MILLER INSTITUTE NEWSLETTER

ISSUE
Spring 2013

Miller Fellow Focus: Timofey Frolov

Materials Interfaces

The pursuit of new technologies for cleaner energy conversion and more efficient energy utilization has generated increased interest in the development of advanced metallic alloys and ceramics that can operate safely at high temperatures and in aggressive environments. The properties of materials used in such contexts are generally dictated by the complex mesoscale variations in composition and structure that are inherited from their synthesis and processing. In particular, the performance of advanced structural materials is often strongly influenced by the presence of internal interfaces. In general, temperature, chemical composition, mechanical stresses and radiation change the properties of internal interfaces, which in turn influence the macroscopic properties of the materials in which they exist. Thus, to enable the rational design of materials, it is crucial to develop a framework for predicting the properties of internal interfaces in crystalline solids.

The term interface is very broad and describes a wide variety of boundaries in materials. Interfaces can be formed between two different phases, in which case they are called phase boundaries. By joining two identical solid phases with different crystal orientation we form an interface called a grain boundary (GB). In crystalline systems an infinite number if interfacial structures can be formed between the same bulk phases by varying interface orientation. The enormous variety of structures that can be formed in crystalline systems makes the behavior of interfaces in these materials incredibly rich and complex. Even though the properties of an interface can be highly distinct from the phases on either side of it, we should not think of it as some messy region. In equilibrium it adopts unique properties with enormous variations in structural and chemical complexity.

The thermodynamic description of interfaces was developed by J. Willard Gibbs over a century ago. To account for the heterogeneous nature of properties across interfaces Gibbs defined interfacial excess properties and derived relations between them. The original formulation of interfacial thermodynamics by Gibbs was mainly devoted to fluid systems. Since the time of Gibbs there has been important advances in our fundamental understanding of interfaces involving solids. Despite enormous progress the general theory of such interfaces remains incomplete. During his

CALL FOR NOMINATIONS

Miller Fellowship nominations
due Thursday, September 12, 2013

Miller Research Professorship applications
due Thursday, September 19, 2013

Visiting Miller Professorship Departmental nominations
due Friday, September 20, 2013

Please see pages 3 & 7 for details. For complete information on all our programs, visit: http://millerinstitute.berkeley.edu

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graduate studies at George Mason University Dr. Timofey Frolov worked in the group of Professor Yuri Mishin on the development of a thermodynamic theory of crystalline interfaces, which describes new variations of state that cannot be realized in fluids due to the absence of an underlying crystal lattice and introduces new excess properties. During his tenure as a Miller Fellow in the group of Professor Mark Asta in the Department of Materials Science and Engineering, Dr. Frolov is interested in studying different GB phases, their equilibrium and phase transformations between them using atomistic simulations. He uses insights obtained from modeling to generalize the thermodynamic theory of interfaces and interface phase equilibria.

It has been recognized for some time that just like bulk materials interfaces can have different phases. Different phases are associated with different atomic structures, compositions, or other interfacial excess properties. Advanced experimental probes, such as electron microscopes and X-ray scattering have given us critically important insights into the structure, composition and chemical bonding at interfaces, but detailed characterization of interfacial free energies and variations with respect to bulk thermodynamic variables remains an outstanding challenge. The complications come from the fact that interfaces are atomically sharp objects buried inside the material. Consequently, much of our knowledge about interface behavior comes from atomistic computer simulations. These simulations can provide us with fine details of atomic structure, and the ways in which this structure can be manipulated by varying composition and temperature.

As in experiment, atomistic modeling of interfaces face many fundamental challenges. A central issue surrounds the determination of the atomic structure of the interface when two crystals with different orientation are joined together. Traditionally, atomistic simulations employ periodic supercells. While such a methodology is natural for solid-fluid systems, in the case of grain boundaries it imposes an unphysical constraint by restricting variations in atomic density in the GB region.

What is the correct simulation methodology that allows us to observe different GB phases and phase transformations? The crucial step required to observe true GB behavior was to break away from the conventional methodology that employs periodic boundary conditions. Through a different arrangement within a molecular dynamics simulation, it became possible for the interface to equilibrate with a source or sink of atoms at the surface. After the constraint was removed, the structure and behavior of the boundary changed dramatically. Figure 1 demonstrates a bicrystal with a grain boundary terminated at an open surface. The initial GB structure disappears as a new GB phase nucleates at the surface and propagates into the bicrystal. During the transformation large number of atoms diffuse from the surface inside the GB to make this transformation possible. The two GB phases can be clearly identified due to different atomic arrangements at the interface. This particular boundary has been extensively studied by simulations for more than two decades, but the transformation has not been observed until now due to artifacts associated with previous simulation methodologies that constrained the atomic density.

It appears that existence of multiple GB phases can be a lot more common than previously thought. The first-order phase transition between such phases implies that grain-boundary mobilities, diffusivities, and compositions may show abrupt changes with temperature, with important consequences for properties ranging from ionic conductivities to mechanical behavior. Such abrupt changes were in fact observed experimentally and now can be explained due to insights obtained from modeling. Structural transformations at interfaces are also of profound fundamental interest as complex examples of phase transitions in low-dimensional systems. In the nucleation and growth of a new GB phase within another, the interfacial phases are separated by one-dimensional line defects that can be considered as an interface within an interface. The role of this defect on GB phase transformations and GB properties is currently unknown. Due to atomistic simulations and new simulation methodology it will now be possible to characterize it.

The discovered properties of GBs may shed new light on our understanding of how interfaces interact with point defects. The first-order nature of these transformations implies the presence of metastable states accessible to a GB with highly different atomic densities. To transition between two different interface structures GB has to absorb or emit large number of atoms. This novel property can be exploited to improve performance of polycrystalline materials under extreme conditions. For example, in metals subject to radiation by energetic particles, large numbers of point defects such as vacancies and interstitials are formed. These point defects then move inside the material and eventually coalesce creating voids, stacking-fault tetrahedra and other

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The Adolph C. and Mary Sprague
Miller Institute for Basic Research in Science
University of California, Berkeley

Call For Miller Research Fellowship Nominations
2014-2017 Term

Nomination Deadline: 12 September 2013

The Miller Institute for Basic Research in Science invites department chairs, faculty advisors, professors and research scientists at institutions around the world to submit nominations for Miller Research Fellowships in the basic sciences. The Miller Institute seeks to discover and encourage individuals of outstanding talent, and to provide them with the opportunity to pursue their research on the Berkeley campus. Fellows are selected on the basis of their academic achievement and the promise of their scientific research. The Miller Institute is the administrative home department for each Miller Fellow who is hosted by an academic department on the Berkeley campus. All research is performed in the facilities provided by the UC Berkeley academic department. A list of current and former Miller Research Fellows can be found at: http://millerinstitute.berkeley.edu/all.php?nav=46

Miller Research Fellowships are intended for exceptional young scientists of great promise who have recently been awarded, or who are about to be awarded, the doctoral degree. Normally, Miller Fellows are expected to begin their Fellowship shortly after being awarded their Ph.D. A short period as a post-doctoral fellow elsewhere does not exclude eligibility. However, applicants who have already completed substantial postdoctoral training are unlikely to be successful except in unusual circumstances. A nominee cannot hold a paid or unpaid position on the Berkeley campus at the time of nomination or throughout the competition and award cycle. Nominees who are non-US citizens must show eligibility for obtaining J-1 Scholar visa status for the duration of the Miller Fellowship. The Miller Institute does not support H1B visa status. The Fellowship term must commence between July 1 and October 1, 2014. Eligible nominees will be invited by the Institute to apply for the Fellowship. Direct applications and self-nominations are not accepted.

*All nominations must be submitted using the Online Nomination System at http://millerinstitute.berkeley.edu

Nominators will need the following required information to complete the online nomination process:

- Nominee's complete full and legal name
- Nominee's current institution
- Nominee's complete and current **active** E-mail address, current mailing address and telephone number
- Nominee's Ph.D. Institution and (expected) Date of Ph.D. (month & year required)
- Letter of recommendation and judgment of nominee's promise by the nominator (saved in pdf format). The Executive Committee finds it helpful in the recommendation letter to have the candidate compared with others at a similar stage in their development.
- Nominator's current **active** E-mail address, title, and professional mailing address (include zip code/campus mail code)

The Institute will provide a stipend of $61,000 with annual increases and a research fund of $12,000 per annum. There is provision for travel to Berkeley for Miller Fellows and their immediate families and a maximum allowance of $3,000 for moving personal belongings. Benefits, including medical, dental, vision and life insurance are provided with a modest contribution from the Miller Fellow. All University of California postdocs are represented by the UAW. Fellowships are awarded for three years, generally beginning August 1, 2014 and ending July 31, 2017. Approximately eight to ten Fellowships are awarded each year. Candidates will be notified of the results of the competition starting in mid-December, and a general announcement of the awards will be made in the spring.

We are grateful for your thoughtful participation in this process and hope that you regard the time you may devote to this effort justified by the contribution you will be making to the careers of distinguished young scientists.

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Miller Research Fellowship Awardees 2013-2016

The Miller Institute is pleased to introduce the 2013-2016 Miller Research Fellows. Each year, the Miller Institute seeks to discover individuals of outstanding talent and to bring to Berkeley young scholars of great promise. Candidates are nominated for these awards and are selected on the basis of their academic achievement and the potential of their scientific research. The Fellows will be working with Berkeley faculty hosts for a three-year term beginning in the 2013 academic year. A full list of all past and present Miller Fellows is available on our website.

Gokhan Barin
Ph.D. - Northwestern University
Berkeley Dept.: Chemistry
Faculty Host: Jeff Long

The development of multifunctional porous materials has the potential to address grand challenges, particularly selective gas capture/storage and catalytic conversions, in energy research. Gokhan is interested in achieving light-driven chemical transformations using porous materials, known as metal-organic frameworks, decorated with catalytically active sites. His research efforts will focus on the development of novel heterogeneous photocatalysts and understanding their fundamental principles in order to establish a structure-property relationship.

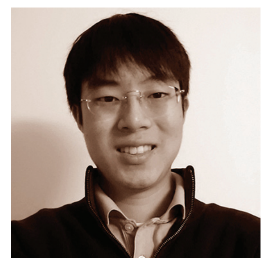
Rebekah Dawson
Ph.D. - Harvard University
Berkeley Dept.: Astronomy
Faculty Host: Eugene Chiang

It was once thought that all planets form in situ and subsequently follow their orbits like clockwork. But this simple picture cannot explain the exotic orbits of the majority of the hundreds of confirmed "extra-solar planets" (planets orbiting other stars). Using evidence from the orbits of extra-solar planets and small, rocky bodies in our own solar system, Rebekah is investigating how planets "migrate" from where they formed to where we observe them today and whether this migration is a smooth or violent process.

Brooke Gardner
Ph.D. - UC San Francisco
Berkeley Dept.: MCB
Faculty Host: Andreas Martin

Eukaryotic cells utilize membrane-bound organelles to perform specialized chemical reactions. Peroxisomes, one class of organelle, can be created de novo within the cell and thus present a compelling opportunity to understand organelle biogenesis. As a Miller Fellow, Brooke will study the mechanistic details of peroxisome biogenesis with the ultimate goal of repurposing these steps to create custom organelles.

Justin Kim
Ph.D. - MIT
Berkeley Dept.: Chemistry
Faculty Host: Carolyn Bertozzi

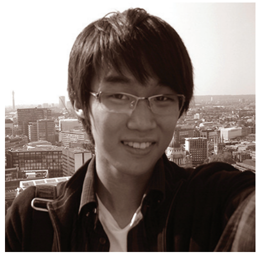


The study of biological systems at a molecular level can be greatly facilitated by the development and application of bioorthogonal reactions. These are chemical reactions that neither interfere nor interact with native biochemical processes, are non-toxic to living organisms, and involve a selective reaction between a pair of reaction partners on biologically relevant time scales. Justin's research will be focused on the development of new bioorthogonal tools and their potential applications to protein engineering and glycobiology.

Christopher Martin
Ph.D. - UC Davis
Berkeley Dept.: ESPM
Faculty Host: Erica Rosenblum

Chris is broadly interested in the evolution and ecology of adaptive radiations, rapid bursts of ecological, phenotypic, and species diversification spread unevenly across the tree of life. His research integrates field measurements of natural selection, functional morphology, behavioral ecology, phylogenetics, genetic mapping, and population genetics with a focus on replicated adaptive radiations of fishes in the Caribbean and West Africa. By mapping the complex relationship between fitness, phenotype, genotype, and environment, he hopes to gain a predictive understanding of one of the major processes driving the evolution of biodiversity.

Sung-Jin Oh
Ph.D. - Princeton University
Berkeley Dept.: Mathematics
Faculty Host: Daniel Tataru



At the heart of many physical theories are Partial Differential Equations (PDEs), which are often nonlinear. Sung-Jin is interested in rigorously understanding the regularity and long term behavior of solutions to such equations, with an emphasis on geometric evolutionary equations such as the Einstein gravitational field equations, Yang-Mills equations and Chern-Simons gauge theories. These PDEs possess rich geometric and analytic structure, and ideas drawn from a wide variety of fields, such as geometric flows, Riemannian and Lorentzian geometries and Fourier analysis, naturally come together in their study.

Shayan Oveis Gharan
Ph.D. - Stanford University
Berkeley Dept.: EECS
Faculty Host: Umesh Vazirani

Optimization problems arise in a wide range including logistics, planning, marketing, advertising and policy-making. The main focus of Shayan's research is to study the approximability of classical NP-hard optimization problems. This area of research is motivated by the fact that many important problems are known to be NP-hard, i.e., under standard conjectures they can not be solved optimally with polynomial time algorithms. Instead, one can hope to efficiently find an approximate solution. Shayan is generally interested in developing mathematical tools and use them to design efficient algorithms that can guarantee a near optimal solution. He wants to rigorously prove that the cost of the solution of an algorithm is very close to the cost of the optimum in the worst case or in the average case.

Ashivni Shekhawat
Ph.D. - Cornell University
Berkeley Dept.: Materials Science & Engineering
Faculty Host: Robert Ritchie

In Ashivni's research he studies the science of fracture, or how things break, and how to keep them from breaking. Some of the specific questions that he is interested in are about the emergent distribution of fracture strengths, the spatial distribution of pre-fracture damage, the path that a crack follows in a given material, and the description of fracture from a statistical mechanics point of view. As a Miller Fellow Ashivni will endeavor to study the fracture properties of specific material systems, such as biological materials, or nano-scale devices. He hopes that his research will help develop the next generation of stronger and smarter materials.

Blake Sherwin
Ph.D. - Princeton University
Berkeley Dept.: Physics
Faculty Host: Uros Seljak

Most of the matter in our universe is made up of invisible dark matter, which is distributed within enormous web-like structures throughout the cosmos. These dark structures can be mapped by measuring small distortions caused by their gravity in the observed image of the cosmic microwave background. Using these distortions - known as gravitational lensing - to map and study the large-scale dark matter structures, Blake hopes to gain insight into some of the key questions of modern cosmology, such as the nature of dark energy, the properties of fundamental particles known as neutrinos, and the relation between dark matter and the luminous matter within stars and galaxies.

Amy Shyer
Ph.D. - Harvard University
Berkeley Dept.: MCB
Faculty Host: Richard Harland

A change in the shape of any structure, including a biological one, must ultimately be explained in terms of the forces exerted on it. For instance, in developing tissues, densely packed layers of cells, or epithelia, both experience and exert mechanical forces as they move, bend, and fold into patterned structures. Amy's long-term goal is to understand such morphogenesis at the level of mechanical forces. An excellent model system for these studies is epithelial wound closure in the Xenopus embryo. As a Miller Fellow, Amy will ask: What physical mechanisms govern wound closure? How do molecular pathways drive changes in forces and physical properties, and how do these forces in turn impact molecular signaling events? Finally, why do some wound closures result in scars while others do not?

Barbara Meyer Named 2013 Miller Senior Fellow

Counting from one to two is among the first things that young children learn to do. How hard could it be? Yet for a cell, determining whether there is one or two copies of certain molecules is difficult, and in come cases, a matter of life or death. Professor Barbara Meyer, recently selected as the fifth Miller Senior Fellow, is a world expert on the most critical counting mechanism, which is how cells tell if they have one X sex chromosome or two. More on counting in a moment, but first, let us introduce Barbara to the Miller Community.

Barbara Meyer

Barbara's ascent to the highest ranks of biologists began with an undergraduate degree at Stanford followed by a Masters in Molecular Biology at Berkeley. She then earned a Ph.D. at Harvard with Mark Ptashne, producing a famous Ph.D. thesis that laid out much of the logic by which a virus of bacteria chooses between different developmental fates. For postdoctoral training she moved to Cambridge, England where she trained under Nobelist Sydney Brenner, one of the most celebrated molecular biologists, at the legendary Laboratory of Molecular Biology of the Medical Research Council. It was here that Barbara launched the line of investigations that have come to beautiful fruition in her lab over the succeeding years. She was recruited to the MIT faculty in 1982, and was recruited to Berkeley as a Professor in 1990, along with her husband Professor Tom Cline, also a biologist. She is presently an Investigator of the Howard Hughes Medical Institute, and a member of the National Academy of Science, the American Academy of Arts and Sciences and has served on many national and international advisory committees including the UC President's Council on the National Labs.

In Cambridge she began her studies on the nematode worm C. elegans, now a charter member of the pantheon of model organisms that drive so much of basic research in biology. At the time she started her work, there were only a handful of labs in the world working on C. elegans. She set out to understand how genes determine the two sexes of C. elegans, males and hermaphrodites. Here is where counting to two comes in. Unlike us, in which females have two X chromosomes and males have an X and Y chromosome, C. elegans animals with one X chromosome become males and animals with two X chromosomes become hermaphrodites. So counting X chromosomes is pretty important to these lovely worms, but even more important than it first appears. In all organisms with sex chromosomes, levels of proteins encoded by genes on X chromosomes must be balanced between males and females (or hermaphrodites). Barbara has tackled this question as well and found that molecular machines, co-opted from the ancient process of chromosome segregation, can compact the X chromosomes of hermaphrodites to alter their expression level. Barbara's discoveries have elucidated a new principle in the biology of sex through a series of experiments that began with classical genetic studies, and in the ensuing years have been at the forefront of molecular biology, cytology, biochemistry and genetics.

The Adolph C. and Mary Sprague
Miller Institute for Basic Research in Science

Call for Applications & Nominations

Miller Research Professorship

Applications from UC Berkeley faculty for Miller Research Professorship terms in the 2014-15 academic year will be accepted online beginning in June 2013. The purpose of the Professorship is to release members of the faculty from teaching and administrative duties and allow them to pursue research on the Berkeley campus. Appointees are encouraged to follow promising leads that may develop in the course of their research.

Applications are judged competitively and are due by Thursday, September 19, 2013. It is anticipated that between five to eight awards will be made.

Visiting Miller Professorship

The Advisory Board of the Miller Institute for Basic Research in Science invites Berkeley faculty to submit online departmental nominations for Visiting Miller Research Professorship terms in Fall 2014 or Spring 2015. The purpose of the Visiting Miller Professorship is to bring promising or eminent scientists from any place in the world to the Berkeley campus on a short-term basis for collaborative research interactions.

Online nominations will be accepted beginning in June 2013 and are due by Friday, September 20, 2013.

For more information please visit: http://millerinstitute.berkeley.edu

Miller Fellow Focus (Continued)

(continued from page 2)

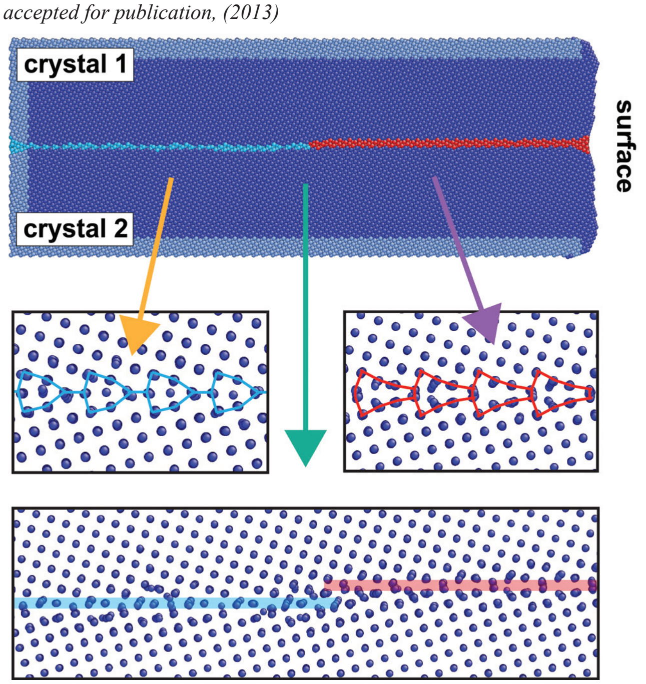
defect complexes degrading the material properties. Interfaces can potentially accommodate interstitials and vacancies by transitioning between different states and heal the material.

The new simulations summarized above establish an unexpected complexity in a relatively simple and well-studied GB system. The type of interfacial phase transformation raises many new questions and challenges current thermodynamic theories, calling for their generalization. For example, in related simulations we have shown that interfaces are not perfect sources or sinks for point defects in crystals, as often assumed. Each interfacial phase can store a certain finite amount of atoms/vacancies before it undergoes a transformation. Thus, variation of concentration of point defects represents a new degree of freedom in addition to temperature, chemical composition and mechanical stresses. This motivates us to introduce this new state variable into theories of crystalline interfacial thermodynamics.

Currently, the topic of GB phase equilibrium is completely unexplored. Two interfaces with the same free energy should coexist in equilibrium. The fact that there are additional degrees of freedom implies larger coexistence phase space. What role will point defects will play in this equilibrium? Can two different GB phases with different solubilities of point defects coexist in equilibrium while exchanging atoms? Dr. Frolov is working on theoretical frameworks that will guide future simulations and experimental work to answer these outstanding fundamental questions.

When not studying interfaces Timofey enjoys biking, running and hiking.

Figure 1: First order phase transition of the interface. New GB phase nucleates and grows from the surface. The two GB phases have different atomic densities. During the transformation extra atoms diffuse inside the GB to make the transformation possible. Frolov et al., Nature Communications, accepted for publication, (2013)



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Spring 2013
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1-36299-24810-44

Next Steps

The Miller Institute congratulates the following Miller Fellows on their next endeavors.

Chang Liu - Assistant Professor
Department of Biomedical Engineering, Center for Complex Biological Systems, UC Irvine

Alexander Hayes - Assistant Professor
Department of Astronomy, Cornell University

Meredith Hughes - Assistant Professor
Department of Astronomy, Wesleyan University

Kirk Lohmueller - Assistant Professor
Department of Ecology & Evolutionary Biology, UCLA

Jun Zhao - Professor
Department of Physics, Fudan University, China

Correction

In the Winter 2013 issue of this newsletter, we inadvertently missed the Miller Professorship announcement of James Graham, Department of Astronomy.

Birth Announcements

We are very happy to welcome the following babies born to Institute members since January:

Son Finn to Nick Piro (Miller Fellow 2009-2012) and his wife Christine.

Daughter Talia to Ian Agol (Miller Professor Fall 2012) and his wife Michelle.

Son Eliot to Marcus Roper (Miller Fellow 2008-2011) and his wife Mechel.

Daughter Io Maria to Tom Sullivan (Staff 2007-2008) and his wife Tina.

Obituaries

Donald Glaser (Miller Professor 1962-64) passed away on February 28, 2013.

Garniss Curtis (Miller Professor 1959-61, a member of the inaugural group of Miller Professors) passed away on December 18, 2012.

John Forte (Miller Professor 1981-82) passed away on November 19, 2012.

The Miller Institute is "dedicated to the encouragement of creative thought and the conduct of research and investigation in the field of pure science and investigation in the field of applied science in so far as such research and investigation are deemed by the Advisory Board to offer a promising approach to fundamental problems."