User and Student Highlights

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Although it may be impossible to capture the excitement and breadth of research done by visitors to CHESS, it is fun trying! With a bias towards the most recent half year or so, this brief article will show some of the rich flavor of work done by established scientists as well as aspiring undergraduates. CHESS "shows off" the successes of our users in a number of ways, using this magazine (of course), short highlights posted on the CHESS web site, editorial coverage on official Cornell news outlets, and in international arenas using highlights posted at www.lightsources.org. We frequently stream highlights to the National Science Foundation, and some of the more colorful stories get posted on their web site and news channels. Please keep us informed about your successes so that we can to spread information to our wide CHESS community of users and supporters.

This past January **Debashis Ghosh**'s lab at the Hauptman-Woodward Medical Research Institute (HWI) in Buffalo, New York published the three-dimensional structure of aromatase, the key enzyme required for the body to make estrogen[1]. This structure plus those of two other enzymes involved in controlling estrogen levels provide the first means to visualize the mechanism of synthesizing estrogen; the enzymes also offer targets for drugs to treat some types of breast cancer. Ghosh added[2]; "Now that we know the structures of all three key enzymes implicated in estrogen-dependant breast cancers, our goal is to have a personalized cocktail of inhibitors customized to the specific treatment needs of each patient. Our knowledge about these three enzymes will enable us to develop three mutually exclusive inhibitors customized to each patient's needs which will work in harmony together with minimal side effects."

Media channels lit up February 17th with a stunning image (fig. 1) and story about a three year project by Rice University scientist **Jane Tao** and collaborators, who mapped out the coat of the PsV-F virus, one of very few viruses containing double-stranded RNA to be studied at the atomic level. Many diffraction images were needed to create this detailed picture, which appeared online Feb. 25 in the journal Proceedings of the National Academy of Sciences[3]. The packing of molecules in the PsV-F coat proved to be surprisingly different from that in related viruses, a finding that will ultimately help researchers to understand the structure and function of viruses and uncover ways to fight viral infections[4-6]. Rice University press said: "If a picture is worth a thousand words, then Rice University's precise new image of a virus' protective coat is seriously undervalued. More than three years in the making, the image... could help scientists find better ways to both fight viral infections and design new gene therapies. The stunning image…was painstakingly created from hundreds of high-energy X-ray diffraction images and paints the clearest picture yet of the viruses' genome-encasing shell called a 'capsid'."

Changing channels to metallurgy and mechanical engineering, **Matt Miller** (Cornell) has been selected to receive the ASM Henry Marion Howe Medal for 2009 for his publication[7], *"Measuring Stress Distributions in Ti-6 Al-4V Using Synchrotron X-ray Diffraction."* This award honors the author whose paper has been selected as the best of those published in the journal *Metallurgical and Materials Transactions* for the prior year. Miller, who reports on his group's many efforts in the cover article of this newsmagazine, points out that the paper cited for the award covers some of the first titanium data taken at CHESS and was the basis of the third chapter of graduate student Joel Bernier's Ph.D. thesis. Now that work is responsible for him having to rent a tuxedo!

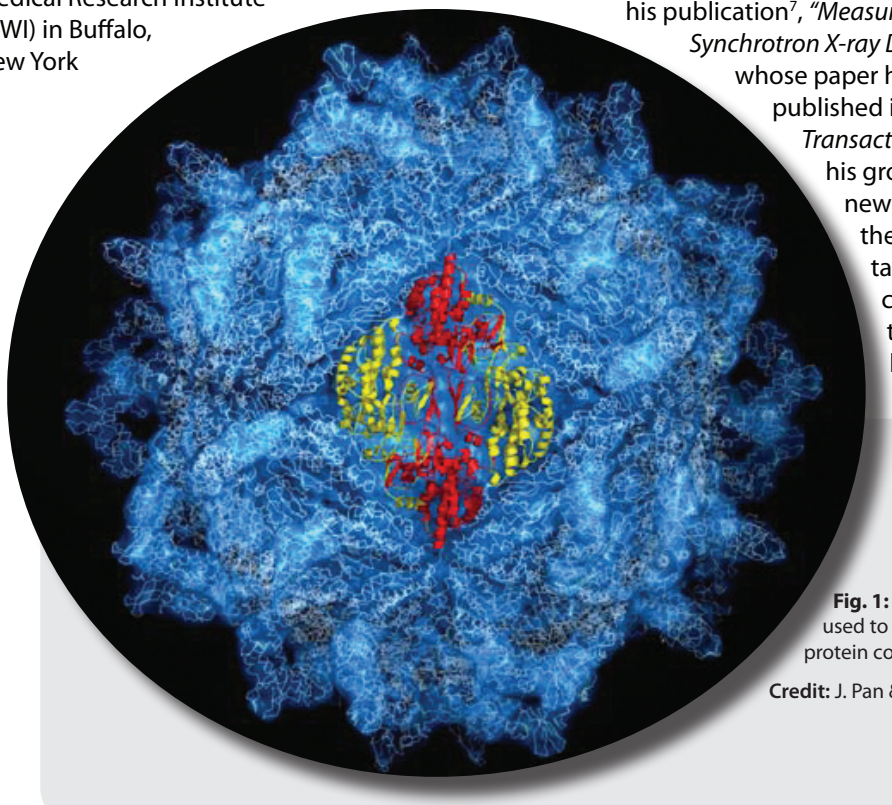

Fig. 1: High-energy x-ray diffraction was used to reveal the structure of the protective protein coat of PsV-F.

Credit: J. Pan & Y.J. Tao/Rice University[1]

The end of August saw news channels saturated with stories about a discovery of a "hidden treasure" in the art world. **Jennifer Mass**, chemist and senior scientist at Delaware's Winterthur Museum and Country Estate, gave a keynote presentation on x-ray fluorescence to study buried painting layers at the August 19th, 2009 American Chemical Society (ACS) meeting symposium, "Practical Applications of Surface Chemistry: Art and Sensing Applications." Her presentation recounted work enabled by a collaboration with CHESS scientists Arthur Woll, Don Bilderback and Sol Gruner to develop a confocal x-ray fluorescence (CXRF) microscope to examine the chemistry – and ultimately see the color palette – of layers of paint buried beneath a later portrait. X-radiography of an N. C. Wyeth family portrait (c. 1922-1924) revealed the presence of a second painting buried underneath the surface. CXRF was able to identify the chemistry of the buried paint layers and, ultimately, help Mass reconstruct the color palette. Mass added: "to date, there have been no published studies on N.C. Wyeth's painting materials and methods, and so this research will not only elucidate a buried painting but also contribute to the extant N.C. Wyeth art historical scholarship and attribution decisions. The Cornell University synchrotron source is currently the only facility for the joint confocal XRFand XRF intensity mapping of buried paintings." This story received streaming video coverage of the ACS press meeting and was the topic of the NPR Science Friday radio interview as well as print coverage by the Cornell Chronicle, CHESS and lightsources.org[8-12].

This summer saw a particularly large (and welcomed!) group of undergraduate student research interns at Wilson Laboratory. CHESS and MacCHESS hosted 7 students in research projects, who filled out an unusually large summer community of 41 undergraduates including 11 participating in the CLASSE Research Experiences for Undergraduates (REU) program, 18 students in a CMS program in high-energy physics and 6 students providing technical support and upgrades for the CESR-TA program. One REU student, **Elizabeth Brost**, worked with scientists Peter Revesz and Don Hartill on "Vibration Studies at CHESS." Liza, a Physics major at Grinnell College, configured a test station using a seismic accelerometer with fast-fourier-transform analysis to characterize mechanical vibrations and component stability at a number of critical locations – e.g. x-ray optics and beam position monitors - around the lab. **Peter Melich** and **Adam Putzer** formed a "dynamic duo" working with Arthur Woll to upgrade the confocal x-ray fluorescence scanning stage to perform "topographic" measurements. Peter and Adam, both Cornell juniors majoring in Applied and Engineering Physics, wrote Labview programs and machined and configured translation stages, encoders, and automated dial indicators to create topographic-like scans of 3-dimensional objects, similar to skimming across a surface as an atomic-force microscope does. Their hope is to dramatically speed up x-ray fluorescence scans of surfaces by following the interfacial surface directly, rather than having to scan an entire 3D volume (fig. 2).

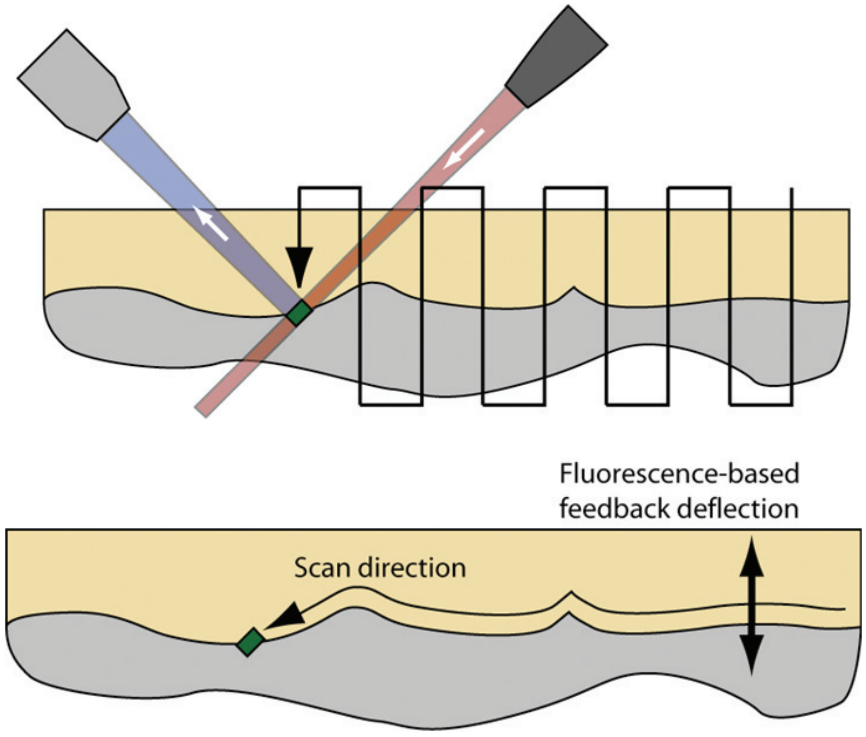

Fig. 2: Rapid, "topographic-like" x-ray fluorescence imaging involves following the surface (below) instead of having to scan the full 3D volume of the specimen (top).

Michael Lyons, a Cornell junior majoring in Electrical and Computer Engineering, worked with Phil Sorensen, Bob Seeley and Ernie Fontes to help design and build a computer-automated apparatus that will be used to carefully control the heating and cooling process of vacuum equipment. The so-called "bakeout" process is used to heat vacuum equipment to high temperatures to accelerate the removal of adsorbed or trapped water from vacuum vessels and parts. Mike made progress using the EPICS control system to automate heating and reading temperatures and pressures. **Paul Grigas**, a junior studying Operations Research at Cornell, worked with Laura Houghton, Kathy Dedrick, Phil Sorensen and Ernie Fontes to examine ways to improve web-enabled databases to track the user community at CHESS. CHESS uses databases to keep track of the hundreds of student and scientist visitors each year who share dozens of scientific instruments. Paul explored modern software options and identified three candidate packages that are being considered for a next generation system.

Gavrielle Untracht, a Cornell junior majoring in Applied and Engineering Physics, worked with Tom Szebenyi and Don Bilderback to improve the fabrication of tapered-glass capillary x-ray optics. She learned how to run the computerized glass puller that makes x-ray optics for CHESS use (the optics make micron diameter x-ray beams for our staff and our users). She has also spent a considerable amount of time writing Labview code to analyze the far-field x-ray intensity patterns formed by imperfect glass capillaries, hoping that

those patterns can be used to pinpoint the sources of error in the figure and surface perfection of the glass. **Rachel Pauplis**, a Cornell junior in Physics and Asian studies, worked with Irina Kriksunov, Chae Un Kim and Marian Szebenyi to study the process of pressure freezing protein crystals using a new apparatus being commissioned for MacCHESS users. Pressure freezing crystals is a fairly new technique that often results in better protein crystallography data by avoiding the need to use cryoprotectant additives, among other benefits. Rachel, a neophyte at the start, helped pinpoint necessary improvements to the apparatus and procedures which should, ultimately, make it easier to apply pressure cooling to users' crystals on a routine basis.

As you can see, this year we had a sizable group of productive Cornell students working on research projects. For the coming years, CHESS has requested support for programs that would allow us to continue to recruit Cornell students as well as those from wider regional and national pools. We look forward to continuing our summer tradition of working with enthusiastic young scientists in training.

Rachel Pauplis

References:

1. Debashis Ghosh, Jennifer Griswold, Mary Erman, and Walter Pangborn; *"Structural Basis for Androgen Specificity and Oestrogen Synthesis in Human Aromatase"*, Nature **457** (7226), 219-223 (2009)
2. The original news release can be found at: http://www.hwi.buffalo.edu/newsroom/Press_Release_09/January/1_8_09.pdf
3. Published online before print February 25, 2009, doi: 10.1073/pnas.0812071106; PNAS 106 no. 11, 4225-4230 March 17, 2009
4. Read the original Rice Report here: http://www.media.rice.edu/media/NewsBot.asp?MODE=VIEW&ID=12128
5. Visit the Tao research group for more information: http://www.bioc.rice.edu/~ytao/index.html
6. See an interesting video explanation of virus structure and function that includes quotes from eminent CHESS user Michael Rossmann: http://www.livescience.com/health/090217-virus-coat.html
7. J.V. Bernier, J.-S. Park, A.L. Pilchak, M.G. Glavicic, and M.P. Miller; *"Measuring Stress Distributions in Ti-6Al-4V Using Synchrotron X-Ray Diffraction"*, Metallurgical And Materials Transactions A **39a**, 3120 (2008)
8. The ACS meeting archived video news conference is here: http://www.ustream.tv/recorded/2009896
9. NPR Science Friday radio interview with Jennifer Mass: http://www.npr.org/templates/story/story.php?storyId=112105590
10. Coverage of the development of the technique is here: http://news.chess.cornell.edu/articles/2007/WollWyeth.html
11. Science writer Anne Ju of the Cornell Chronicle wrote the following summary (PDF): http://www.news.cornell.edu/stories/Aug09/WyethColor.html
12. Lightsources.org coverage (PDF): http://www.lightsources.org/cms/?pid=1003645