Crystallography 2017

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Keynote Forum

Day 1

Dieter Herlach, Struct Chem Crystallogr Commun, 3:2
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Dieter Herlach

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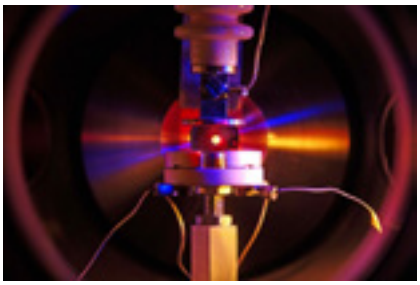
Crystal nucleation and growth in undercooled melts of metals and alloys

An undercooled melt possesses an enhanced free enthalpy that gives access to crystallize metastable solids. Crystal nucleation selects the crystallographic phase whereas the subsequent crystal growth controls the microstructure evolution. Electromagnetic and electrostatic levitation techniques are very efficient to produce a highly undercooled melt since heterogeneous nucleation on container-walls is avoided. Moreover, a freely suspended drop is accessible for *in situ* observation of crystallization far away from equilibrium. We combine levitation technique with the diagnostic means of neutron scattering to investigate short range order in undercooled melts and energy dispersive X-ray diffraction of synchrotron radiation to observe phase selection processes upon undercooling. Measurements of the statistics of nucleation undercooling are performed in order to study the physical nature of crystal nucleation. Nucleation is followed by crystal growth. In undercooled melts, the crystal grows with dendritic morphology since a planar interface is destabilized by the negative temperature gradient ahead the solid liquid interface. In highly undercooled melts, dendrites propagate very rapidly. A high speed camera is used to record the advancement of the solidification front. Dendrite growth velocities are measured as a function of undercooling of pure metals, solid solutions and intermetallics. Non-equilibrium crystallization effects are evidenced. Crystal growth is governed by heat and mass transport. To explore the influence of convection on dendrite growth comparative experiments in microgravity are performed using an electromagnetic levitator on board in the International Space Station. Metals show dendritic growth in a mesoscopic scale with a rough interface at the microscopic scale. In case of semiconductors the solidification front is facetted in a mesoscopic scale with a smooth interface in a microscopic scale. The entropy of fusion of the compound Ni_2B is located in between that of metals and semiconductors. A transition from dendritic to facetted growth is observed induced by convection in the undercooled drops.



Biography

Dieter Herlach as studied Physics at the RWTH Aachen and received Doctoral degree as Dr. rer. nat. at the same university. He became private lecturer upon a Habilitation at the Ruhr-University Bochum RUB. Presently, he is Group Leader at the Institute of Materials Physics in Space and Senior Scientist of the German Aerospace Center, Germany. He is a Full Professor of Physics at RUB. He has authored over 300 scientific publications in refereed journals. He is author and Editor of six books and Co-Editor of *Advanced Engineering Materials*. He leaded and leads projects of the German Research Foundation, the German Aerospace Center-Space Management, the European Space Agency and was the Principal Investigator of NASA during three spacelab missions. He is an Honorary Professor of three universities and received Chinese Friendship Award in Beijing in 2000 and the Lee Hsun Lecture Award of the Chinese Academy of Sciences in 2007. He has chaired the Division of Metal and Materials Physics of the German Physical Society DPG and was elected as Member of the Council of DPG. He was an elected Member of the General Review Committee of DFG and Deputy Chairman of the German Society of Materials Science and Engineering.

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Eui-Hyeok Yang, Struct Chem Crystallogr Commun, 3:2
DOI: 10.21767/2470-9905-C1-001

Eui-Hyeok Yang

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Synthesis of 2D flatlands beyond graphene

I will present one of our primary research topics, focusing on our development of the chemical vapor deposition (CVD)-growth of 2D materials; we develop a direct growth process to enable localized, patterned, single crystalline or large-scale polycrystalline monolayers of TMDs, including MoS_2, WS_2, WSe_2 and $MoSe_2$, along with their heterostructures. TMDs are emerging graphene analogues with unique properties for optoelectronic applications, but they are prone to rapid oxidation in air, presenting a critical roadblock in practical device applications. In attempts to overcome this issue of TMD oxidation, we study CVD-growth and perform extensive material characterization to illuminate the role of dissimilar 2D substrates in the prevention of interior defects in TMDs, thus uncovering the conditions for anti-oxidation. This research provides a detailed look into the oxidation and anti-oxidation behaviors of TMDs, which corroborates the role of underlying 2D layers in the prevention of interior defects in TMDs. We furthermore show the epitaxial growth of TMDs on hBN and graphene, as well as vertical/lateral heterostructures of TMDs, uniquely forming in-phase 2D heterostructures, and we examine the resulting quality and integrity of differing heterostructure. If the technique could be developed to be highly reliable and high fidelity, it could have a high impact on the future research and commercializability of TMD-based devices.

Biography

Dr. E. H. Yang is a full professor of Mechanical Engineering Department at Stevens Institute of Technology. He received Ph.D. degrees from Ajou University, Korea. After his postdoctoral training at University of Tokyo and at California Institute of Technology, he joined NASA's Jet Propulsion Laboratory where he became a Senior Member of the Engineering Staff. At JPL, he received a number of awards, including NASA ICB Space Act Awards, Bonus (Level B and C) Awards and a number of Class 1 NASA Tech Brief Awards. In recognition of his excellence in advancing the use of MEMS-based actuators for NASA's space applications, he received the prestigious Lew Allen Award for Excellence at JPL in 2003. His scholarly leadership has been recognized by peers. Examples of these efforts include being appointed as an Associate Editor and/or Editorial Board of several journals including Nature's Scientific Reports, and being elected as the Division Chair of the ASME MEMS Division. Since joining Stevens in 2006, he has been responsible for obtaining competitive research funding from several federal agencies including NSF, AFOSR, US Army, NRO, NASA and DARPA (including 6 NSF and 3 AFOSR grants, and 5 NASA and 3 NRO contracts). Dr. Yang holds over 12 patents issued or pending. Dr. Yang is the director of the Micro Device Laboratory, a Stevens's multi-user microfabrication facility.

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Joseph Orgel, Struct Chem Crystallogr Commun, 3:2
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Joseph Orgel

Illinois Institute of Technology, USA

X-ray diffraction reveals the mechanical load tolerance of mammalian nerve, muscle and tendon in traumatically induced injury and the vertebrate identity of fossilized T-rex bone

Those living with traumatically induced injuries, including but not limited to, Traumatic Brain Injury (TBI), face an elevated risk for developing chronic health issues including Alzheimer's disease (AD) or AD-like dementia and depression. One of the most serious impediments to the study of traumatic injury is the lack of meaningful primary mechanical damage criteria at the molecular level. This study addresses this, through the use of novel imaging technologies such as a newly developed X-ray Diffraction (XRD) scanning methodology, applied to systemically loaded animal models of both brain and connective tissue injury and accompanied by conventional microscopy for cross-correlation of observations. Interestingly, this same technique reveals the state and status of soft tissue preserved in T-rex fossilized bone.

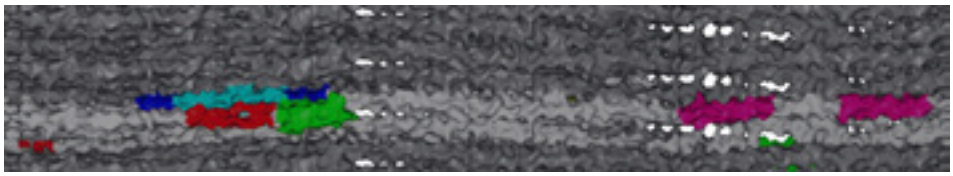

Figure-1: Molecular representation of connective tissue structure

Biography

Joseph Orgel is a British American Scientist based at the Illinois Institute of Technology with past and present appointments in Biology, Physics and Biomedical Engineering and Applied Health Sciences at UIC as Visiting Faculty. His research interests are concerned with fundamental structural biochemistry problems that have direct links to the understanding and treatment of disease. He leads investigations of brain pathological diseases such as Alzheimer's and Traumatic Brain Injury in collaboration with the US Army and connective tissue conditions including heart disease and arthritis at the National Institutes of Health Biotechnology Research Resource, BioCAT, as Associate Director. He is an awardee of the United States National Science Foundation's CAREER Award. He has been Biochemistry Section Editor of the Public Library of Science Journal, PloS ONE since 2008 and joined the board of Directors of the National Museum of Health and Medicine (Chicago) in December of 2012.

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Meir Lahav, Struct Chem Crystallogr Commun, 3:2
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Meir Lahav

Weizmann Institute of Science, Israel

Structure, design and function of pyroelectric crystals

Pyroelectricity, a phenomenon first discovered in 314 BC by the Greek philosopher Theophrastus, who noticed that a mineral, presumably tourmaline, attracts or repels ash, when exposed to a temperature change. It was not until the 17th century, that it was determined that pyroelectricity is the ability of some crystals to generate a temporary voltage which is followed by attraction of depolarization charges from the surrounding. It was generally considered, that such property is confined exclusively to the polar directions of the 10 out of 32 crystal classes. Experimental observation of pyroelectricity associated with surface polarity was thought impossible because surface polarity attracts very little depolarization charges to be detectable. During the last decade; however, improvement in instrumentation provided means to measure accurately pyroelectric currents of few pico-amperes and pyroelectric coefficients of the order of 10^{-13} C/(cm^{2}K), which is 1:10000 with respect to commercially important materials. This opens interesting opportunities to apply the pyroelectric effect as a tool for searching disorders in crystals or for acquiring structural information about near polar surfaces of non-polar crystals. One of the important advantages of the pyroelectric technique is that it allows studying a large variety of materials including rough surfaces. Mechanistic studies of the formation of mixed crystals by intentional doping or by occluded impurities had demonstrated reduction in the symmetry of the non-polar hosts by converting the latter into mixed crystals composed from polar sectors. Furthermore, the occluded guests create constrained polar-domains within the host crystals, which determine their macroscopic properties. The structure of such domains can be elucidated at the molecular level by pyroelectric measurements combined by computational techniques such as DFT (density functional theory) calculations and MD (molecular dynamics) simulations. Here are described the application of these concepts for the following examples: (1) The structure of the polar domains of the doped centrosymmetric α-glycine crystals with other α-amino acids, in concentrations less than 1%, were determined at the molecular level by pyroelectric measurements combined with theoretical calculations. (2) The riddle of the anomalous pyroelectricity from the centrosymmetric α-glycine crystals is resolved by considering the landing of large clusters, present in the supersaturated solutions, during the growth of the crystals, in keeping with the non-classical mechanisms of crystal growth. (3) The detection of enantiomeric disorder, by pyroelectricity along the non-polar directions, in the racemic crystals of D,L alanine and D,L aspartic acid, which is not detectable by the diffraction techniques. (4) Freezing experiments performed on the surfaces of $LiTaO_3$ studied in a specially designed set-up, revealed that positively charged surfaces enhance, whereas negatively charged surfaces delay freezing. Differences in the operation of the pyroelectric effect on inducing ice nucleation on hydrophilic and hydrophobic surfaces will be presented.

Biography

Meir Lahav has completed his PhD and Postdoctoral and then joined the Weizmann Institute. His scientific interests comprise solid-state and surface chemistry, stereochemistry, the properties of polar crystals and the emergence of homochirality on Earth. He shared with Prof. L. Leiserowitz the Prelog Medal for Stereochemistry from ETH, the G. Aminoff Prize for Crystallography from the Swedish Academy of Science and the Israel Prize.

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Day 2

Paolo Scardi, Struct Chem Crystallogr Commun, 3:2
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Paolo Scardi

University of Trento, Italy

Static and dynamic atomic disorder in nanocrystalline systems

Much is known about the effect of size and shape of metal nanocrystals on their catalytic activity. Size effect may appear obvious for the direct relation with the total surface area exposed to the environment, whereas shape is a major factor controlling selectivity of the catalytic reaction. Palladium nanocrystals, for example, can catalyze a variety of oxidation reactions, but the yield of the process is strongly influenced by the exposed nanocrystal facets: Better O_2 activation occurs on (100) than on (111) facets, for the differences in the O-O bond stretch and spin charge density. As a consequence, Pd nanocubes are much more effective than nanooctahedra in oxygen-related catalytic reactions. The different, generally lower coordination of surface atoms reflects in an excess surface energy, which in many metals gives shorter bond distances between surface atoms, causing an average shrinking of the nanoparticle. The atomic displacement influences electronic properties, leading to d-band center modification and, in general, surface properties differing from corresponding bulk materials. Change in bond distances is largest on the surface, gradually decreasing toward the nanoparticle core; therefore, the displacement field is inhomogeneous and depends on nanocrystal size and shape. In addition to the static component, dynamic displacement in nanocrystals is also peculiar: Phonon confinement arises from the finite size, capping longest possible phonon wavelengths, while additional effects are due to the amplitude of thermal vibration, changing toward the surface for the decreasing coordination. The present contribution shows how X-ray spectroscopies can shed light on the behavior of metal nanocrystals, influenced by complex relations between size, shape, surface atomic coordination and bond distances. Atomistic approaches are indispensable to go beyond the limits of traditional crystallography, clearly inappropriate to deal with small crystals. In particular, we show how X-ray diffraction, applied to powders of nanocrystals with definite shape and little size dispersion can provide detailed information on atomic disorder.

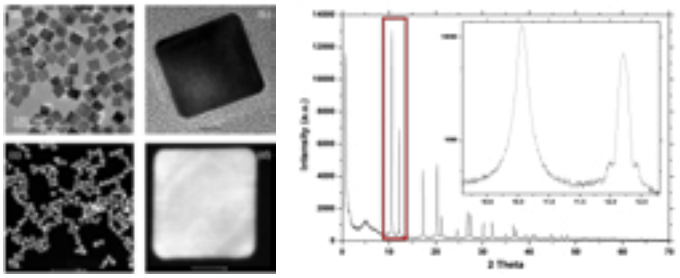

Figure-1: Pd nanocubes (left) and corresponding XRD powder pattern (right).

Biography

Paolo Scardi is a Full Professor of Material Science and Technology and Head of the PhD School in Civil, Environmental and Mechanical Engineering at the University of Trento, Italy. He is the author of more than 250 papers and his main interest concerns diffraction and crystallography with applications to materials science. His recent work focuses on thin films and highly deformed materials, photovoltaic devices, residual stress analysis and atomistic modeling of nanocrystalline materials.

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Xavier Feaugas, Struct Chem Crystallogr Commun, 3:2
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Xavier Feaugas

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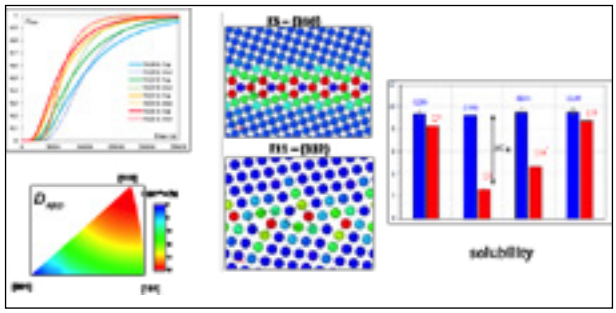
Hydrogen diffusion in nickel single- and poly-crystals: The effects of self-stress

Hydrogen diffusion and trapping has an important role in solute-dependent hydrogen embrittlement in metals and metallic alloys. In spite of extensive studies, the complexity of hydrogen diffusion in solids remains a phenomenon that needs to be clarified. The effects of the grain boundaries (GBs), and several defects (dislocations, vacancies …) and their interactions with hydrogen on the mechanisms of metal damages remain a controversy. Actually, several works suggest that the grain boundaries represent preferential paths for hydrogen diffusion, and this kind of hydrogen diffusion along GBs is higher than the interstitial diffusion. However, grains and GBs contain different defects, particularly, dislocations and vacancies. These defects are able to trap hydrogen affecting the diffusion mechanisms. Although a number of theories have been proposed to describe the role of GBs for hydrogen diffusion and segregation, none of them is able to give an exact answer. In present work we report our recent works, which support the investigation of diffusion in pure nickel single crystals and poly-crystals using both an experimental approach and a thermodynamic development. We have studied at the first time some nickel single crystals. We evaluate the hydrogen diffusion and trapping mechanisms using the electrochemical permeation (EP) coupled to the thermal desorption spectroscopy (TDS). Later, we propose to screen several bi-crystals of pure nickel with different grain boundaries. For each ones, the hydrogen diffusion and segregation are studied using EP and TDS analyses. In addition, Molecular Dynamics (MD) simulations have become a useful method to comprehend the becoming of hydrogen in these types of GBs. The results allow us to associate the short-circuit diffusion and trapping phenomena to the grain boundaries and defect characters (excess volume, defects density and distribution …). In each situation, we highlight the importance of the self-stress on the processes of diffusion and segregation.



Biography

Professor Xavier Feaugas has published over three hundred papers, and several collective books in the field of physics, mechanics and metallurgy. His research interests lie in the area of physical bases of solid plasticity and crack initiation with a focus on interactions between plasticity and surface reactivity to understand the inception of hydrogen embrittlement and stress corrosion cracking. The main research topics are: physical bases of solid plasticity and crack initiation (dislocation pattern, slip activity, slip, irreversibility, local approach of fracture …) - Interaction between plasticity and surface reactivity (dissolution, hydrogen adsorption, passivity…) - Multi-physics modeling (ratcheting, cyclic over-hardening, hexagonal slip plasticity, thermo-kinetic modeling, polymer and composite degradation, diffusion …) - Hydrogen Embrittlement/Stress Corrosion Cracking - Crystallographic defects (dislocation, vacancy, grain-boundaries, …), length scales, internal stresses – physical and metallurgy thermodynamic. More recent trend of its works is focus on the different aspects of the interactions between the hydrogen solute and the crystallographic defects formalized in thermodynamic framework.

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Yimei Zhu, Struct Chem Crystallogr Commun, 3:2
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Disentangle phonon modes using ultrafast electron diffraction and timely-resolved electron crystallography

Polaron transport, in which electron motion is strongly coupled to the underlying atomic lattice, is crucial to understanding the electrical conductivity in many solids. The accompanying atomic displacements are themselves coupled through phonons, but the specific phonon modes responsible for the dynamics of polaron motion have rarely been identified. In this presentation, I will first give an overview on the 2.8 MeV ultrafast electron diffraction instrument and the time resolved electron crystallography method we developed at BNL, then focus on its application to understand charge, orbital and lattice coupling and interaction in strongly correlated electron systems. A detailed example will be given on quantifying the dynamics of both electronic and atomic motion in the $LaSr_2Mn_2O_7$ manganite. Using photoexcition to set the electronic system in motion, we find that Jahn-Teller-like O, La/Sr, and Mn^{4+} displacements dominate the lattice response and exhibit a dichotomy in behavior overshoot-and-recovery for one sub-lattice versus normal behavior for the other. This dichotomy, attributed to slow electronic relaxation, proves that polaron transport is a key process in doped manganites. Our technique with the access to high-order reflections and being sensitive to phonons promises to be applicable for specifying the nature of electron-phonon coupling in many complex materials.

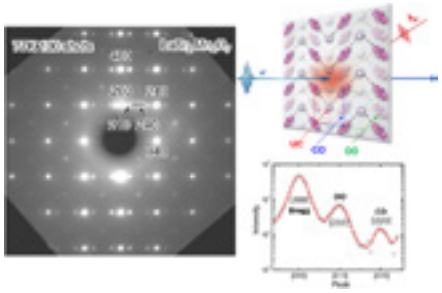

Figure-1: An electron diffraction pattern of $LsSr_2Mn_2O_7$ at 77K obtained from the BNL 2.8MeV-130fs UED (Left). Schematic of the ultrafast pump-probe approach is shown in the top panel (Right). The Bragg, orbital-ordered (OO) and charge-ordered (CO) reflections are marked and quantified in the bottom panel.

Biography

Yimei Zhu is a Senior Physicist at Brookhaven National Laboratory (BNL) and Adjunct Professor at Columbia University and Stony Brook University. He has received his BS from Shanghai Jiaotong University in 1982, MS and PhD from Nagoya University in 1987. He joined BNL as an Assistant Scientist in 1988, rising through the rank to become Tenured Senior Physicist in 2002. He is the Founding Director of the Institute for Advanced Electron Microscopy and Facility Leader of the Functional Nanomaterials at BNL. His research interests include electron crystallography of condensed matter physics of strongly correlated electron systems and advanced electron microscopy including ultrafast microscopy instrumentation. He is an Inaugural Fellow of Microscopy Society of America, a Fellow of American Physical Society and a Fellow of American Association for the Advancement of Science. He has published more than 500 peer-reviewed journal articles and delivered more than 300 invited talks at international conferences.

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