

INTERACTIONS

DEPARTMENT OF PHYSICS 2016



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Using X-Ray Vision to Generate a Revolution in Understanding of Materials



R.M. Suter

A revolution in X-ray sources

The increase in the brilliance of synchrotron-generated X-ray beams since 1960

is significantly ahead of Moore's law. "Brilliance" is a measure of useful flux: photons per second per unit source area per unit angular divergence per fractional energy (or wavelength) bandwidth. The increase is roughly 18 orders of magnitude over the "high power" source in my X-ray lab in Wean Hall! The brightest sources are the new X-ray free electron lasers (FEL), such as the Linac Coherent Light Source at Lawrence Berkeley Laboratory (portal.slac.stanford.edu/sites/lcls_public/Pages/Default.aspx), that reach the diffraction limit, at least for soft X-rays — that means that the source size times the divergence (or transverse momentum) is as small as physics allows. The next step down is the synchrotron electron storage rings that use periodic magnetic lattice devices (undulators) to generate X-rays (www1.aps.anl.gov, www.bnl.gov/ps/nsls2/about-NSLS-II.php). The advantage here is that since the electrons travel around the ring, there are many opportunities to place undulator sources, so one facility can feed many X-ray beam lines and many experiments simultaneously. Keep in mind that it is the relativistic Lorentz

transformation that makes extreme brilliance possible: radiation emitted in the electrons' frame of reference emerges in a small cone in the direction of the velocity vector; the cone opening angle is $\approx 1/\gamma$, with γ being the usual relativistic factor. For the 7 GeV electrons used at the Advanced Photon Source at Argonne National Laboratory, this corresponds to 0.004 degrees. In fact, new synchrotron sources are using a new technology to reach toward the FEL limit and many existing sources are being upgraded to do the same. The revolution in applications of these X-ray sources is still underway; people are inventing new types of measurements that would have been impossible a few years ago.

The Materials Genome Initiative

At Carnegie Mellon in June of 2011, President Barack Obama announced a new initiative that aims to enable "businesses [to] discover, develop and deploy new materials twice as fast" as was possible previously. (www.whitehouse.gov/mgi). In many critical technological areas, as much as 20 years or more are required due to extensive trial and error formulations and repeated testing requirements. The initiative points out that, if one could model materials properties from the basic physics level, this could greatly accelerate such development cycles. The problem is that such predictive models do not exist for materials relevant to many technologies. In fact, what you probably think of as "low tech" materials

like steels, titanium or aluminum alloys, fall into precisely this category: current models cannot predict mechanical and thermal properties well enough to predict changes due to new processing routes or modified compositions. One clear reason for this lack is the fact that these properties depend on internal structure and its evolution, and it has not been possible to look inside these materials and watch how they respond — until quite recently. We need X-ray vision!

Using revolutionary X-ray sources to assist model development for polycrystalline materials

My research group has helped to develop new synchrotron X-ray based microscopies that allow us to study structural responses. Unfortunately, for the above described reasons, these measurements are almost impossible to perform with a laboratory source. We use high energy X-rays (typically $30 < E < 100$ keV photons) at the Advanced Photon Source (and other high electron energy synchrotrons) that penetrate through millimeter distances in typical metallic or ceramic materials. The schematic diagram in Fig. 1 shows the experimental setup for what is now termed "near-field High Energy Diffraction Microscopy" (nf-HEDM). The sample (green) is placed on a high precision rotation stage and a planar cross-section is illuminated by a micron-high by millimeter-wide beam (red). As the sample rotates, a high resolution two-dimensional imaging detector (gray), placed several millimeters

behind the sample, senses Bragg scattered X-rays (blue) and, by measuring at two sample-to-detector distances, encodes both the position of origin of the scattered beam and its direction (2θ and η). Measurements are performed on many sample cross-sections in order to generate three-dimensional structural information. In a typical measurement, we detect 10^5 to 10^6 Bragg peak images from thousands of crystals that are typically tens of microns in size. We use high-performance computing algorithms, developed entirely at CMU, to reconstruct from the imaged sets of Bragg peaks the crystallographic lattice orientation field that generated those images. In hard materials, the measurement is nondestructive, so we can remeasure the same material volume multiple times in successive states as the sample is annealed or mechanically altered. Two example measurements are shown in Figures 2 and 3.

We currently interact with academic, national laboratory and industrial scientists and engineers to both perform and interpret the measurements. The nf-HEDM technique has been combined with a far-field HEDM method that adds information on the elastic strain state of the local crystal structure and with tomographic methods that yield three dimensional information on cracks, pores and impurity precipitation. These correlated data sets showing materials three-dimensional responses present rigorous challenges for model development to meet the goal of, for example, the Materials Genome Initiative.

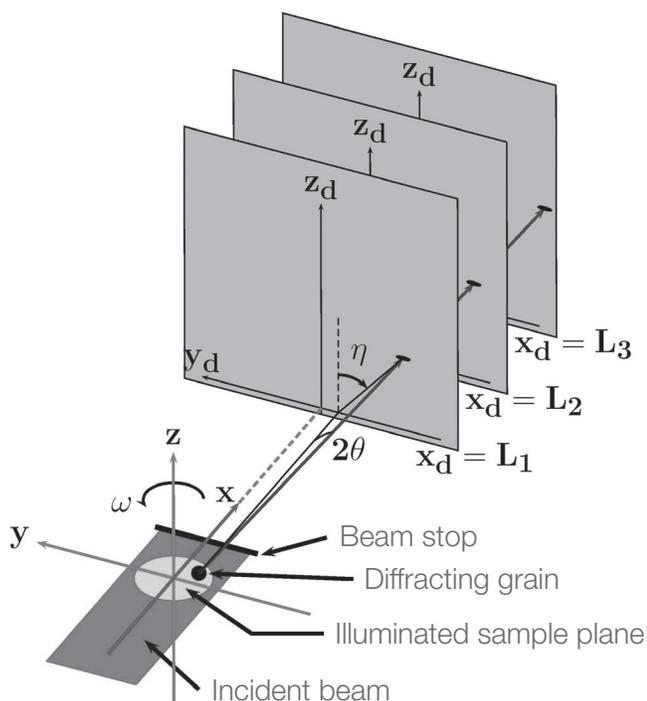


Fig. 1: Schematic of the near-field High Energy Diffraction Microscopy technique. See text for explanation.

The development of the techniques described here has relied heavily of the work of graduate students and the assistance of many undergraduate research students. In the early days, we collaborated closely with Ulrich Lienert of the Advanced Photon Source. The first implementation of both hardware and software, along with first demonstration measurements, were the work of then graduate students Chris Hefferan, Frankie Li and Jon Lind. More recent students, David Menasche, Reeeju Pokharel, Siddarth Maddali, among others, have demonstrated increasingly complex applications as well as, in the case of Menasche, performing careful calibration and error analysis work. We continue to work to extract additional types of information from these rich data sets as well as applying the measurements to a wider range of sample conditions and applied problems.

For more information, see my website at www.andrew.cmu.edu/user/suter or, feel free to contact me directly at suter@cmu.edu.

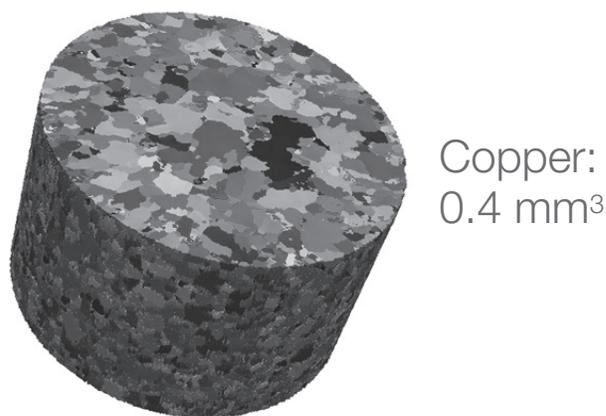


Fig. 2: Reconstructed microstructure of a copper sample. Crystal orientations are mapped to RGB colors, so regions of uniform color correspond to similar crystal orientations. The cylindrical sample was 1 millimeter in diameter. Subsequently, the sample was stretched along the cylinder axis and heterogeneous crystal rotations were tracked. (R. Pokharel, J. Lind, S.F. Li, P. Kenesei, R.A. Lebensohn, R.M. Suter, A.D. Rollett, In-situ observation of bulk 3D grain evolution during plastic deformation in polycrystalline Cu, *Int. J. of Plasticity*, 67, 217-2343 (2015).)

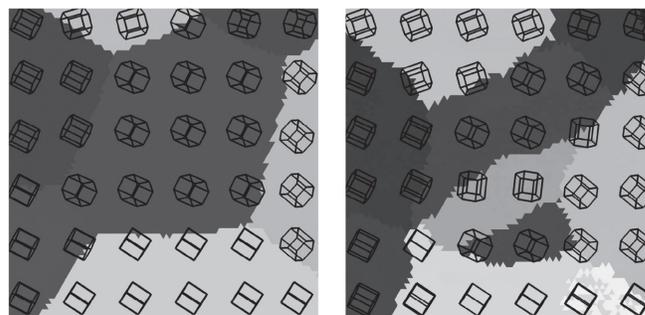
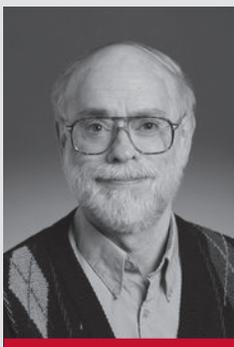


Fig. 3: A region (~100µm across) of a single layer of a zirconium sample in two states of deformation. Lattice orientations are again shown by RGB colors. The superimposed hexagons show the crystal unit cell orientations relative to the viewing direction. The left image shows the initial, well-annealed state while in the right image, the sample has been pulled in tension by 14%. The pink region is a deformation twin that formed within the purple crystal. The geometry of this twin and correlated deformation in neighboring grains has been followed in three dimensions. (J. Lind, S.F. Li, R. Pokharel, U. Lienert, A.D. Rollett, R.M. Suter, Tensile twin nucleation events coupled to neighboring slip observed in three dimensions, *Acta Materialia*, 76, 213-220 (2014).)

From the Department Head



Steve Garoff

Friends,

The Physics Department has had a very eventful year since our last edition of Interactions. We continue to produce outstanding research results in all our subfields, and we support and develop educational programs that provide physics students with the skills and knowledge they need to contribute to society in an incredibly wide range of fields.

Our graduate and undergraduate programs are thriving and continue to be a source of pride for the Department. I am especially pleased to tell you that Professor Kunal Ghosh won CMU's Undergraduate Advising Award, joining our legacy of eighteen faculty members winning one or more of the College or University level education awards. I am sure some of you remember his boundless enthusiasm and unfailing dedication to mentoring physics undergraduates. In the past year, the Department conferred twelve Ph.D. degrees, twelve M.S. degrees, twenty-six B.S. degrees and twenty-two minors in Physics. Our graduation ceremony on June 15 was a great celebration of our graduates' accomplishments and a source of excitement for them, their families as well as for the faculty - another generation of bright minds who will go out into the world, full of knowledge, enthusiasm, and idealism. We are all eager to witness the great things they will accomplish in their future.

New, important initiatives, as well as great scientific results, continue to come out of every one of our research groups in Cosmology, High Energy Physics, Quark Interactions (the new name for our Medium Energy Group), Nanophysics, and Biological Physics. You can find out about some of the highlights in this newsletter or by browsing through the many press releases we have published on our Department's webpage during the past year. Our faculty are members of national advisory boards, where they influence science and policy decisions, and they hold leadership positions in major national facility construction projects and within large scientific collaborations. Moreover, our groups continue to forge and lead new alliances within CMU, for instance with computer science, engineering, and biology. We are particularly proud that Professor Emeritus Luc Berger's great work in magnetism has been recognized by a second national award, the Institute of Electrical and Electronics Engineers (IEEE) Magnetics Society achievement Award, having also been recognized by the 2013 Buckley Condensed Matter Physics Prize of the American Physical Society.

Three faculty have left our Department this year. Rich Holman, a long time member of our High Energy Theory group, has assumed the position of Dean of Computational Sciences at the Minerva Project, and Alex Evilevitch, a member of our Biological Physics initiative, has accepted a position at the Department of Pathobiology at the University of Illinois at Urbana Champaign. We wish them good luck and much success in their new responsibilities. Tom Ferguson, a member of our High Energy Experiment group, has retired. While he will continue to be around and share his knowledge and experience, we are sure he will enjoy the less stressful life of an emeritus professor!

We look forward to two new faculty, Diana Parno and Sergey Kuposov, joining us just as this newsletter is being sent out. Diana joins us from the University of Washington's Center for Experimental Nuclear Physics and Astrophysics and will be exploring the properties of one of nature's most elusive known particles, the neutrino. Sergey joins us from Cambridge University and will be studying dark matter in dwarf galaxies as part of our McWilliams Center for Cosmology. Look for articles about them and their work in the next edition of Interactions.

I again want to invite all of you to renew and strengthen your ties to our Department. We would love to hear from you, telling us what you are doing and commenting on how the Department has helped in your career and life. You can write to me at physics@andrew.cmu.edu. We would love to post some excerpts from your notes on our new Alumni web page, provided this is OK with you (please let us know!).

If you are ever in Pittsburgh and can stop by the Department, let me know when you will be here. I would love to talk to you in person. In these times of electronic social and professional connections I also encourage you to join our new LinkedIn page at: [linkedin.com/grp/home?gid=8434243](https://www.linkedin.com/grp/home?gid=8434243) and connect with other alumni and current faculty and students.

Our Department has a rich heritage going all the way back to 1906 and an accomplished group of faculty and students, past and present. Alumni and friends of our Department have been remarkably generous in donating to our mission, and we are enormously grateful for that. We need these contributions to provide resources for new initiatives in research and enable new opportunities for our students. Our new giving page on our website, cmu.edu/physics/giving/index.html, has just gone live. It allows you to target your donation to various areas in the Department if you wish, and it makes it easy to complete the process.

I wish you all the best for an excellent new year,

Steve Garoff



McWilliams Center for Cosmology Hosts Large Synoptic Survey Telescope Hack Week

CMU recently hosted a meeting of the Dark Energy Science Collaboration (DESC), a group that is preparing to analyze data from the Large Synoptic Survey Telescope (LSST) survey. The LSST is now being constructed in Chile, and in the 2020s, will conduct a ten-year-long survey of the sky that will map tens of billions of galaxies. The LSST survey will enable a broad range of scientific investigations, from detection of asteroids within our solar system, to mapping the structure of the Milky Way, to studies of dark matter and dark energy. The goal of the DESC is to prepare the research infrastructure that will be needed to learn about dark energy using data from the LSST.

This particular meeting was the DESC's first-ever "hack week." Unlike a traditional workshop, a hack week does not include any formal presentations. Instead, it's an opportunity for groups of collaborators within the DESC to sit in one place and work together on their ongoing projects.

As part of an international collaboration, members of the DESC found the opportunity for face-to-face interaction to work on projects highly useful. Of the 550 DESC members, 65 came to Pittsburgh during the week of November 7–11 for this meeting and made substantial progress on 10 high-priority projects. These projects include use of the LSST data analysis software (still in preparation) to analyze real data from existing telescopes, as a way of testing the software and spurring future software development; development of software to simulate LSST data and test our understanding of the telescope and detectors; and writing software for classifying different types of supernovae, explosions of stars in distant galaxies that can be used to test the expansion rate of the universe. The consensus of meeting participants is that hack week was a success in every sense: the group accomplished what it set out to accomplish and had fun working together at the same time.

The head of scientific and local organization of the hack week was Professor Rachel Mandelbaum, who is part of the management team of the DESC. A team of graduate students and postdoctoral researchers from CMU (Sukhdeep Singh, François Lanusse, Danielle Leonard) and the University of Pittsburgh (Lluís Galbany, Yao-Yuan Mao, Kara Ponder) formed the rest of the local organizing committee. This meeting took place thanks to support from the LSST Corporation, which provided travel support for junior meeting participants (graduate students and postdoctoral researchers); from the McWilliams Center for Cosmology, which provided food and equipment to enable the workshop to occur without a registration fee; and from CMU's Department of Physics, which provided administrative support for the meeting.

Pictured above: Professor Rachel Mandelbaum (right) converses with postdoctoral researcher, François Lanusse, at the first-ever DESC "hack week."

Summer Undergraduate Experience



During the course of last summer, I was involved with the Pennsylvania Governor's School for the Sciences (PGSS), where I worked as a teaching assistant and

residential assistant for 60 high school seniors from across Pennsylvania. The PGSS program was a six-week program on the CMU Pittsburgh campus, including a week of pre-program staff training. I worked under PGSS Program Director Dr. Barry Luokkala (S 2001), who also served as the coordinator of the physics team research projects. I was a teaching assistant for physics core course instructor Dr. Hael Collins, and for physics

department alumna Lisa Milan (S 1993), who taught the physics laboratory course.

At PGSS, there were two teaching assistants for each scientific subject: chemistry, computer science, biology, theoretical mathematics and physics. I attended the students' physics core lecture class, labs and electives, and offered academic guidance as they worked on problems involving special relativity and quantum mechanics. After classes, the counselors provided daily social activities, followed by help with homework, lab work and team research project work. At the end of the program, each group of research project partners presented their independent team projects in a formal symposium, attended by faculty, parents and members of the Pennsylvania Department of Education. One of the computer science groups even tied seven world records for efficiency in solving an artificial intelligence problem.

Each TA/counselor received a stipend, a food allowance and housing in the dormitory with the PGSS students. I had heard of the opportunity through an email announcement sent to physics students by our assistant department head and head of advising, Kunal Ghosh. Shortly after submitting my application, I was called for an interview.

The goal of the PGSS program was to expose advanced high school students to topics they would not otherwise see in a traditional high school setting and to encourage them to pursue careers in the sciences. As a result of my participation as a TA/counselor in PGSS, I was able to determine whether I would be interested in eventually becoming a professor to college-level students, and I experienced a fun social environment as well. I would highly recommend this to anyone with an interest in the sciences beyond just the classroom.

Physics Diploma Ceremony 2016



Oz Amram received this year's Richard E. Cutcosky Award. Pictured left to right are Stephen Garoff, Oz Amram, Barry Luokkala and Kunal Ghosh



Group photo of this year's degree recipients

News Briefs

GRADUATE STUDENT HONORS



Shadab Alam received the 2016 Guy C. Berry Graduate Research Award.



Michelle Ntampaka received a 2016 Bruce McWilliams Presidential Fellowship in the Mellon College of Science.



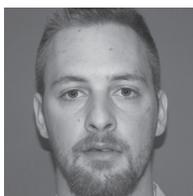
Sergio de la Barrera received the 2016 J. Michael McQuade Nanophysics and Energy Fellowship.



Siddharth Satpathy received the 2016 Physics Departmental TA Award.



Aklant Bhowmick received the 2016 John Peoples, Jr. Presidential Fellowship in Physics.



Bradley Treece received the 2016 Physics Departmental TA Award.



Alex Moskowitz received the 2016 George E. (S 1945) and Marjorie S. Pake Presidential Fellowship in Physics.

FACULTY HONORS



Professor Emeritus **Luc Berger** received the IEEE Magnetics Society Achievement Award.



Professor **Sara Majetich** was elected a Fellow of the IEEE.



Teaching Professor **Kunal Ghosh** received the 2016 Carnegie Mellon University Award for Outstanding Contributions to Academic Advising and Mentoring.



Associate Professor **Di Xiao** received a 2016 Cottrell Scholar Award for his work on Topological Excitronics in Gapped Dirac Materials.

Faculty Promotions

Markus Deserno promoted to Professor

Shirley Ho promoted to Associate Professor

Rachel Mandelbaum promoted to Associate Professor with Indefinite Tenure

Hy Trac promoted to Associate Professor

Di Xiao promoted to Associate Professor

Faculty Retirements

Thomas Ferguson
Richard Holman

Newly-Appointed National Leadership Positions

Curtis Meyer to Chair, JLab Director's Review of the SoLiD experiments

Brian Quinn to Chair, Coordinating Committee of Super BigBite Spectrometer Collaboration

Reinhard Schumacher to Chair, 2017 APS Division of Nuclear Physics Annual Meeting

Robert Swendsen to Associate Editor, Journal of Statistical Mechanics

Degrees Granted in 2016

DOCTOR OF PHILOSOPHY IN PHYSICS

Onur Albayrak
Patrick Michael Diggins IV
Marilia Cabral Ramos Do Rego Barros
Qin Gao*
Robert Haussman
Dao Ho*
Michael Stephen Jablin*
William Levine
Siddharth Maddali
David Benjamin Menasche
Patrick C. Mende*
Ying Zhang

MASTER OF SCIENCE IN PHYSICS

Nicholas Agia
Aklant Kumar Bhowmick
Bojun Feng
Siyu He
Yuchi He
Michael F. Matty
Karpur A. Shukla
Michael Sinko
Abel Sun
Larisa Thorne
Dacen Waters
Xiaouo Zhang

UNDERGRADUATE HONORS

Oz M. Amram, *University Honors, Phi Beta Kappa, Phi Kappa Phi*
Ernest Kin Hoe Chiew, *University Honors, Phi Kappa Phi*
Zachary Dell, *University Honors, Phi Beta Kappa*
Yongshan Ding, *University Honors, College Honors*
Raghav Gupta, *University Honors*
Alexander Barratt Gurvich, *University Honors, College Honors, Phi Beta Kappa*
Bridget Megan Haas, *University Honors*
Paul Cotter Hamerski, *University Honors, College Honors, Phi Beta Kappa*
Shae T. Hart, *College Honors*
Jeremy R. Hyde, *University Honors, College Honors, Phi Beta Kappa*
Joseph W. Kania, *University Honors, College Honors*
Lachlan T. Lancaster, *University Honors, College Honors, Phi Kappa Phi*
Michael Prijatelj, *University Honors, College Honors, Phi Kappa Phi*

Vijay A. Sampath, *University Honors*
David B. Sisson, *University Honors*
Julia H. Yang, *University Honors, College Honors, Resnick Honorable mention*
Weichen Yin, *University Honors, College Honors, Phi Beta Kappa, Phi Kappa Phi*

UNDERGRADUATE DEGREES

Bachelor of Arts in Physics
Vijay A. Sampath
Bachelor of Science and Arts in Physics and Drama
Lina Pulgarin-Duque
Bachelor of Science: Double Degree in Mathematics and Physics
Zachary R. Dell
Bachelor of Science: Double Degree in Physics and Computer Science
Yongshan Ding
Bachelor of Science: Double Degree in Physics and Mathematics, Minor in Computer Science
Paul Cotter Hamerski

Bachelor of Science: Double Degree in Physics and Statistics
Ernest Kin Hoe Chiew

Bachelor of Science in Electrical and Chemical Engineering, Additional Major in Physics
Raghav Gupta

Bachelor of Science in Materials Science and Engineering, Additional Major in Physics
Julia H. Yang

Bachelor of Science in Physical and Digital Systems, Minor in Robotics
Carter Sharer

Bachelor of Science in Physical Science, Double Minor in Cognitive Neuroscience and Physics
Paul D. Popa*

BACHELOR OF SCIENCE IN PHYSICS

Mark S. Dyehouse
William B. Griffin
Bridget M. Haas
Michael Prijatelj
David Sisson*
Weichen Yin
Bachelor of Science in Physics, Additional Major in Computer Science
Connell P. Donaghy

Bachelor of Science in Physics, Additional Major in Philosophy
Craig R. Morey

Bachelor of Science in Physics/Astrophysics Track
Alexander B. Gurvich
Joseph W. Kania*

Bachelor of Science in Physics/Astrophysics Track, Minor in Computer Science
Shae T. Hart

Bachelor of Science in Physics/Astrophysics Track, Minor in Mathematics
Lachlan T. Lancaster

Bachelor of Science in Physics/Biophysics Track
Michael S. Woolford

Bachelor of Science in Physics/Computational Physics Track
Anthony Ko

Bachelor of Science in Physics, Minor in Computer Science
Jeremy Hyde

Bachelor of Science in Physics, Minor in Philosophy
Oz M. Amram

MINORS IN PHYSICS

Terence An
Andrew N. Butko
Patrick G. Chang
Tanner J. Douglas
Anna L. Etzel
Yeshar I. Hadi
Kevin H. Hunter
Alaaddin Ismail
Matthew D. Nulph
Cheul Young Park
Benjamin J. Plaut
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INTERACTIONS

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