

Crystallography 2017



2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Scientific Tracks & Abstracts

Day 1

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Non-destructive studies of microstructure and elemental composition of crystalline materials through energy-resolved neutron imaging

Anton S Tremsin¹, Didier Perrodin², Adrian S Losko³, Sven C Vogel³, Mark A M Bourke³, Gregory A Bizarri², Edith D Bourret², Takenao Shinohara⁴, Kenichi Oikawa⁴, Winfried Kockelman⁵, S Ganguly⁶ and Yan Gao⁷¹University of California at Berkeley, USA²Lawrence Berkeley National Laboratory, USA³Los Alamos National Laboratory, USA⁴Japan Atomic Energy Agency, Japan⁵STFC-Rutherford Appleton Laboratory, UK⁶Cranfield University, UK⁷GE Global Research, USA

Energy-resolved neutron imaging provide unique possibilities to study materials non-destructively in situations, where other more conventional techniques fail due to opacity of materials or their surrounding equipment (e.g., high temperature furnaces in case of crystal growth). Microstructure of both polycrystalline and single crystal materials can be investigated due to the presence of Bragg scattering of neutrons with wavelengths comparable to crystal lattice parameters. At the same time the elemental composition and temperature of the material can be mapped remotely with ~0.1 mm resolution through the analysis of neutron resonance absorption at epithermal energies, all from one measurement with no need to scan through the sample and thus allowing quantitative studies of relatively slow dynamic processes, such as crystal growth. In this paper we demonstrate the unique capabilities of energy-resolved neutron imaging to measure strain and some texture variation within metal welds, loaded fastener assemblies and metal samples produced by additive manufacturing. In situ diagnostics of crystal growth parameters such as shape and location of liquid/solid interface, mapping the elemental composition and visualization of macroscopic crystal defects and crystal mosaicity are also shown for the growth of single crystal gamma scintillators. For some compound materials, such as Cs₂LaLiBr₆:Ce and BaBrCl:Eu, we directly observed dynamics of phase separation within the liquid phase as well as dynamics of liquid/solid interface and dopant segregation during crystal growth at 550 °C and 850 °C temperatures, respectively. These novel studies became possible with the recent progress in novel high resolution neutron fast counting detectors and bright pulsed beamlines at spallation neutron sources, as well as development of novel data analysis tools capable of processing hundreds of thousands neutron transmission spectra in acceptable time, both of which will be briefly described in the paper.

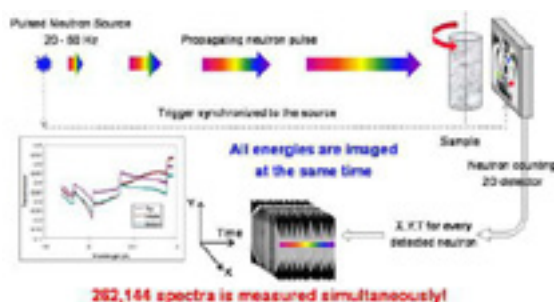


Figure-1: Schematic diagram of energy-resolved neutron imaging experimental setup

Biography

Anton S Tremsin is currently working on the development of novel non-destructive testing techniques utilizing unique combination of high resolution event counting neutron detectors and bright pulsed neutron sources. The detectors developed by him enable simultaneous detection of >250 thousand transmission spectra in each 55×55 μm² pixel, enabling studies of microstructure of crystalline materials and mapping of their elemental composition, both ex situ and even in situ, as these materials are being grown at high temperatures. A wide range of new state-of-the art experimental techniques in combination with data analysis tools have been demonstrated by him over recent years in the field of materials science, structural engineering, single crystal growth and characterization, studies of magnetic phenomena, geosciences and many others, result of which were presented at many international conferences and published in more than 200 research papers.

ast@ssl.berkeley.edu

2nd International Conference on

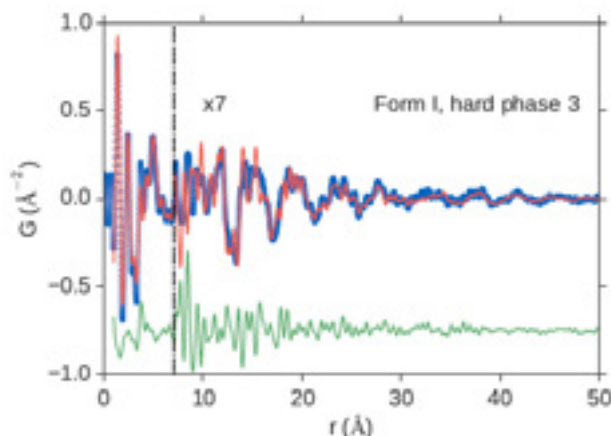
APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Crystal structures of polymers: Will PDF paves the way to greater understanding?

Bernd Hinrichsen¹, Maxwell W Terban² and Robert E Dinnebier³¹Ludwigshafen, Germany²Columbia University, USA³Max Planck Institute for Solid State Research, Germany

Industrial polymers (plastics) are a fundamental part of modern society. The global production of polymers has been growing steadily from the tentative beginnings in the 1940s to 322 million tons in 2015. This immense and ubiquitous use of polymers has led to dramatic pollution issues and legislation curtailing use of environmentally detrimental polymers. Surprisingly little is known about the solid-state structure of these megaton products. Nuclear magnetic resonance studies elucidate the molecular structure in a liquid solution, transmission electron microscopy gives an inkling into the solid-state microstructure; however the chemistry involved in polymeric structures are only well characterized for a few examples by X-ray diffraction studies. Often these are performed on idealized samples, not necessarily representative of the real-life material. We will be presenting works that have been carried out and illustrate the potential which the PDF method brings to polymer research with special focus on challenging subjects such as biodegradation.



Biography

Bernd Hinrichsen has his scientific foundation in crystallography, having attained his PhD at the Max Planck Institute for Solid State Research under the supervision of Robert E. Dinnebier. He spent some time at Bruker AXS as an Application Scientist for powder X-ray diffraction before taking over the responsibility of the powder X-ray diffraction lab at the main research site of BASF in Ludwigshafen, Germany. He is currently responsible for PXRD, Solid-State, NMR, TEM and SEM labs.

bernd.hinrichsen@basf.com

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Observation of π -electron in metal hexaboride through X-ray charge density

Eiji Nishibori

University of Tsukuba, Japan

Metal hexaborides MB_6 , where M is an alkaline earth or rare earth metal exhibit metallic and semiconductor properties by changing the M ion. The metal hexaborides have a B_6 octahedron in the structure. The M ion is located at the body-center surrounded by the B_6 octahedra. The B_6 octahedron has 18 valence electrons. Two electrons per B_6 octahedron are required to fulfill the bonding orbital of B_6 . Metal hexaborides with divalent metal ions are considered to be semiconductor and with the trivalent ions are metal from the consideration. Theoretical study suggests that the π -electron like an anti-bonding orbital of B_6 contributes electrical conductivity in the metallic trivalent MB_6 . We investigated the charge densities of divalent and trivalent metal hexaborides, semiconducting BaB_6 and metallic LaB_6 using the $d > 0.22 \text{ \AA}$ ultra-high resolution synchrotron radiation X-ray diffraction data by a multipole refinement and a maximum entropy method. High resolution powder diffraction data were measured at SPring-8. The strong inter-octahedral and relatively weak intra-octahedral boron-boron bonds were observed in the charge densities. A difference of valence charge densities between LaB_6 and BaB_6 was calculated to reveal a small difference between isostructural metal and semiconductor. The weak electron lobes distributed around the inter B_6 octahedral bond were observed in the difference density. We found the electron lobes are the conductive π electrons in LaB_6 from the comparison with the theoretical charge density. We have successfully visualized very small amount of conductive π electrons from X-ray charge density. Electron density distribution is now one of the most information-rich observable owing to the great improvement of experimental situation such as synchrotron X-ray source.

Biography

Eiji Nishibori is currently a Professor of Division of Physics, Faculty of Pure and Applied Sciences, University of Tsukuba, Japan. He has received his Bachelor's and Master's degree from Nagoya University, Japan. He was appointed an Assistant and Associate Professor at Nagoya University. He was then appointed as the Director of RIGAKU-RIKEN collaboration center at SPring-8. His main research field is structural science using a synchrotron radiation X-ray including a development of experimental and analytical system. He has received several awards including Young Scientists' Prize, the Commendation for Science and Technology by the MEXT, the CrSJ Young Scientist Award and the Crystallographic Society of Japan.

nishibori.eiji.ga@u.tsukuba.ac.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Atomic view of the histidine environment stabilizing higher-pH conformations of pH-dependent proteins

Franck Artzner

CNRS and Rennes University, France

External stimuli are powerful tools that naturally control protein assemblies and functions. For example, during viral entry and exit changes in pH are known to trigger large protein conformational changes. However, the molecular features stabilizing the higher pH structures remain unclear. Here we elucidate the conformational change of a self-assembling peptide that forms either small or large nanotubes dependent on the pH. The sub-angstrom high-pH peptide structure reveals a globular conformation stabilized through a strong histidine-serine H-bond and a tight histidine-aromatic packing. Lowering the pH induces histidine protonation, disrupts these interactions and triggers a large change to an extended β -sheet-based conformation. Re-visiting available structures of proteins with pH-dependent conformations reveals both histidine-containing aromatic pockets and histidine-serine proximity as key motifs in higher pH structures. The mechanism discovered in this study may thus be generally used by pH-dependent proteins and opens new prospects in the field of nanomaterials. This work is based on three complementary x-ray techniques: Single crystal solving at 0.85 Å, Fiber diffraction at wide angles that gives insight into the molecular structures, and, SAXS, Small Angle X-ray Scattering that illuminates the packing and the radial electron density profiles of the nanotubes. The full x-ray analysis that reveals both nanostructures at the molecular scale will be detailed. *Céline Valéry, Stéphanie Deville-Foillard, Christelle Lefebvre, Nuria Taberner, Pierre Legrand, Florian Meneau, Cristelle Meriadec, Camille Delvaux, Thomas Bizien, Emmanouil Kasotakis, Carmen Lopez-Iglesias, Andrew Gall, Stéphane Bressanelli, Marie-Hélène Le Du, Maité Paternostre, Franck Artzner*, Nature Communications 6: 7771 (2015). <https://www.nature.com/articles/ncomms8771>.

Biography

The Franck Artzner's bio-inspired self-assemblies group addresses materials issues from fibrillation of pharmaceutical peptides to the colloids crystallization by fibrillar proteins. The group has an expertise in technical development as well as crystallographic characterization of structures by unconventional X-ray scattering techniques, SAXS, Fiber Diffraction. A Joint Laboratory with IPSEN and Maité Paternostre is headed by Franck Artzner and investigates commercial formulation of self-assembled peptides. FA was the chairman of the National brain storming group on Bio-inspired Nanotechnologies at OMNT. He is involved in the review committees of synchrotrons : SOLEIL, ESRF, NSLS I. He received the Young Investigator Award of the Physical Chemistry Division of the French Chemical Society (SFC) and the French Physical Society (SFP) in 2015, and the Delalande prize from the French Pharmaceutical academy in 2016.

franck.artzner@univ-rennes1.fr

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

On the application of molecular simulation tools in studies of organic molecular crystals (i.e., modeling disorder and other crystalline properties)

Eric J Chan

Bristol Myers Squibb, USA

Analysis and prediction of physical properties of crystalline materials is of crucial importance. For example, a pharmaceutical crystal form must satisfy a target profile with respect to process-ability as well as bioavailability. In the material development arena, undesirable physical phenomena offer non-trivial challenges. Such phenomena include polymorphism, disorder, solvation/de-solvation, disproportionation and variation in the crystal particle size shape; because these phenomena impact the physical structure and related properties of a material, challenges also exist analytical and characterization perspective. Nowadays varieties of atomistic simulation techniques are useful to support analysis, provide further chemical/physical insight and for risk assessment/predictive capabilities. The once active laboratory chemical crystallographer may be forced to seek refuge *in silico*. Such computational activities are facilitated by a plethora of commercial and community software tools and codes. However, in some cases workflows and tools are not as streamlined and options are limited, the former experimentalist then takes the role of a computer scientist. We discuss a selection of case studies where such former mentioned novel molecular simulation hackwork is applied to small molecule crystallography, the majority being pharmaceutically relevant. Example workflows include atomistic simulation methods (MC or MD) useful for interpreting supplementary scattering features like diffuse and satellite intensities from single crystal X-ray diffraction. One study demonstrates insight into de-solvation processes. For understanding the interplay between different solvents within the crystal structure, a Grand Canonical Monte Carlo (GCMC) model was developed combining crystal structure, molecular mechanics models and SSNMR data. This was useful to estimate site occupation parameters for solvent bound to a crystal. We argue the supplementary knowledge of molecular level interactions provides a simple means for prediction of the corresponding thermodynamic properties such as the solvent activities and temperatures required to remove or replace unwanted lattice solvent. Another example includes *in silico* screening for solvent effect on crystal morphology.

Biography

Eric J Chan has completed his graduate studies in Organic Chemistry/Biochemistry, PhD in coordination chemistry of metal-organic complexes and chemical crystallography and Post-doctoral study in X-ray single crystal diffuse scattering interpretations, molecular models, and Monte Carlo methods for molecular simulation, solid state organic chemistry and analysis of organic solids. He has expertise in crystallography, solid-state or materials chemistry and molecular simulations. He has interest in computational physics approaches used in chemistry. Graduate in organic chemistry/biochemistry, PhD: coordination chemistry of metal-organic complexes and chemical crystallography.

Eric.Chan@bms.com

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

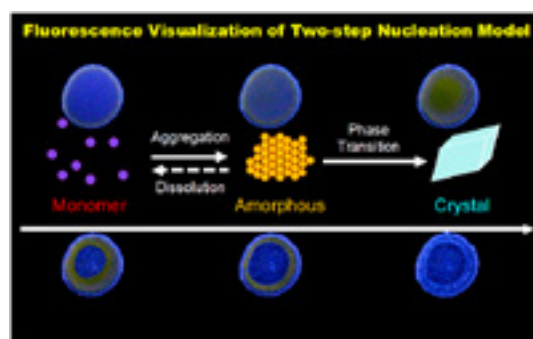
October 16-17, 2017 | Chicago, USA

Visualization of evaporative crystallization dynamics probed by fluorescence color changes

Fuyuki Ito

Shinshu University, Japan

Crystal formation from a solution is necessary for the fabrication of organic solid material. In solution crystallization, the formation of crystal nuclei plays an important role in determining crystal structure, size and polymorphism, and their crystal quality. Recently, a two-step nucleation model was developed to explain protein crystallization; involving a liquid-like cluster intermediate before nucleation, which has been shown to be of more general validity. The two-step nucleation model replaces the classical model of crystallization that is molecules are added on one by one to extend the crystal lattice and form embryo clusters in a one step process. Liquid-clusters are believed to originate from disordered liquids or amorphous metastable clusters in homogeneous solutions. We have focused the fluorescence detection for crystal formation process. The fluorescence spectra of the materials are sensitive to molecular environment and aggregation. In principle, the evolution of the molecular assembly can be assessed by fluorescence spectroscopy on the scale of only a few molecules or a bulk process scale. We have investigated fluorescence spectral changes of perylene and cyanostilbene derivatives showing aggregation-induced emission during solvent evaporation by fluorescence microscopy. We have claimed that the information on molecular assembly and crystal nucleation and growth processes is obtained by studying the concentration-dependent fluorescence spectral change of organic fluorescent dyes in the polymer film and solvent evaporation. In this paper, we investigate the fluorescence properties of 4,4'-di-*tert*-butyldibenzoylmethane boron difluoride (BF₂DBMb) solutions during evaporative crystallization. BF₂DBMb exhibits mechanofluorochromism, which originates from the different emission properties of its amorphous and crystalline states.



Biography

Fuyuki Ito received his Ph.D. in 2004 from Tohoku University under the direction of Prof. Shozo Tero-Kubota. He worked as a postdoctoral fellow at Osaka University. He moved to Kyushu University in 2005 as a research associate. In 2009 he moved to Shinshu University and became an associate professor in 2010. His research interests photochemistry of molecular-assembly system and crystal formation process of organic molecules.

fito@shinshu-u.ac.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Understanding interface and surface structures of nano-phases in natural Fe-oxyhydroxide and Fe-bearing olivine minerals

Huifang Xu, Seungyeol Lee and Shiyun Jin
University of Wisconsin-Madison, USA

Understanding interface structures, nano-precipitates, vacancies, impurities and adsorbed atoms on mineral surfaces are important to elucidate formation mechanism and reactions of minerals in the earth environments. Aberration-corrected Z-contrast imaging can provide chemical images with sub-Å resolution. Z-contrast images are HAADF images with atomic resolution. Multiple diffraction effects that appear in high-resolution transmission electron microscopic (HRTEM) images can be eliminated or minimized in Z-contrast images, because Z-contrast imaging uses non-coherent elastically scattered electrons at high scattering angle. We can obtain positions of atoms directly over a large range of thickness with Z-contrast to help distinguish columns of different atoms and their occupancies along the beam direction. Interface structures and crystal structures of nano-minerals and nano-precipitates can be solved by combining the Z-contrast imaging and *ab initio* calculation using density functional theory (DFT) methods. Vacancies, impurities, adsorbed heavy atoms can be also revealed directly. Vacancy ordering in Fe-bearing olivine and Fe-sulfides, adsorbed heavy metals (e.g., As, Au, U) on Fe-oxyhydroxide minerals are resolved clearly. Z-contrast images of the Fe-oxyhydroxides show ordered FeOOH proto-goethite nano-domains intergrown with nanophase goethite. The FeOOH nanophase is a precursor to the goethite. DFT calculations indicate that goethite is more stable than proto-goethite. Our results suggest that ordering between Fe and vacancies in octahedral sites result in the transformation from feroxyhyte to goethite through a proto-goethite intermediate phase. Combining Z-contrast images and TEM-EDS reveals that arsenate (AsO_4^{3-}) tetrahedra are preferentially adsorbed on the proto-goethite (001) surface.

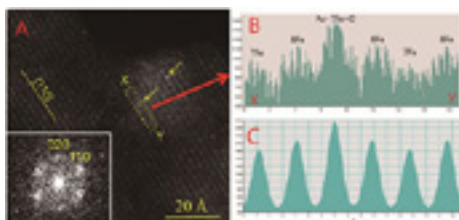


Figure-1: (A) a [001]-zone-axis Z-contrast image of proto-goethite, bright spots are positions of Fe atom columns. Very bright spots are adsorbed arsenic (As) atoms on the surface right above Fe; (B) the intensity profile of an outlined area from X to Y; (C) the intensity profile of simulated Z-contrast image showing the peak with As atom above an Fe atom column.

Biography

Huifang Xu has received his Bachelor's degree from Nanjing University and PhD degree from The John's Hopkins University in field of Mineralogy and Crystallography. He has completed his Postdoctoral studies at Arizona State University in area of Electron Crystallography. He is a Faculty Member in the Department of Geoscience and Materials Science Program at the University of Wisconsin-Madison. His research interests are studies of incommensurately modulated structures and nano-phase structures using e-beam imaging, X-ray diffraction and neutron scattering methods. He has published more than 100 papers in fields of mineralogy, crystallography and inorganic materials. He is an elected Fellow of Mineralogical Society of America.

hfxu@geology.wisc.com

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Interplay between H-bonding and charge ordering in $\text{Fe}_3(\text{PO}_4)_2(\text{OH})_2$ barbosaliteJ Rouquette¹, J Haines¹, V Ranieri¹, M Poienar², A Guesdon³ and C Martin³¹Université Montpellier, France²CRISMAT, France³Laboratoire Léon Brillouin, France

Charge Ordering (CO) in transition metal oxides is an important parameter for obtaining original magnetic and/or electric properties. That was largely shown within the framework of the studies on colossal magneto-resistance in manganese perovskites and it again seems to be at the origin of the ferroelectricity in $\text{CaMn}_7\text{O}_{12}$ or LuFe_2O_4 . The mixed valence of iron in the system is a particular motivation in view of the long lasting research on the understanding of the effects of pressure on charge order/magnetic order in iron compounds such as the LuFe_2O_4 new charge ordered state and the pressure dependence of its magnetic order. Here we focus on $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2$ barbosalite single crystal, an hydroxyphosphate of iron which exhibits a mixed valence state. High pressure behavior of barbosalite was successfully characterized based on single crystal X-ray diffraction, Raman and infrared spectroscopies. $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2$ presents two phase transition at close to 3 and 8 GPa respectively which are clearly governed by an interplay between H-bonding and electron delocalization. Moreover the temperature reaction $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \rightarrow \text{Fe}^{3+}_3(\text{PO}_4)_2(\text{OOH})$.

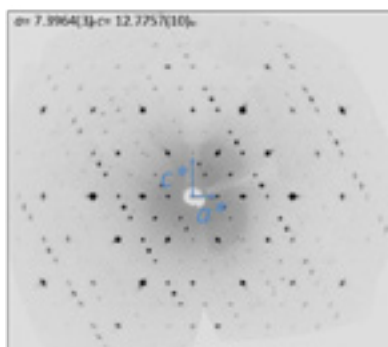


Figure 1: $h0l$ reconstruction of the reciprocal space of incommensurate $\text{Fe}^{3+}_3(\text{PO}_4)_2(\text{OOH})$.

Biography

J Rouquette has obtained his PhD in Julien Haines' group in Materials Science (Condensed Matter) from University of Montpellier, France in 2004 and was a Postdoctoral Fellow in Leonid Dubrovinsky's group at the Bayerisches Geoinstitut in Bayreuth University, Germany for two years. He has joined the CNRS as a Researcher in 2004 in the field of ferroelectrics/multiferroics and he defended his Habilitation in 2012 entitled "*in situ* structural studies of ferroic materials as a function of P,T,E,B. He has published more than 50 research papers in these areas.

jerome.rouquette@umontpellier.fr

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Applications of crystallography data in force-field and density functional theory calculations: JARVIS database

Kamal Choudhary

National Institute of Standards and Technology, USA

Crystal structure information can be used to characterize material-properties using quantum density functional theory and classical force-field calculations. JARVIS database is a part of Materials Genome Initiative at National Institute of Standards and Technology (NIST) enabling users to access material property calculation data through easy web-interface. JARVIS-FF database currently consists of 3248 entries including energetics and elastic property calculations and it is still increasing. We also include computational tools for convex-hull plots for DFT and FF calculations. The data covers 1471 materials and 116 force-fields. A major feature of this database is that the web interface offers easy look up tables to compare at a glance the results from different potentials (for the same system). In addition, both the complete database and the software coding used in the process have been released for public use online. JARVI-DFT database consists of more than 5000 DFT calculations for three-dimensional (3D) bulk and single layer 2D materials data for structural, electronic and elastic properties. We use lattice-constant criteria to identify potentially novel 2D materials. We predicted at least 1485 2D materials based on relative error in lattice constants obtained from semi-local DFT and Inorganic Crystal Structure Database (ICSD) data. We calculate exfoliation energy as a verification of our lattice-constant criteria.

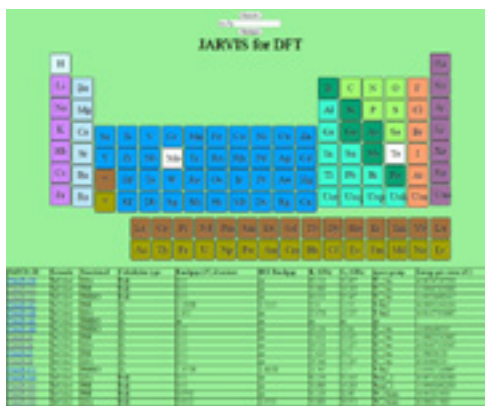


Figure-1: JARVIS database online

Biography

Kamal Choudhary has expertise in molecular dynamics, density functional theory and machine-learning based calculations. He has built JARVIS database at NIST to enable users access classical and quantum mechanical data of material free of cost to enable future materials discovery. He was graduated with PhD in Materials Science and Engineering from University of Florida in 2015 under the guidance of Dr. Susan B Sinnott.

kamal.choudhary@nist.gov

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structural study of sulfide glassy electrolytes for all-solid-state batteries

Koji Ohara¹ and Shinya Shiotani²¹Japan Synchrotron Radiation Research Institute, Japan²Toyota Motor Corporation, Japan

Sulfide glass ceramics are of interest for use as solid electrolytes in lithium ion batteries, because the realization of an all-solid-state battery will enable the miniaturization of battery packages and reduce safety issues. In general, the crystallization of glassy materials results in a decrease in the conductivity, although it increases in a few sulfide glasses owing to the crystallization of a highly conductive new phase. Significant progress has been made so far with the discovery of numerous sulfide crystalline compounds with high ionic conductivities such as $\text{Li}_7\text{P}_3\text{S}_{11}$, $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$, $\text{Li}_7\text{P}_2\text{S}_8\text{I}$ and $\text{Li}_{10}\text{SnP}_2\text{S}_{12}$. Their conductivities are higher than those of the corresponding sulfide glasses. Recently, we reported that $75\text{Li}_2\text{S}-25\text{P}_2\text{S}_5$ glass in the binary $\text{Li}_2\text{S}-\text{P}_2\text{S}_5$ system with strongly polarized sulfur has high ionic conductivity. In the sulfide glasses as presented here, an interesting improvement in the conductivity is observed during annealing, which appears in the glassy phase. In this presentation, we report the local glassy structure with a mixture of glass and crystalline phases by using synchrotron X-ray pair distribution function (PDF) analysis. The differential pair distribution function is utilized as a methodology for the mixed materials in our work to extract the glassy structure in the $75\text{Li}_2\text{S}-25\text{P}_2\text{S}_5$ sulfide glass ceramic. This method quantitatively reproduced the fraction of mixed phases, which was in agreement with the result of NMR. The extracted glassy structure exhibited no changes during the annealing treatment. Owing to the crystallization of the majority phase, the ionic conductivity in this glass decreased after crystallization. We observed the formation of a nanocrystalline phase in the diffraction pattern obtained during the annealing. Thus, our present finding of minority component is expected to lead to further understanding for the development of solid electrolytes with high ionic conductivity.

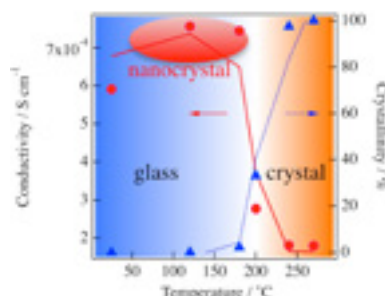


Figure-1: Crystallinity obtained from the pair distribution function under each annealing condition and the lithium ionic conductivity.

Biography

Koji Ohara has received his PhD in Condensed Matter Chemistry and Physics from Kyushu University of Japan, working with Prof. S. Takeda. He then did his Post-doctoral research with S. Kohara at Japan Synchrotron Radiation Research Institute (JASRI), where he studied elemental specific pair distribution function (PDF) analysis using anomalous X-ray scattering for disordered materials. After two years at JASRI, he moved to the position of Research Assistant Professor at Office of Society-Academia Collaboration for Innovation of Kyoto University in 2012. He has worked on structural studies of electrolytes in lithium ion batteries. He has been working as a Researcher at JASRI since 2015.

ohara@spring8.or.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Designing chiral metal-organic assemblies

Michal Lahav

Weizmann Institute of Science, Israel

Coordination-based polymers and metal-organic frameworks (MOFs) have been explored since their serendipity discovery by a Berlin color-maker named Diesbach at the beginning of the 18th century. These intriguing materials combine metal-coordination chemistry with the often complex formation of large supramolecular structures and may exhibit optical, catalytic, redox and magnetic functions derived from their metallic elements. Such materials are currently generated by the dozens in a gold-rush-type search for unique properties mainly related to the storage and release of energy (e.g., hydrocarbons, dihydrogen) at ambient temperatures and pressures. How the molecular components, metal salts and experimental conditions control the dimensions, shapes and homogeneity of these coordination-based materials is barely known. Moreover, the formation of chiral MOFs and MOFs confined on surfaces is especially challenging. We demonstrated the controlled generation of various homogeneous MOF structures from solution and on surfaces. Using a versatile ligand system that binds late-transition metals in a defined manner, we address various challenging issues related to the mechanism underlying the formation of such homogeneous structures at the (sub)-microscale, their magnetic and electronic properties and other functions. These new chiral materials have been characterized by a series of complementary methods, including electron microscopy, X-ray powder diffraction, atomic force microscopy and synchrotron X-ray reflectivity.

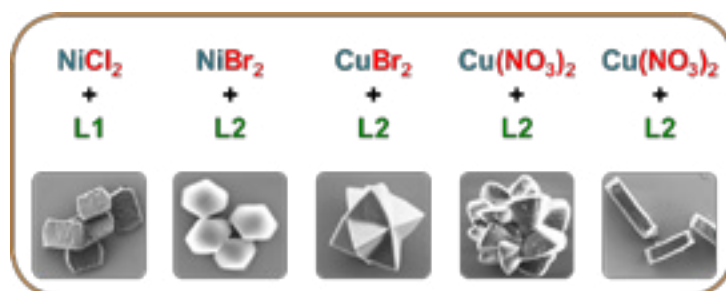


Figure-1: Examples of metal-organic frameworks (MOFs).

Biography

Michal Lahav has completed her BSc and PhD studies in Chemistry from the Hebrew University of Jerusalem, Israel. She was a Postdoctoral Researcher at the Weizmann Institute of Science for two years before she moved to Harvard University, where she studied nanochemistry. After two years of postdoctoral work in the United States, she returned to Israel and started to work as a Scientific Advisor at the Weizmann Institute of Science. She was appointed as an Associate Staff Scientist in the Department of Organic Chemistry in 2011. Her interdisciplinary materials chemistry research is related to the self-assembly of metallo-organic materials for energy storage and for electrochromics whose products are now being patented. Her work is related to fundamental understanding of the formation and electronic properties of these metallo-supramolecular architectures. Her prizes and honors include the Dr. Maxine Singer Prize for Outstanding Staff Scientists.

michal.lahav@weizmann.ac.il

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Old forces to create new materials

Milko E van der Boom
Weizmann Institute of Science, Israel

Enabling and understanding new methodologies to fabricate molecular assemblies driven by intermolecular interactions is fundamental in chemistry. Such forces can be used to control crystal growth and enable surface-confinement of these materials, which remains challenging. In the 1960s, the late Gerhard M. J. Schmidt from the Weizmann Institute of Science discovered that some molecules are unusually closely arranged in organic crystals. This spatial arrangement turned out to be a result of an unexplored weak intermolecular interaction, termed “halogen bonding” many years later by other scientists. Such interactions play a key role in organic processes (in a cell or organism) that are necessary for sustaining life. For example, thyroid hormones use halogen bonding to bind to receptors in order to regulate the development, growth and metabolism of the cells in our body. We demonstrate a solvent-free on-surface crystal-to-co-crystal conversion process driven by halogen bonding (XB). By exposing a polycrystalline organic material, consisting of a XB-acceptor moiety, to the vapors of a complementary XB-donor compound, the corresponding halogen-bonded co-crystals were formed. Furthermore, we show that this approach can also be utilized for non-crystalline materials to afford surface-confined organic composites. Our stepwise vapor-based approach offers a new strategy for the formation of hybrid supramolecular materials.

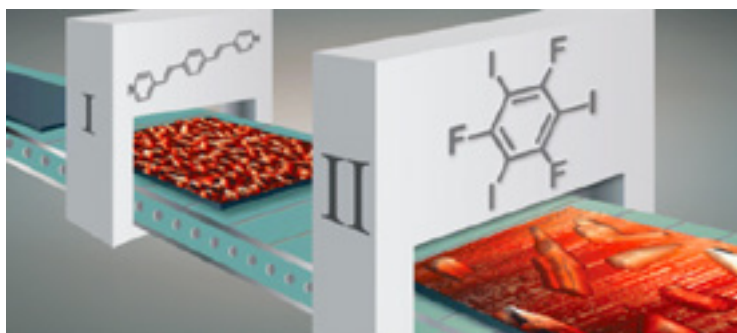


Figure-1: Consecutive formation of halogen bonded crystals.

Biography

Milko E van der Boom has completed his BSc in Chemical Engineering at the Amsterdam University of Applied Sciences and his MSc degree in Inorganic Chemistry at the University of Amsterdam. In 1994, he was enrolled as a Doctoral student at the Weizmann Institute of Science, where he studied Organometallic Chemistry and was awarded his PhD degree with distinction in 1999. After three years of Postdoctoral work at Northwestern University, where he studied the formation of functional organic films, he returned to the Weizmann Institute's Department of Organic Chemistry in 2002. His interdisciplinary materials chemistry research focuses on metalloorganic-oriented synthetic and mechanistic studies. His prizes and honors include an Alon Fellowship from the Israel Council for Higher Education.

milko.vanderboom@weizmann.ac.il

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

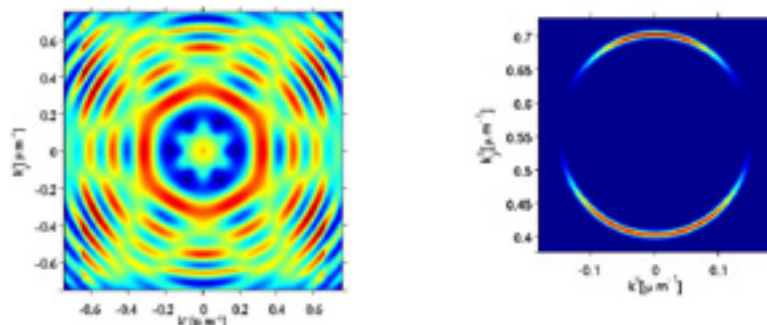
October 16-17, 2017 | Chicago, USA

Nonlinear crystallography with structured light: Classical and quantum optics effects

Rocio Jáuregui

Universidad National Autonomy de México, México

An alternative to diffraction techniques is the characterization of the point symmetry group of a crystal by its effects on the nonlinear optical response encoded in the susceptibility tensors. In this work, we show that it is possible to perform complementary symmetry studies of nonlinear materials by using nonlinear processes besides second harmonic generation. We also show that structured light can enhance the tracks of the symmetry of a crystal on its nonlinear optical properties. We focus on the usage of light beams that can be described as the superposition of plane waves with wave vectors confined in a cone and with cylindrical symmetry on the angular spectrum (Bessel beams). This is equivalent to observing the crystal simultaneously from many different angles. The polarization structure of these beams out of the paraxial regime allows to incorporate information from all the components of the susceptibility tensors using a single structured illumination beam. The crystallographic analysis is exemplified for the parametric down conversion process. It is shown that, for an uniaxial birefringent nonlinear crystals, a proper orientation of a non paraxial Bessel beam induces the emission of photon pairs in directions that reflect directly the point symmetry. Both the flux rate of signal photons (with a clear classical analog) and coincidence detections (with a pure quantum interpretation) exhibit traces of the crystal symmetries.



(i) Angular dependence of the flux rate of signal photons; and maximal flux rate of idler photons detections in coincidence with a signal photon for type I spontaneous parametric down conversion of GaSe illuminated by a Bessel pump beam with an axicon angle of 0.097.

Biography

Rocio Jáuregui performed her graduate and postgraduate studies at the Universidad Nacional Autónoma de México. (UNAM). She has worked on the interaction of light and matter from diverse points of view: high precision atomic spectroscopy, effects of boundary conditions on the electromagnetic field, pair creation and modification on atomic transition rates due to moving boundaries, classical and quantum description of structured electromagnetic fields and their effect on thermal and ultracold atomic samples, simulations of ultracold bosonic and fermionic atoms, and the analysis of quantum nonlinear optical response of different media. Her work has been supplemented by teaching activities. Nowadays, Prof. Jáuregui coordinates the Laboratorio Nacional de Materia Cuántica which incorporates 11 Mexican research institutions and chairs the Department of Quantum Physics and Fotonics of Instituto de Física (UNAM).

rocio@fisica.unam.mx

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Fabrication of single crystal silicon nanowires by metal assisted chemical etching with nanoimprinted barrier patternSeok-min Kim and Jonghyun Ju
Chung-Ang University, Republic of Korea

To fabricate the silicon nanowires, various methods such as vapor-liquid-solid growth, reactive ion etching with barrier pattern, oblique angle deposition and metal assisted chemical etching (MACE) have been developed. The MACE can provides a high aspect ratio and undamaged single crystal silicon nanostructures using low-cost wet etching process. In the MACE process, a patterned noble metallic structure etches the silicon substrate anisotropically in aqueous solutions containing hydrogen fluoride and an oxidant, and an isolated single crystal vertical silicon nanowires are obtained. Since the geometrical structure of silicon nanowire is mainly determined by the initial metallic pattern, the fabrication of metallic nanostructure on a silicon substrate is the key technology in the MACE process. To obtain highly ordered nanowires with precisely controlled diameter and distribution, the various metal patterning method such as electron beam lithography, photolithography and nanosphere lithography were suggested. In this study, we fabricated a highly ordered large area ultraviolet (UV) nanoimprinted etch barrier pattern on an Au catalyst layer with low cost for MACE process. A silicon nanodot master having 500nm pith, 250nm diameter and 125nm height was prepared by KrF laser scanning lithography. A transparent flexible mold was UV replicated from the silicon master, and a nanodot barrier pattern was UV imprinted on a PMMA lift-off layer coated silicon wafer. After RIE process with O₂ gas, the silicon surface was exposed except nanodot barrier patterned area. An Au layer was deposited on silicon wafer using thermal evaporator and UV imprinted nanodot barrier were lift-offed with PMMA layer in acetone solution with ultrasonication process. Finally, Au nanohole array was fabricated and MACEed in hydro fluoride and hydrogen peroxide mixed aqueous solution. Depending on the etching time, 300 – 8000 nm heights silicon nanowire arrays were successfully demonstrated.

This study was supported by a grant of the Korean Health Technology R&D Project, Ministry of Health & Welfare, Republic of Korea. (HI14C2687), and the Technology Transfer Development Program (S2334634) funded by the Small and Medium Business Administration(SMBA, Korea).

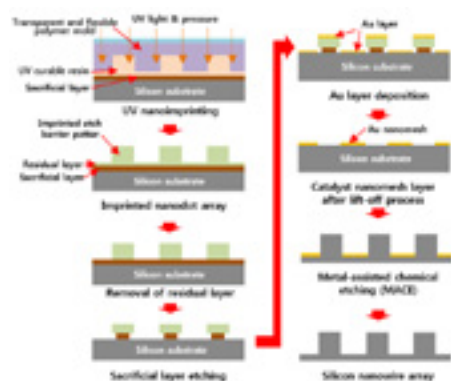


Fig. 1 Proposed MACE process with nanoimprinted etch barrier

Biography

Seok-min Kim received his PhD degree from the School of Mechanical Engineering at Yonsei University, Seoul, Republic of Korea. He is currently an associate professor in the School of Mechanical Engineering at Chung-Ang University, Seoul. His current research interests include design and fabrication of micro/nanostructures for optical component, gas/bio sensors, micro fluidic chips, and enhanced boiling heat transfer surface.

smkim@cau.ac.kr

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

'Crystal genes' in metallic liquids and glasses

Feng Zhang

Ames Laboratory US Department of Energy, USA

It has been widely speculated that dominant motifs, such as short-range icosahedral order can influence glass formation. Less well understood is how these motifs (crystal genes) in the liquid can influence phase selection upon devitrification. These 'crystal genes' are the underlying structural order that transcends liquid, glass and crystalline states. By comparing the amorphous states of the same alloy compositions formed by sputtering and rapid solidification, and their devitrification pathways, we can quantify the distribution of the common packing motifs in the liquid or glass and in stable and metastable phases which form. We will discuss how this approach brings new insight into the origin of vitrification and mesoscopic order-disorder transitions in condensed matter. A genetic algorithm is applied to search for the energetically favorable stable and metastable crystal structures of complex metallic compounds, and a cluster alignment method reveals the most common packing motifs in crystalline and non-crystalline structures.

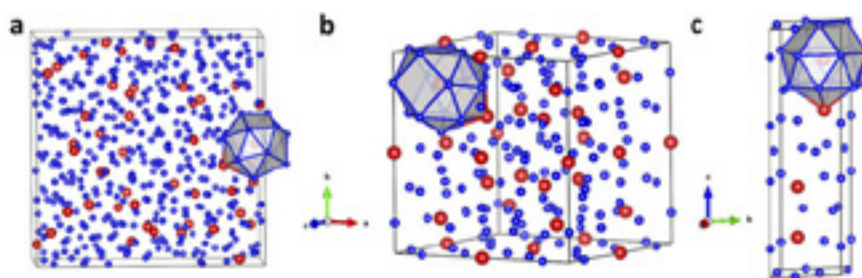


Fig. The commonly shared "3661" motif in AlSm glass and devitrified metastable crystal structures.

Biography

Feng Zhang is an Assistant Scientist III at the Ames Laboratory, US DOE. He received his Ph.D. in physics from Penn State University in 2008, and held a postdoctoral fellow position at Georgia Institute of Technology before joining Ames Lab. His current research interest lies in the structure and dynamics of metallic liquids and glasses, and phase selection during transformations into crystalline structures.

fzhang@ameslab.gov

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structural and functional studies of actin interacting protein 5, a novel actin assembly regulator in *Saccharomyces cerevisiae*

Sun Jialin^{1,2}¹Agency for Science, Technology and Research, Singapore²Nanyang Technological University, Singapore

Aip5 is a newly identified member of the polarisome complex found in yeast. It acts as actin assembly regulator via binding to other protein partners in the polarisome complex. Polarisome complex helps to establish the polarity of the cell, which is critical for cell growth and division. It is also responsible for actin filament assembly in the cell that contributes to the tissue organization and cell motility. All in all, polarisome is crucial for the survival and division of a yeast cell. Being a new member of the polarisome complex, Aip5 is most likely recruited by its binding partner Spa2 to the tip of the yeast bud during polarized cell growth, to regulate actin filament assembly. Deletion of Spa2 led to the complete loss of localization signal of Aip5 to the polarized region in the cell, while deletion of Aip5 C-terminal had similar effect. These results indicate that Aip5, most probably interact with other polarisome proteins via its C-terminal. Thus it is critical to elucidate the structure of Aip5 given its importance in aiding the actin filament assembly. In this study, we have successfully solved the structure of Aip5 C-terminal at atomic resolution of 1.8 Å. It consists of a dimer per asymmetrical unit, which is consistent with the gel filtration chromatography result. This indicates that Aip5 possibly functions as a biological dimer as well. Preliminary results have shown that the oligomer state of Aip5 might play a part in actin filament assembly. More studies will be conducted to further investigate on the effect of Aip5 oligomer state with to its function.



Figure-1: Structure of Aip5 dimer and side view of Aip5 monomer depicting four beta chains flanked by three alpha helices in its surrounding.

Biography

Sun Jialin is currently a PhD student majoring in Structural Biology from Agency for Science, Technology and Research and Nanyang Technological University in Singapore. She had a Diploma in Pharmacy Science and found her passion in structural biology later during her undergraduate study. Her focus of work mainly revolves around the structural and functional studies of plant enzymes and actin interacting proteins in yeast. She has expertise in molecular cloning, and as well as X-ray crystallography.

jsun009@e.ntu.edu.sg

Notes:

Crystallography 2017



2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Scientific Tracks & Abstracts

Day 2

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

The difference in the P- and T-induced dynamics in breathing crystals

Victor Ovcharenko
ITC, Russian Federation

Reactions between the paramagnetic transition metal ions and nitroxides are convenient and effective methods for the preparation of heterospin crystals. The presence of several paramagnetic centers in heterospin molecules stirred the growing interest in their magnetic properties because these compounds are convenient objects for studying the fine distinctions in exchange interaction channels and revealing valuable magneto-structural correlations. When the temperature (or pressure) changes, the solid compounds undergo structural rearrangements accompanied by magnetic effects similar to spin crossover. The observed anomalies are caused by the reversible spatial dynamics of Jahn-Teller coordination units. The high mechanical stability of the crystals, i.e., their ability of being reversibly compressed and expanded in the temperature range of phase transition, underlies the term breathing crystals. When the cooling–heating cycles are repeated in the range 5–325 K the phase transformations of the heterospin crystals may be accompanied by deep coloring of the solid phase, which is an unusual effect. The possibility of creating spin devices whose working unit is an exchange cluster that changes multiplicity under the action of temperature, pressure, or light was discussed. The effect of a change in the external pressure on the character of the temperature dependence of the effective magnetic moment is discussed. Noteworthy, external pressure variation and temperature variation have essentially different effect on the magneto-structural correlations.

Biography

Victor Ovcharenko has his expertise in design of molecular magnets and investigation of spin transitions, “breathing crystals” and magneto-structural correlations in heterospin compounds. He developed new methods of selective synthesis of highly dimensional heterospin systems based on metal complexes with stable organic radicals, investigated magneto-structural correlations inherent in heterospin compounds, created a new type of breathing crystals and explained mechanical activity of these crystals (breathing crystals, jumping crystals, dancing crystals).

Victor.Ovcharenko@tomo.nsc.ru

Notes:

2nd International Conference on

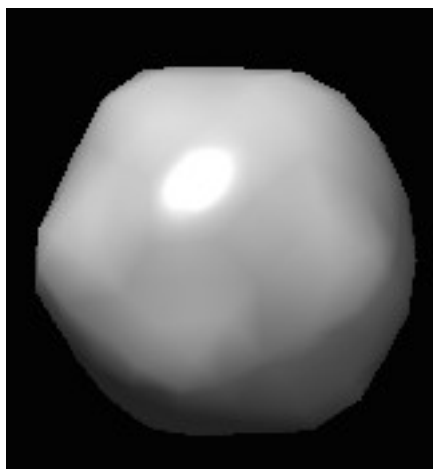
APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structure of viruses from experimental data from an X-ray free electron laser

Dilano K Saldin and F Jamaludin
University of Wisconsin-Milwaukee, USA

The X-ray Free Electron Later (XFEL) is a brand new machine capable of delivering X-ray to a sample some 10 billion times brighter than a conventional source. The question is whether one can exploit the ultra-brightness of the source to enable structure determination of identical randomly oriented particles delivered to the beam by means of a sample delivery system specifically designed for this purpose. The particles will be delivered to the XFEL in a specially designed apparatus that delivers identical particles in random orientation. The question is whether one can determine the structure of the particles from the collection of diffraction patterns even though one does not know the precise orientation of the particle in each. We demonstrate a solution with experimental data for the icosahedral virus PR772 from an XFEL. What we exploit is the fact that the angular correlations amongst the intensities are independent of particle orientation. Consequently an average over all diffraction patterns of the angular correlation merely increases the accuracy of the angular correlation measurement. We have developed a method of extracting the X-ray diffraction volume from accurately determined angular correlations. An iterative phasing algorithm then recovers the electron density of the viruses from the diffraction volume.



Biography

Dilano K Saldin is a Professor at the Physics Department of the University of Wisconsin-Milwaukee, where he started as a Surface Physicist, but has over the past 10 years turned his attention to the problem of structure determination in the XFEL particularly of viruses.

dksaldin@uwm.edu

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structural changes in type-I collagen from non-enzymatic glycation revealed by isomorphous X-ray diffraction

Rama S Madhurapantula and Joseph Orgel
Illinois Institute of Technology, USA

The process of non-enzymatic glycosylation, i.e., glycation, is rather slow resulting in the formation of sugar-mediated crosslinks, also known as Advanced Glycation Endproducts (AGEs), within the native structure of type-I collagen. This process occurs in all animals but is accelerated in diabetics. However, the exact locations or regions of high propensity for the formation of these crosslinks within the packing structure of collagen are largely unknown, despite our knowledge of the underlying chemistry. The results obtained showed the location of possible crosslinks and correlate the effects of crosslinks to the structural and functional sites present on the D-periodic arrangement of collagen into fibrils. Prolonged treatment with iodine, as a wound disinfectant, is detrimental to the structure of collagen underlying the wound site. Diabetic patients are more prone to injuries to limb extremities. Wounded extremities are commonly amputated to prevent the spread of infection to the rest of the body followed by low dose iodine application to the wound site. We will present results to demonstrate specific disintegration of collagen fibrils in rat tail tendons from a short iodine treatment.

Biography

Rama S Madhurapantula is a Senior Postdoctoral Research Associate at Dr. Joseph Orgel's research group at the Illinois Institute of Technology, USA. He is currently involved with work on the changes in molecular packing in myelin and cytoskeleton caused by traumatic brain injury and understanding stress-strain relations in the muscle tendon junction using X-ray diffraction. He also specializes in HPLC method development and has collaborated with various research groups from Chicago to develop new methods for measuring analytes in various samples.

rmadhura@iit.edu

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Non-covalent interactions that control the self-assembly of organic molecular crystals

M Sithambaresan

Eastern University, Sri Lanka

Non-covalent interactions (NCI) are of paramount importance in chemistry and especially in bio-disciplines since they set up the force-field scenario through which chemical species interact with each other without a significant electron sharing between them. They represent, in fact, the machinery through which molecules recognize themselves and establish how molecules will approach and eventually pack together. These kinds of weak interactions become important in determining the properties of substances and therefore we have explored some of the novel organic molecular crystals to study the non-covalent interactions and their behavioral patterns during packing of molecular crystals. Animated pictures and videos are used to explore the nature of these interactions. This study provides better understanding of various non-covalent forces such as classical and non-classical hydrogen bond, $\pi \dots \pi$, C-H... π interactions etc. thereby demonstrating the packing forces for designing novel materials having certain interesting physical properties.

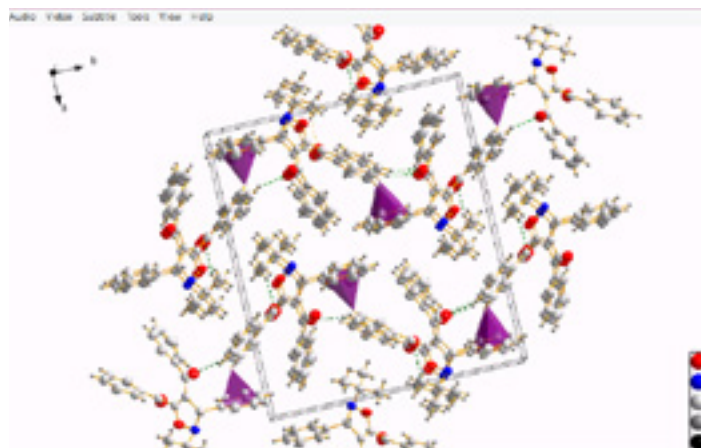


Figure-1: Crystal packing diagram of 3,5-dihydro-5,9 b-o-benzonaphtho [1,2-c] furan-1-one viewed along a axis.

Biography

M Sithambaresan has his expertise in synthesis and characterization of transition metal complexes and single crystal studies of organic ligands and metal complexes. His works on crystal studies on ligands and metal complexes creates new pathways for improving characterization of novel complex molecules and designing of new materials with required properties to enlighten the development of sensor for medical, pharmaceutical and various other fields.

msithambaresan@gmail.com

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Three parameter crystal-structure prediction for sp-d valent compounds

Thomas Hammerschmidt
Ruhr-Universität Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges in materials design. We use a cluster analysis of experimentally observed crystal structures and derive structure maps that are systematically optimized to reach high predictive power. In particular, we present a three-dimensional structure map for compounds that contain sp-block elements and transition metals in arbitrary composition. The structure map predicts the correct crystal structure with a probability of 86% and has a confidence of 98% that the correct crystal structure is among three predicted crystal structures. The three parameters that span the structure map are physically intuitive functions of the number of valence electrons, the atomic volume and the electronegativity of the constituent elements. We test the structure map against standard density-functional theory calculations for 1:1 sp-d-valent compounds and demonstrate that our three-parameter model has comparable predictive power. We show that the identified parameters are valid for off-stoichiometric compounds and they separate binary and ternary crystal-structure prototypes.

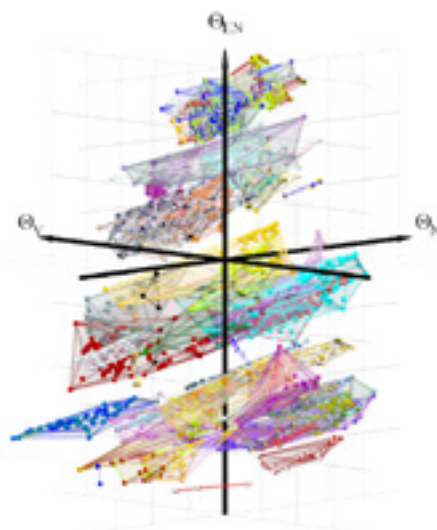


Figure-1: Three-parameter structure map for sp-d valent compounds. The colored polyhedrons correspond to different crystal-structures. The three descriptors are physically intuitive functions of electron count (N), atomic size (V) and electro-negativity (EN).

Biography

Thomas Hammerschmidt has his expertise and passion on the reliable and robust prediction of structural stability and phase stability of technologically relevant materials. In order to make direct contact to experiments, he includes finite temperature, complex microstructures and multi-component chemistry. His focus is particularly the development, implementation and application of analytic bond-order potentials for large scale atomistic simulations.

thomas.hammerschmidt@rub.de

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Novel magnetism and local symmetry breaking in a mott insulator with strong spin orbit interactions

Vesna F Mitrovic
Brown University, USA

Study of the combined effects of strong electronic correlations with spin-orbit coupling (SOC) represents a central issue in quantum materials research. Predicting emergent properties represents a huge theoretical problem since the presence of SOC implies that the spin is not a good quantum number. Existing theories propose the emergence of a multitude of exotic quantum phases, distinguishable by either local point symmetry breaking or local spin expectation values, even in materials with simple cubic crystal structure such as $\text{Ba}_2\text{NaOsO}_6$. Experimental tests of these theories by local probes are highly sought for. Our local measurements designed to concurrently probe spin and orbital/lattice degrees of freedom of $\text{Ba}_2\text{NaOsO}_6$ provide such tests. We show that a canted ferromagnetic phase which is preceded by local point symmetry breaking is stabilized at low temperatures as predicted by quantum theories involving multipolar spin interactions. Specifically, we find that the ferromagnetic state is in fact a type of canted ferromagnet with two sub-lattice magnetizations and that cubic symmetry breaking occurs at a temperature above the Néel temperature and it involves deformation of oxygen octahedra presumably reflecting a complicated pattern of staggered orbital order. Our findings are in startlingly good agreement with theoretical predictions based on quantum models. Thus, our results, to be presented, establish that such quantum models represent an appropriate theoretical framework for predicting emergent properties in materials with both strong correlations and SOC, in general.

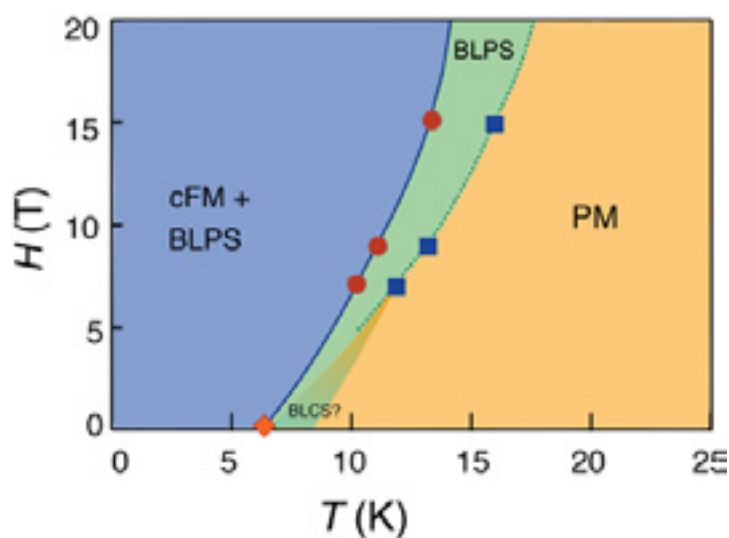


Figure 1: Phase diagram based on nuclear magnetic resonance measurements. The square symbols data indicate onset temperature for the local cubic symmetry breaking. Circles denote transition temperature into canted ferromagnetic (cFM) phase. The solid line indicates phase transition into the cFM state. The dashed line denotes cross-over to the broken local point symmetry (BLPS) phase.

Biography

Vesna F Mitrovic has her expertise in study of microscopic properties of materials using magnetic resonance techniques. She is a graduate of Illinois Institute of Technology and received her PhD from Northwestern University in 2001. Her thesis work was on magnetic resonance studies of high temperature superconductor. In 2003, she joined the Brown Physics Department and she was named Alfred P. Sloan Fellow in 2007 and Fellow of American Physical Society in 2015 for her pioneering contributions to NMR study of low energy excitations in emergent quantum phases.

vemi@brown.edu

2nd International Conference on

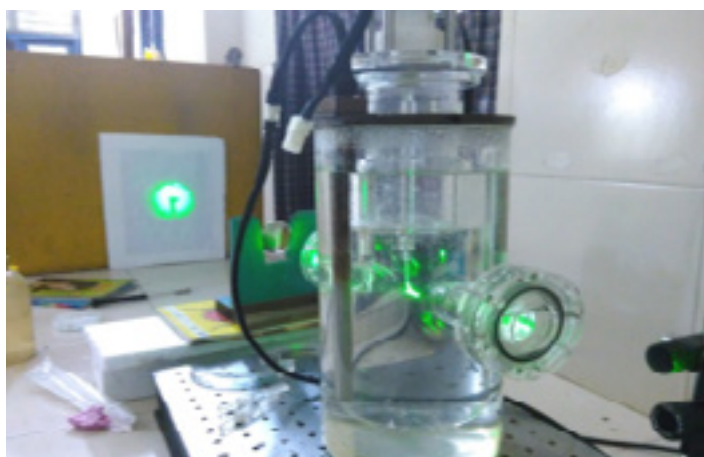
APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Growth and growth rate analysis of potassium succinate crystal

Vijeesh P^{1,2}, Annieta Philip K¹ and Supriya M H²¹The Cochin College, India²Cochin University of Science and Technology, India

Single crystals of potassium succinate-succinic acid were grown by slow-cooling method. The growth of the crystal is recorded using shadowgraph and the growth rate is evaluated using image processing. The growth rate analysis showed that slow cooling rate enhances the quality of crystal obtained. Also the *in situ* image analysis of the crystal gives a better method for controlling the growth parameters of the crystal. Semi organic non-linear optical materials play an important role in many fields of science such as information storage systems, data processing systems, information technology, telecommunication, utility equipment development, etc. Their properties like high melting point, dielectric and mechanical stability, second harmonic generation, etc. made them suitable for many applications. Semi organic non-linear materials are developed to overcome the shortcomings of organic non-linear materials such as low transparency and short optical band gap. Semi organic materials formed with ionic salts offer wide range of frequencies. Also it is much easier to grow semi organic materials. This paper presents the design and realization of a crystallizer and its use to synthesize from aqueous solution, structure, crystal growth and growth rate analysis of Potassium Succinate (KS) crystal which belongs to monoclinic system. Even though the evaporation techniques were used for the growth of KS, the slow cooling solution growth of KS is not much tried so far. This method provides comparatively easier and faster method to grow crystals. The solution growth of KS is not much represented in the literature. A crystallizer for slow cooling solution growth is designed and realized and a single crystal of potassium succinate is grown using slow cooling solution growth technique. The growth rate analysis is done by shadowgraph image analysis. The image analysis showed the growth rate of different faces of the crystal.



Biography

Vijeesh P is currently an Assistant Professor in the Department of Physics, The Cochin College and Research Scholar in Cochin University of Science and Technology. His major research area is crystallography.

namastheviji@gmail.com

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structural insights into Crenezumab's mechanism of action

Weiru Wang
Genentech, USA

Crenezumab is a fully humanized immunoglobulin isotype G4 (IgG4) monoclonal antibody that binds to monomeric as well as aggregated A β forms (oligomers, fibers and plaques). Notably, crenezumab binds with higher affinity to A β oligomers over monomers and *in vitro* studies have demonstrated crenezumab's ability to block A β aggregation and promote A β disaggregation. To understand the structural basis for this activity and crenezumab's broad binding profile, we determined the crystal structure of crenezumab in complex with A β . The structure reveals a sequential epitope and the conformational requirements for epitope recognition, which include a subtle but critical element that is likely the basis for crenezumab's versatile binding profile. We find interactions consistent with high affinity for multiple forms of A β , particularly oligomers. Crenezumab also sequesters the hydrophobic core of A β and breaks an essential salt-bridge characteristic of the β -hairpin conformation, eliminating features characteristic of the basic organization in A β oligomers and fibrils, and explains crenezumab's inhibition of aggregation and promotion of disaggregation. These insights highlight crenezumab's unique mechanism of action, particularly regarding A β oligomers and provide a strong rationale for the evaluation of crenezumab as a potential treatment for patients with Alzheimer's disease.

Biography

Weiru Wang has completed his PhD in Biophysics from Cornell University and Post-doctoral studies from University of California, Berkeley. He is currently a Senior Scientist and a Group Leader in the Structural Biology Department at Genentech, a member of the Roche Group. His research focuses on understanding of molecular basis of protein-drug interactions using biophysical methods, primarily macromolecular crystallography.

wang.weiru@gene.com

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Light-induced crawling motion of azobenzene crystals on a glass surface

Yasuo Norikane

National Institute of Advanced Industrial Science and Technology, Japan

Creating self-propelled motion in nano- to macroscopic sized objects has been of interest to scientists. Physical or chemical energy has been used to obtain motion of liquid droplets or solid objects in various media. Using light as an energy source, photochromic molecules have been utilized to induce various mechanical motions of objects. In many cases, the mechanical motions involve the photochemical reactions of azobenzene molecules, which exhibit photoisomerization between trans and cis isomers. So far, various type of motion has been reported; however, photo-induced translational motion of crystals on solid surfaces is unknown. Recently, we have been interested in photochemically-induced phase transitions between solid and liquid phases in photochromic organic compounds such as macrocyclic or rod-shaped azobenzene derivatives. Materials' showing the phase transition has been of interest because of its interesting properties such as photocontrollable adhesives, photoresists and motion on water surface. Here, we report the novel crawling motion of crystals of simple azobenzenes such as azobenzene and 3,3'- dimethylazobenzene on a glass surface. The motion is directional and continuous when irradiated simultaneously with two different wavelengths (365 and 465 nm). Our method is simple as crystals move on a bare glass surface using a light-emitting diodes or Hg lamp as light sources in a fixed position. The direction of the motion can be controlled by the position of the light sources and the crystals can even climb vertical surfaces. The motion proceeds without changing the crystal orientation, despite the large deformation of the crystal shape. There is a no need for any special treatment such as chemical modification, spatial gradient or application of ratchet potential of the solid surface. It is presumed that the motion is driven by crystallization and melting at the front and rear edges of the crystal, respectively, via photochemical conversion between the crystal and liquid phases induced by the trans-cis isomerization of azobenzenes.

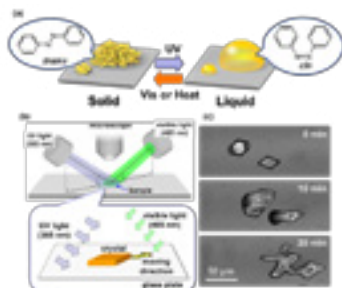


Figure 1 (a) Schematic representation of the photoinduced phase transition. (b) Schematic diagram of the experimental set-up and the crystal motion. (c) Laser microscope images for the translational motion of 3,3'-dimethylazobenzene crystals on a glass surface.

Biography

Yasuo Norikane has received his PhD in 2001 from University of Tsukuba, Japan, for investigating the photochemistry of intramolecularly hydrogen-bonded molecules, under the supervision of Professor Tatsuo Arai. From 2001-2003, he carried out his Postdoctoral research on novel crystal structure and photo-isomerization in macrocyclic azobenzenes with Dr. Nobuyuki Tamaoki at AIST. After serving as a second Post-doctorate with Professor M. Reza Ghadiri at the Scripps Research Institute, he began his carrier as a Researcher in AIST. He was awarded a Commendation for Science and Technology by The Minister of Education, Culture, Sports, Science and Technology, Japan. He is currently a Group Leader at Electronics and Photonics Research Institute and an Associate Professor at Department of Chemistry, University of Tsukuba. His research focuses on organic photochemistry especially in design and synthesis of photofunctional materials using photochromic compounds such as azobenzene.

y-norikane@aist.go.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Recent developments in single crystal diffuse scattering: Imaging nanoscale disorder in reciprocal space

Stephan Rosenkranz, Matthew J. Krogstad, Raymond Osborn, Peter Zapol, and Justin M. Wozniak
Argonne National Laboratory, USA

Correlated defects are responsible for the functional properties of many materials that underpin energy-related technologies. Single-crystal diffuse scattering using x-rays or neutrons offers a powerful probe of such short-range order in crystalline lattices, but its use has been limited by the experimental challenge of collecting data over a sufficiently large volume of reciprocal space and the theoretical challenge of modeling the results. However, instrumental and computational advances at both x-ray and neutron sources now allow the efficient measurement and rapid transformation of reciprocal space data into three-dimensional pair distribution functions, providing model-independent images of nanoscale disorder in real space. We discuss how these recent developments of efficient methods of measuring single crystal diffuse scattering provide new insights into cation disorder in electrode materials. Large volumes of measured diffuse scattering in reciprocal space are transformed into 3D difference pair distribution functions (3D- Δ PDF) that image defect-defect correlations in real space, allowing a model-independent view of short-range order. We demonstrate this with data on β - $\text{Na}_x\text{V}_2\text{O}_5$ with $x=0.2$ and 0.4 over the temperature range 100K to 500K. The sodium intercalants partially occupy sites on two-rung ladders penetrating the framework of vanadium oxide pyramids and octahedra, with no long-range order at room temperature and above. However, at $x=0.4$, the length scale of sodium-sodium correlations increases significantly below 200K with the emergence of forbidden Bragg peaks below an order-disorder transition. The 3D- Δ PDF directly reveal that the sodium ions occupy alternate sites on each ladder rung, with a zig-zag configuration that is in phase with neighboring ladders. The growth in the length scale of sodium-sodium correlations with decreasing temperature is clearly seen in real space images that allow a quantitative determination of the interionic interactions that impede ionic mobility.

Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering. Research conducted at ORNL's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US. Department of Energy. Research conducted at the Cornell High Energy Synchrotron Source (CHESS) was supported by the NSF & NIH/NIGMS via NSF award DMR-1332208.

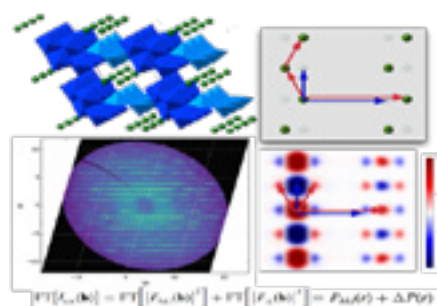


Figure 1: Transformation of the measured diffuse scattering from $\text{Na}_x\text{V}_2\text{O}_5$ and the 3D- Δ PDF transform, which reveals the freezing of the Na ions in a zigzag chain.

Biography

Stephan Rosenkranz is a Senior Physicist in Materials Science Division at Argonne National Laboratory, USA. He has completed his Ph.D. in Physics in 1996 at ETH Zurich. His Diploma in experimental physics in 1992 at ETH Zurich. His research interest is on Structure and dynamics of strongly correlated systems, in particular the role of phase competition in generating complex phenomena. Investigation of long-range order and excitations and short-range correlations and fluctuations due to the presence of ground states with competing order.

srosenkranz@anl.gov

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Structural response to pressure in 1111-type iron-based superconductor $\text{LaFeAsO}_{1-x}\text{H}_x$

Kensuke Kobayashi

High Energy Accelerator Research Organization, Japan

Iron-based superconductor (iron pnictides) and cuprates are most well-known types of superconductor with critical temperature (T_c) higher than 50 K. In iron-based superconductors, the relation between the maximum T_c and structural parameters of FePn_4 (Pn = pnictide) has been proposed as follows: the highest T_c is achieved when the Pn-Fe-Pn bond angle ($\alpha_{\text{Pn-Fe-Pn}}$) approaches 109.5° as in a regular tetrahedron of FePn_4 or when the Pn height from Fe plane (h_{Pn}) $\sim 1.38 \text{ \AA}$. The application of pressure is a direct and clean way to modify the local geometry of FePn_4 without the degradation of the crystal in comparison to the chemical substitution; hence, the detailed crystal structure under pressure warrants further investigation. A systematic study of the crystal structure of a layered iron oxypnictide $\text{LaFeAsO}_{1-x}\text{H}_x$, with a unique phase diagram of two superconducting phases and two parent phases, as a function of pressure was performed using synchrotron X-ray diffraction. We established that the $\alpha_{\text{As-Fe-As}}$ widens on application of pressure due to the interspace between the layers being nearly infilled by the large La and As atoms. This behavior implies that the FeAs_4 coordination deviates from the regular tetrahedron in our systems, which breaks a widely accepted structural guide albeit the increase of T_c from 18 K at ambient pressure to 52 K at 6 GPa for $x = 0.2$. In the phase diagram, the second parent phase at $x \sim 0.5$ is suppressed by low-pressure at $\sim 1.5 \text{ GPa}$ in contrast to the first parent phase at $x \sim 0$, which remains robust to pressure. We suggest that the spin/orbital fluctuation from the second parent phase gives rise to the high- T_c under pressure. The pressure responses of the FeAs_4 modification, the parent phases, and their correlation are previously unexplained peculiarities in 1111-type iron-based superconductors.

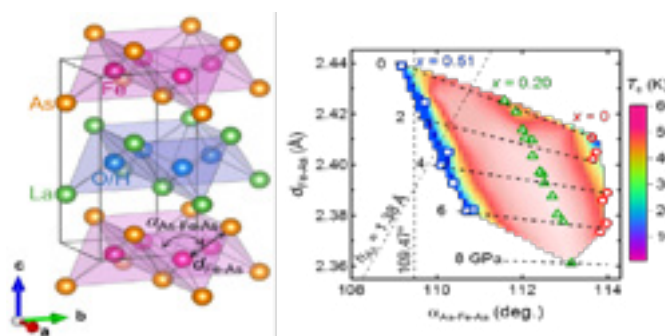


Figure 1: Crystal structure of $\text{LaFeAsO}_{1-x}\text{H}_x$ and the contour plots of T_c as a function of As-Fe-As bond angle ($\alpha_{\text{As-Fe-As}}$) and the Fe-As bond length ($d_{\text{Fe-As}}$).

Biography

Kensuke Kobayashi has received his doctor's degree in science from Osaka City University in 2009. Since April 2010, he has been a researcher at Condensed Matter Research Center (CMRC), Institute of Material Structure Science, KEK. At present, he is a Project Assistant Professor (MEXT Element Strategy Initiative) and worked on experimental studies of the structural and electrical properties of materials by means of synchrotron X-ray diffraction under external fields, such as pressure, electric field and low temperature

kensuke.kobayashi@kek.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Role of crystal structure stability for energy storage applications

A. K. Thakur

Indian Institute of Technology Patna, India

Materials research for energy storage applications has drawn considerable attention in recent years owing to growing alertness on saving earth from impending dangers of pollution, implementation of stricter emission norms across the globe and emerging emphasis on development of clean/green energy alternatives. To meet this challenge, chain of efforts aimed at bringing a paradigm shift in energy research is underway. Potential candidates are solar photovoltaics, fuel cells and storage devices. Further, the best considered and commercially available alternative is solar photovoltaics. However, it cannot act itself as a standalone energy solution. It requires storage devices as backup for providing energy when source of solar energy recedes into background during night. The most sought-after storage devices are high energy density rechargeable batteries, supercapacitors and a hybrid of the two. All energy storage devices are based on conversion of stored chemical energy into electrical energy. Energy storage devices, being multi component system, primarily comprise a separator compartment sandwiched between two electrodes (anode & cathode). Energy storage capability is determined by its crystallographic structure. Crystallographic structure & phase, structural stability and strain bearing capability of these components play a crucial role in determining their suitability as a storage device component. Such applications require a single phase layered crystallographic structure with attributes such as: (a) availability of guest sites for intercalation-deintercalation of cations during charge-discharge cycles, (b) layered tunnel type structure along all the planes in a 3-D geometry, (c) presence of crystalline structure with a flexible framework, (d) sustainability of volume expansion with capability of withstanding lattice strain, (e) phase stability etc. In the present work, we report a review of the crystallographic features of some important material structures used in energy storage applications. State-of-the-art developments in the area covering recent emphasis on development of new generation of materials with structural suitability for high energy density applications is proposed to be discussed with summary of the ongoing work in our laboratory at IIT Patna.

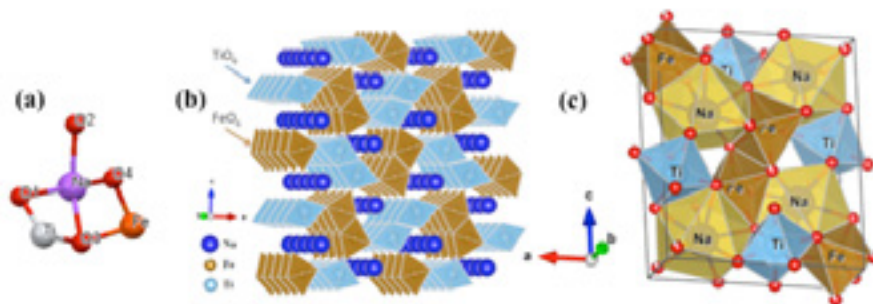


Fig.1: Layered structure with Na⁺ ion intercalation sites in the proposed sodium battery electrode

Biography

A. K. Thakur is currently working at the Department of Physics at the Indian Institute of Technology Patna, India as Associate Professor. His research area is experimental condensed matter physics and applied physics with focus on wide variety of materials including ceramics and polymer composites for device applications including sensors, EMI shielding and renewable energy. His current interest lies in development of new generation of novel functional materials for clean and green energy alternatives.

akt@iitp.ac.in

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Landyne, a software suite for electron diffraction simulation and crystallographic analysis

Xing-Zhong Li

University of Nebraska, USA

Landyne software suite is the 2.0 version of the previous JECP—a Java Electron Crystallography Project. The software suite currently includes eight stand-alone computer programs. Each of them was designed for one topic of application in electron diffraction simulation, crystallographic analysis or experimental data processing and quantification. Figure 1 shows the classification of the computer programs in the Landyne suite according to their functionality. The computer programs have been grouped into a suite to increase the total usefulness and a launcher has been developed for the users to conveniently access all of the computer programs. The purpose of this software suite is twofold: i) as research tools to analyze experimental results, ii) as teaching tools to show students the principles of electron diffraction and crystallography. The software suite was programmed using Java SE Development Kit 8. It has been successfully tested on Microsoft Windows 7, 8 and 10 with a Java virtual machine, i.e. Java 2 Runtime Environment (J2RE). The executable codes, user manuals and a set of crystal structural data are available at <http://www.unl.edu/ncmn-cfem/xzli/computer-programs>. The design and functions of the computer programs will be elucidated in this presentation. Three examples are listed here: SAED is used for simulation and analysis of electron diffraction patterns including twins and two phases with a fixed orientation and the search for the zone axes of experimental patterns; SPICA is for the calculation of stereograms and related applications; LAUNCE is for lattice reconstruction and unit cell determination of unknown crystal phases in TEM experiments. The application of the Landyne suite in our recent research works will be also discussed.

<http://www.unl.edu/ncmn-cfem/xzli/computer-programs>

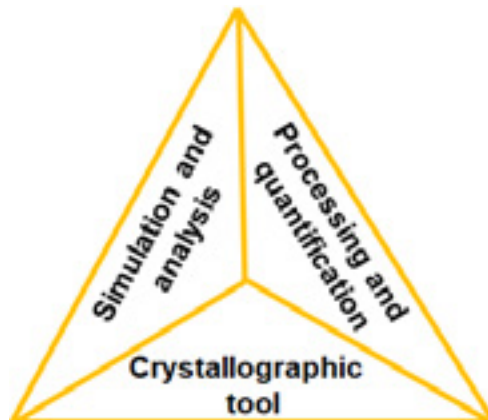


Figure 1: The classification of the computer programs in the Landyne suite according to their functionality and the relationship among the three subgroups.

Biography

Xing-Zhong Li has his expertise in transmission electron microscopy on materials and nanoscience. He started the works on computer programs for electron diffraction simulation and crystallographic analysis a decade ago. He works in Nebraska Center for Materials and Nanoscience, University of Nebraska.

xzli@unl.edu

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Double bragg scattering from highly oriented pyrolytic graphite in small-angle X-ray scattering region

Yoshinori Ohmasa¹, Ayano Chiba²¹Kansai University, Japan²Keio University, Japan

Highly oriented pyrolytic graphite (HOPG) is a form of carbon, which is composed of many crystallites arranged uniaxially. The c-axes of the crystallites are aligned along a single direction, while the a- and b-axes are distributed randomly in the plane perpendicular to the c-axis. HOPG is used in a wide range of scientific and technological areas, for example as a monochromator of X-ray and neutron beams. We measured small-angle X-ray scattering from HOPG and observed radial streak patterns. When the sample is rotated, the number and the direction of the streaks change. The streaks are divided into two categories: (i) A pair of streaks which forms X-shaped pattern. The angle between the two streaks changes with sample rotation, and they appear and disappear in pairs. (ii) A single streak which appears only in a narrow range of the sample rotation angle. Examples of the streak patterns of the type (i) and (ii) are shown in Fig.1 and 2, respectively. We found that the appearance of the streaks is explained by double Bragg scattering. They appear in the small-angle region because the first scattered X-ray is scattered back to the small-angle region. The streaks of the type (i) is caused by the successive Bragg reflections hkl and hkl with $(h,k) \neq (0,0)$, and (ii) is by $00l$ and $00l$. The dependence of the streak directions on the sample rotation angle is in good agreement with theoretical prediction. The double Bragg scattering observed in the present work is an obstacle to obtaining the 'true' small-angle scattering. On the other hand, the intensity profile of the double Bragg scattering pattern itself is interesting because it contains various pieces of information on the sample structure. For example, the width and length of the streaks are related to the distribution of crystallites.

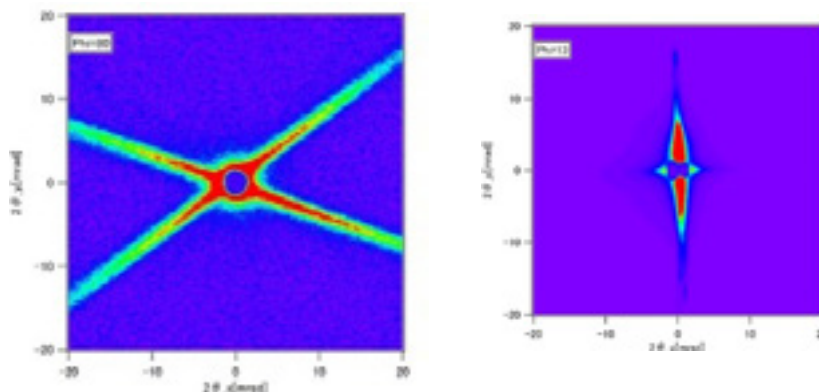


Fig.1(left) Fig.2(right) : Examples of observed streak patterns of the type (i) and (ii), respectively. The scattering in Fig.1 is caused by the successive Bragg scatterings and , and Fig.2 is by and

Biography

Yoshinori Ohmasa studied physics at Kyoto University and received PhD from Kyoto University. His doctoral thesis is about the phase transitions and the structure of halogen mixed crystals under high pressure. He worked at Kyoto University from 1996 to 2008, and moved to Hiroshima Institute of Technology, and then to Kansai University. His research interest covers the field of structurally disordered materials, such as liquid, glass, alloys and disordered crystals. Especially, he has been studying phenomena related to liquid surface, such as wetting and capillary waves.

y_ohmasa@kansaiu.ac.jp

Notes:

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

How does crystallography affect material properties?

Serife Yalcin

Harran University, Turkey

Statement of the Problem: Developments in science and technology have required the production of new materials and design. Knowing the properties of the materials used to obtain them are helpful to design and manufacture of materials that we need. Crystallography studies have been very important for developing of materials because this studies deal with internal structure, in particular the symmetry of crystal. The majority of the solid materials are composed of crystals. This explains how much important crystallography is in material. The purpose of this study is to determine suitable materials for material science need.

Methodology & Results: Crystallography is the science of structure used for characterization of materials and to determine some physical properties with microstructure and texture analyses. It includes the general features of structure and deals with the mapping of all kinds of systems as geometrical representations. The same material with different crystallographic parameter has different properties. It is hardly possible to develop materials science without crystallographic techniques. As a sample, we will focus on structure of calcium carbonate. Calcium carbonate is one of the most abundant and cheap material found in nature. It can be found in three forms: Calcite, aragonite and vaterite. XRD pattern of aragonite, calcite and vaterite shows difference as seen in Figure-1. These patterns show difference depending on crystal structure. When Scanning Electron Microscopy (SEM) image investigate of different forms of calcium carbonate, it has been observed difference among picture. Calcite structure shows square structure while aragonite and vaterite structure show rod and flower type structure, respectively.

Conclusion & Significance: The results have showed difference depending on the form of calcium carbonate. Young modulus has been obtained 76, 89-193 Pa for calcite and aragonite, respectively. Preparation of materials that is needs of human must be in coordination with crystallography.

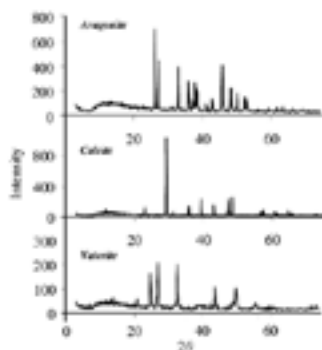


Figure-1: XRD pattern of aragonite, calcite and vaterite calcium carbonate.

Biography

Serife Yalcin has completed her PhD from Erciyes University and Postdoctoral studies from Caen University. She has published more than 40 papers in reputed journals and has been serving as an Editorial Board Member of repute.

serifeyalcin@harran.edu.tr

Notes: