

## Homework 101: collect data 24 hours a day at CHESS!

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There's no better way to teach students about crystallography and diffraction, according to Matt Miller, professor of Mechanical and Aerospace Engineering (MAE) at Cornell, than to assign them a 24 hour per day homework assignment at the local synchrotron x-ray facility. Miller's course, MAE 695: "Special Topic – Diffraction Methods for Understanding the Structure and Response of Crystalline Materials," was an experiment in itself and the first time he had ever attempted to use synchrotron data collection as a pedagogical tool. Five students took the special topics course – one undergraduate, one masters of engineering student, and three Ph. D. candidates. Both teacher and students liked the special topic course so much that it will be reborn as an official departmental course, MAE 711, for Fall 2006.

Miller and his research group have a long history studying the processing and properties of engineering materials – primarily alloys. They have worked on a broad range of metals and alloys including steels, copper and aluminum, titanium and nickel based superalloys. Over the past few years they have developed a large scale load-frame that can stretch solid samples, like millimeter-thick bars of copper, all while collecting x-ray diffraction data. X-rays are sensitive to very small changes atomic order, strain and relaxation dynamics deep inside opaque materials. The load-frame was developed by graduate and undergraduate students, with advice and technical guidance from CHESS, the Cornell High Energy Synchrotron Source. CHESS is the local synchrotron source, of course, and is just a stroll across campus from the MAE department and 60 feet below an outdoor running track and soccer field.

With MAE 695 Miller wanted to offer students an interesting alternative to the usual mechanical testing and transducer design projects. "It [was] a little different for Mechanical Engineers but it would be great to enable them to think of a synchrotron facility as a place for them to obtain material characterization data." The course syllabus was packed with topics covering a variety of materials, from single crystal to polycrystalline, ranging from macroscopic alloys (think I-beams and airplane engines) all the way down to microscopic crystalline structures in microelectronics and micromechanical machines (think memory chips and carbon nanotubes). Students learned about diffraction as a measurement technique using x-rays, neutrons and electrons. They were introduced to stereographic projections, pole figures, measurement of lattice strain and electron backscattering techniques. Naturally, the teacher's favorite topic was included: deformation of materials under mechanical load. That is, stretching and squeezing, and using x-ray data to record the action.

Before the students showed up at CHESS, though, Miller's group spent a whole week setting up and collecting some of their own research data. Graduate students Jun-sang Park and Aaron Vodnick moved the load-frame into the A2 station and worked with CHESS staff scientist Alexander Kazimirov to adjust the x-ray optics and optimize the diffraction instrument. Vodnick is a graduate student in the Materials Science and Engineering department under Prof. Shef Baker, and both have common interests with Miller's group on *in-situ* strain measurements. After a week of around-the-clock data collection they got only a single day to rest before the second week of x-rays began. The MAE 695 students joined into the fray for the last three days.

According to Miller graduate students play an important role in training undergraduates, either in the data collection exercise at CHESS or with the undergraduate help constructing the load-frame apparatus over the two preceding years. "It is sort of an apprenticeship," Miller notes. "Like many faculty I often assign an undergrad to a Ph. D. student. They work closely, working their way up the research ladder. The undergrads learn a lot from their Ph. D. mentors and the grad students equally benefit. There is no better motivator to truly learn a concept than to be assigned to teach it to someone else."

The data the students took involved capturing an x-ray diffraction pattern while the material under study is being compressed or stretched. The changes in the x-ray images can be subtle and so the research group had to develop their own software tools to tease out small but substantial changes. At the atomic scale, the alloys are asymmetric, and might have different chemical bonds and different arrangements of atoms along the three spatial directions. As a result, stretching a material can cause atoms to move closer together in some directions and further apart in others.

To help describe and explain this complicated response, Miller has worked closely with fellow professor Paul Dawson to develop graphical three-dimensional representations of the crystallographic responses. Both support a facility they call the Deformation Processes Laboratory that focuses on quantifying our understanding of the link between the structure of engineering materials and their performance in design applications. They have developed a whole suite of programs for polycrystal simulations that they are willing to share. Using colorful shadings, their software displays physical attributes on the surfaces of spheres, hexagons, octagons, or

other solid volumes. Pole figures and inverse pole figures, related to the stresses and strains applied by the load-frame, can be easily computed from their representations. Red regions on a sphere, for instance, show compressive strain whereas blue areas might denote expansion. Seeing the colors painted on the surface of a sphere immediately conveys differences along the orthogonal crystal axes. The colorful pole figure graphics are compelling and attractive. The computer models seem to unleash the artist in the engineer.

Although Miller's use of CHESS for homework assignments is a first, undergraduate student help is widely praised and valued. Sol Gruner, professor of physics and director of CHESS, recalls his most recent student researcher, Thomas Caswell. "He was really helpful in preparing for, and executing one of the fuel injector data runs." Gruner refers to a recent experiment at CHESS where x-ray images of gasoline squirting from an automobile fuel injector were captured on a pixel-array detectors (PAD) being developed in his lab. "Thomas helped evaluate PAD chips suitable for the run, debug the PAD camera electronics, and collect the data." Richard Gillilan, staff scientist with the MacCHESS group, points out that mentoring requires a serious investment of time, but that sometimes we "hit gold." As an example of "gold" he points to Ismail Degani, a Cornell undergraduate who worked part-time over three years to develop a Java software package. His program allows scientists, from a remote location, to orient and position very tiny protein crystals in the center of small x-ray beams. "His graphical user interface is an essential tool used hundreds of times each day," adds Gillilan, "and we think it is better than anything available at other light sources." "Ismail's program is highly user friendly and helps distinguish CHESS as an x-ray user facility."

Happy with the overall experience, Miller concludes about the students: "Proof was in the pudding – their final reports focused on the CHESS experiments and strain pole figure data they had gathered... The ones who get to come to CHESS feel as though they are doing some pretty exciting science." He also notes that working with novices can have secondary benefits. For instance, the experience prodded his group to improve their data reduction software. The next group will find the homework exercise even more user friendly.



Collecting x-ray data at CHESS. At the A2 experimental station are MAE 695 students Phil Wu (front, right), Helen Durden (back, left), and Hadas Ritz (back, right) are assisted by graduate students Aaron Vodnick (front left) and Jun Park (middle). [Photo: Matt Miller]



Master of Engineering student Phil Wu stands in front of the load-frame inside the A2 x-ray station. The “jaws” in the center of the tilted load-frame hold a copper specimen that is stretched during the x-ray measurement. [Photo: Matt Miller]

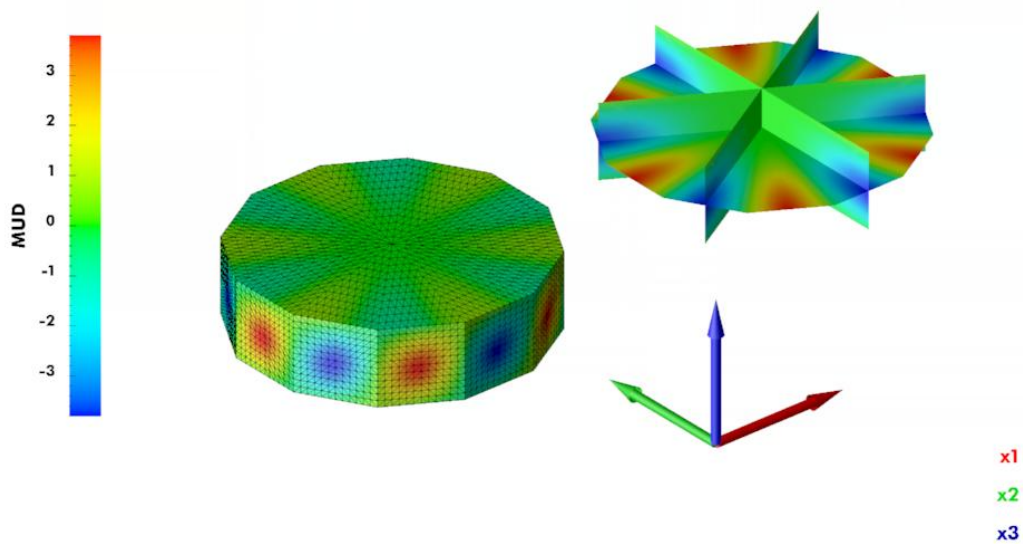


Image of one of the lowest order harmonics for the Orientation Distribution Functions (ODF) with hexagonal symmetry. The harmonics were computed using the Matlab ODF pole figure routines developed by the research groups of Miller and Dawson. The plots were made using the openDX graphics package. [Photo: Don Boyce/Joel Bernier]