the Protein Universe with High Throughput Structural Biology

Ian A. Wilson, *Joint Center for Structural Genomics and Department of Molecular Biology and Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA (USA)*. E-mail: wilson@scripps.edu

The landscape of structural biology has changed significantly over the past decade due to the overwhelming amount of novel sequence data generated from genome sequencing projects and the increased automation and robotics that facilitate protein production through crystallization to structure determination. These advances have unleashed unparalleled opportunities for re-evaluation of the size and diversity of the protein universe via explorations into new environments, such as the human microbiome and, in general, for addressing more challenging biological questions. For over a decade, the Joint Center for Structural Genomics (http://jcsg.org) has been at the forefront of developing tools and methodologies that enable the application of HTP structural biology to a broad range of biological investigations. For example, in the previous phases of the NIH PSI (http://www.nigms.nih.gov/initiatives/psi), we explored structural coverage of uncharted regions of the protein universe [1] as well asa single organism that enabled a complete structural reconstruction of the metabolic network of *Thermotoga maritima*.[2] As we embark on PSI: Biology, the JCSG is leveraging its HTP platform to take on challenging targets in stem cells and T cells that capitalize on our extensive experience to develop the best strategies to enhance chances of success. The emerging field of metagenomics has been particularly enlightening, where the human gut microbiome sequencing projects have already uncovered fascinating new families and expansions of known families for adaptation to particular environments. These high-throughput approaches can be applied to important biological problems not only in large consortia, such as the JCSG, but also in individual laboratories to tackle fundamental biological questions. Examples of the types and range of biological problems that are being tackled by PSI:Biology, as well as examples from my own laboratory on influenza virus and the search for a universal vaccine will be discussed [3]. The JCSG is located at The Scripps Research Institute, the Genomic Institute of the Novartis Research Foundation, U.C. San Diego, Sanford-Burnham Medical Research Institute, and SSRL/Stanford University, and supported by U54 GM094586, and P01 AI058113 and HHSN272200900060C.

[1] Jaroszewski, L. *et al*. **2009** Exploration of uncharted regions of the protein universe. *PLoS Biol.* 7:e1000205. [2] Zhang, Y. *et al*. **2009** Three-dimensional structural view of the central metabolic network

of *Thermotoga maritima*. *Science* 325:1544-1549. [3] Ekiert, D. C., *et al.* **2009**. Antibody recognition of a highly conserved influenza virus epitope. *Science* 324:246-251.

Keywords: structural genomics, high-throughput, influenza

KN11

Acta Cryst. (2011) A**67,** C9

Energy related materials: borohydrides

Yaroslav Filinchuk,[a] [a]*Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve (Belgium).* E-mail: yaroslav.filinchuk@uclouvain.be

Metal borohydrides attract a particular interest as potential hydrogen storage materials, capable to release hydrogen by thermolysis and hydrolysis. Recently, a significant progress was made in synthesis of bimetallic borohydrides, their characterization and in establishing composition-structure-property relations. The structure of these compounds can be rationalized in terms of different bonding schemes between metal atoms and the BH_4 groups, involving various degrees of iono-covalent interaction. Their hydrogen storage properties are not a simple average of the monometallic borohydrides, but depend mostly on the nature of the complex-forming cation. Indeed, the BH_4 group can be considered as a directional ligand which can form complexes with less electropositive metals. In some cases, inorganic frameworks similar to MOFs are obtained, e.g. interpenetrated and porous frameworks, the latter capable to absorb reversibly and selectively guest species. Metal borohydrides reveal rich coordination chemistry and their properties can be changed by chemical modification, for instance by means of so-called "anion substitution", i.e. by using different ligands along with the BH_4 groups.

In-situ powder diffraction is the primary technique to characterize new phases, study their formation, decomposition, and to evaluate a reversibility of hydrogen desorption. Synthetic screening combined with a "decomposition-aided indexing" of the *in-situ* powder diffraction data, followed by a structure solution in direct space and an energy optimization by DFT methods becomes a standard approach to characterize new systems. Diffraction allows to find conditions for reversible dehydrogenation: different decomposition pathways are commonly detected in vacuum, in argon and under hydrogen back-pressure, while the reversibility strongly depends on the nature of decomposition products. Therefore, high throughput diffraction measurements under working conditions become a part of the characterization protocol of a new hydrogen storage system [1]. Naturally, structural information from diffraction methods is combined with data on dynamics from Raman/IR spectroscopies and spin-lattice relaxation NMR measurements [2], physico-chemical characterization by TGA, DSC, PCT etc (see for example Ref. 3).

A large work front is initiated on reactive hydride composites. These systems usually are mixtures of borohydrides, binary hydrides, amides, ammonia borane or metal amidoboranes, metal-coordinated ammonia and sometimes catalytic amounts of transition metal salts. These combinations allow to decrease further dehydrogenation temperatures, increase the useful hydrogen weight content, and suppress the undesirable release of borane and ammonia gases. Information on structure, bonding, properties and reactivity of the individual components, the experimental and analytical protocols to study the reaction composites as well as the use of theoretical methods [4] are the prerequisites for finding a suitable hydrogen storage material in these multicomponent systems.

[1] D.B. Ravnsbæk, Y. Filinchuk, R. Černý, T.R. Jensen, *Z. Krist.* **2010**, *225*, 557-569. [2] A.V. Skripov, A.V. Soloninin, O.A. Babanova, H. Hagemann, Y. Filinchuk, *J. Phys. Chem. C* **2010**, *114*, 12370-12374. [3] D.B. Ravnsbæk, Y. Finchuk, R. Černý, M.B. Ley, D. Haase, H.J. Jakobsen, J. Skibsted, T.R. Jensen, *Inorg. Chem.* **2010**, *49*, 3801-3809. [4] S.V. Alapati, J.K. Johnson, D.S. Sholl, *J. Phys. Chem. C* **2008**, *112*, 5258-5262.

Keywords: Hydride, Synchrotron, Chemistry

KN12

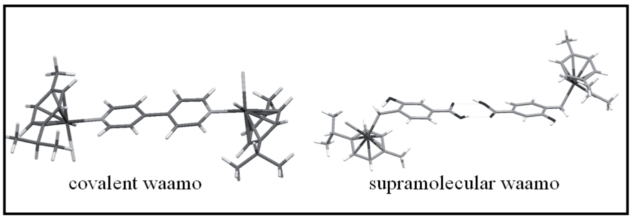
Acta Cryst. (2011) A**67,** C9-C10

Crystal engineering of flexible metallorganic networks

Alessia Bacchi, *Dipartimento di Chimica GIAF, University of Parma, Parma (Italy).* E-mail: alessia.bacchi@unipr.it

During the past twenty years much effort has been devoted to design crystalline species capable of incorporating small molecules into the lattice through weak interactions, which might be broken at will, producing crystalline materials with host-guest properties [1]. These have been classified according to the behavior of the host framework when the guests are removed [2]: first-generation compounds have microporous frameworks that collapse on the removal of guest molecules, second-generation compounds exhibit a permanent porosity also in the absence of included guests, and third-generation compounds have flexible and dynamic frameworks, which rearrange reversibly in response to the presence of guests.

In this contribution the full toolkit of crystal engineering is used to rationalize the design of third generation porous metallo-organic materials with flexible dynamic frameworks, able to create pores on demand to accommodate small guest molecules [2]. The size and shape of the organic ligands are crucial in determining the inclusion propensity of these materials, and we focused on wheel-and-axle (*waa*) systems that are constituted by two bulky groups (wheels) connected by a rigid linear spacer (axle) [3]. In particular, trans-palladium wheel-and-axle complexes of carbinol ligands (*waad*) have shown suitable structural requisites to give host-guest properties, and display reversible vapor solvents uptake without loss of crystallinity [4]. This paradigm has evolved into the class of wheel-and-axle metal-organic systems (*waamo*) based on two ruthenium half-sandwich units (HSRu) playing as wheels, connected by a linear axle that may be covalent or supramolecular [6] (Figure). These compounds combine the inclusion properties of the wheel-and-axle molecular motif with the chemical properties of HSRu complexes, known as catalysts of a variety of important organic transformations, such as the enantioselective reduction of polar bonds under hydrogen transfer conditions. A careful design of both the HSRu unit and the ligands that constitute the molecular axle permits to finely tune the supramolecular properties of the crystalline frameworks. Based on the number of hydrogen bond donors and acceptors and on their nature materials exhibiting a range of inclusion propensities have been obtained, from stiff networks that do not include any guest to extremely dynamic materials that easily transform in the solid state to exchange guests by solid/vapour and solid/liquid processes.



[1] J. W. Steed, J. L. Atwood, Eds, *Supramolecular Chemistry*, Wiley, Chichester, **2000** [2] S. Kitagawa, K. Uemura, *Chem. Soc. Rev.* **2005**, *34*, 109-119 [3] A. Bacchi, M. Carcelli, T. Chiodo, F. Mezzadri, *CrystEngComm*, **2008**, *10*, 1916-1927. [4] A. Bacchi, in *J.C.A. Boyens, J.F. Ogilvie, Eds. Models, Mysteries, and Magic of Molecules,* Springer, **2008***,* 87-108. [5] A. Bacchi, E. Bosetti,