



# CHESS

## SCIENTISTS' HIGH ENERGY X-RAY TOOL

### The Nature of X-rays

Anyone who has visited a dentist's office or hospital knows that invisible x-rays can go right through us and produce shadowy images of our teeth or bones. These common images already portray quite a bit about the nature of x-rays: they are a high energy light that can penetrate deeply into matter; they can be preferentially absorbed by dense matter (like bone); and they make fuzzy grayscale images on film.

### How Small Is Small?

These are just a few of the many properties of x-rays that bring hundreds of scientists—chemists, biologists, physicists, environmentalists, and art historians—to CHESS each year in order to peer inside all sorts of materials. Unlike medical x-ray sources, the CHESS x-ray beams produced by the CESR synchrotron are small, laser-like beams with intensities hundreds of millions of times brighter than radiograph machines. These small, intense beams are perfect for examining extremely small specimens. The typical sample brought to the synchrotron is a millimeter in size, and many are so small, they cannot be seen by eye. In addition, high energy x-rays have very small

wavelengths, typically a tenth of a nanometer or smaller, a length commonly referred to as the Angstrom unit. These wavelengths are 1,000 times smaller than visible light. Because they are so small, x-rays are one of the few tools perfectly adapted to peering inside almost anything to “see” actual arrangements of atoms and molecules.

### From Concrete to DNA

Just about anything can be studied with x-rays—from concrete to DNA. Hundreds of measurement techniques use x-rays. Some are as simple as x-ray absorption (like the medical radiograph), and others are more complicated procedures that measure tiny changes as x-rays pass through a sample. Often, subtle changes reveal the nature of chemical bonds or the charge state of atoms and their surrounding environments. In crystalline materials, such as grains of salt or diamonds, atoms organize themselves into rows and two-dimensional sheets. These sheets act like mirrors and cause incoming x-ray beams to reflect, or diffract, into hundreds or even thousands of separate directions as they exit the crystal, covering a piece of film with hundreds of spots. These spots can be mathematically inverted to locate

**UNLIKE MEDICAL X-RAY SOURCES, THE CHESS X-RAY BEAMS PRODUCED BY THE CESR SYNCHROTRON ARE SMALL, LASER-LIKE BEAMS WITH INTENSITIES HUNDREDS OF MILLIONS OF TIMES BRIGHTER THAN RADIOGRAPH MACHINES.**

each of the atoms inside the crystal and get an extremely accurate measure of the distance from one atom to another. This method, called x-ray crystallography, produces wonderful ball-and-stick models of molecules that show up routinely on the covers of scientific journals and magazines.

### X-ray Beamtime

CHESS has been a National User Facility supported by the National Science Foundation since 1980. One of a few

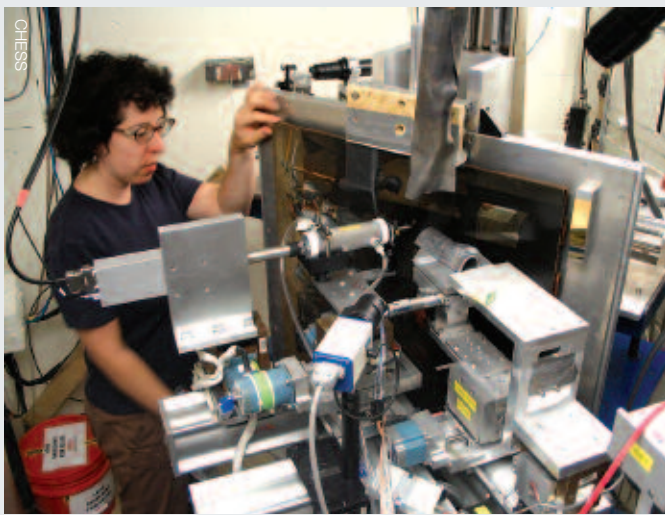
synchrotron radiation sources in the United States, CHESS is the only one located on (actually under!) the central campus of a major research university, and Cornell's educational impact is high. The CHESS staff hosts 400 to 600 scientists per year. More than half the visitors are graduate students working on doctoral research projects, resulting in more than 500 Ph.D.s

during a 25-year history, with 80 more in progress. Cornell faculty and students comprise one-third of the facility use; a group of faculty and students have recently helped to build three new experimental stations that serve a special educational purpose.

X-ray "beamtime," as it is traditionally called, is free to all scientists whose work will be published in the open scientific press. Access is granted to high-quality scientific projects based upon a written proposal subject to external peer review. During a typical five- to seven-week running period—usually three times per year—the lab's operations and scientific staffs work around the clock (24/7) to teach and assist new users in operating the equipment and collecting data. Lab operators must maintain and operate the wide variety of equipment, as well as pursue advanced techniques and projects in vacuum, electronics, computing, and general instrumentation. CHESS's senior staff redesigns instrumentation and continually upgrades and improves the lab's capabilities. CHESS's staff scientists provide oversight of experimental stations, develop their own research programs related to x-ray science, and assist or collaborate with ongoing user research. Staff and users together publish an average of two research papers for every day of x-ray operations.

### X-raying Art

The microbeam and confocal x-ray fluorescence groups at CHESS are engaged in collaborative research projects with the North Carolina Museum of Art, the Getty Museum in California, the Museum of Modern Art in New York, and the Winterthur Museum in Delaware. A special 3-D scanner allows CHESS to mount paintings up to 1.4 meters and move them with a few microns from a small x-ray probe beam. The microscope can determine the chemical makeup of paint layers buried beneath the surface without altering or damaging the valuable surface work. Jennifer Maas of the Winterthur Museum and University of Delaware shows the seventeenth-century Flemish painting, "The Armorer's Shop," under study.



### Pioneering Protein Crystallography at MacCHESS

Two expert user groups work alongside the CHESS staff. MacCHESS, a National Institutes of Health-funded group that supports protein crystallography at CHESS, is one of them. This group builds equipment, develops techniques, and supports visitors who bring tiny protein crystals with hopes of building atomic resolution images of their molecules. Protein molecules can have hundreds of thousands or millions of atoms, so developing three-dimensional atomic models is a monumental accomplishment. Much of the pioneering work and technique development in this area was started at CHESS and MacCHESS.

Protein crystallography has had a huge impact on biology in the last 60 years. As evidence, consider how x-ray images unraveled the mystery of DNA and, for the first time, gave us a picture of the double helix and, more recently, elucidated the structure and function of membrane proteins. MacCHESS can boast that one user—Rod MacKinnon of Rockefeller University, who won the 2003 Nobel Prize in Chemistry—primarily conducted this work at CHESS A1 station, where he collected data on the

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**THE CHESS STAFF HOSTS 400 TO 600 SCIENTISTS EACH YEAR—CHEMISTS, BIOLOGISTS, PHYSICISTS, ENVIRONMENTALISTS, AND ART HISTORIANS—WHO WANT TO PEER INSIDE ALL SORTS OF MATERIALS.**



biological crystals of a nerve membrane. The MacCHESS staff helped MacKinnon, a medical doctor by training, learn how to do x-ray crystallography, and then he astonished the CHESS staff by explaining in detail how potassium ions flow across cellular nerve membranes. Some 10 million ions per second must flow through each protein channel in order to provide the tiny electrical current that the brain uses to say, “My finger feels something.”

### Intense X-ray Optics at G-line

A second group, called G-line, consists of Cornell faculty and graduate students who helped raise funds from Cornell and the NSF in 1999 to add an extension to Wilson Lab and build three new x-ray stations. G-line—so called because it followed the construction of lines A through F—was designed with special x-ray optics to extract the highest possible x-ray intensity from the CESR synchrotron. In this case “high” can mean up to  $10^{14}$  photons per second focused onto a one-millimeter specimen! These high x-ray doses are useful in many ways, including to study very small specimens, record very weak signals, or collect data very, very rapidly. The latter of these opens up the possibility of studying physical phenomena that are changing with time. For instance, a chemist may want to learn how quickly molecules reverse orientation in a liquid crystal display. Another scientist may be studying a single layer of atoms deposited onto a surface of a growing crystal.

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## STAFF AND USERS TOGETHER PUBLISH AN AVERAGE OF TWO RESEARCH PAPERS FOR EVERY DAY OF X-RAY OPERATIONS.

Because x-rays easily travel through the walls of a reaction vessel and do not interfere with ongoing chemical reactions, they are an extremely valuable tool for dynamically watching chemical and physical changes as they take place.

G-line also provides graduate students a unique experience by allowing them to help design, construct, and then support their own x-ray infrastructure. Some students have built as Ph.D. projects experiments to record the fundamental physics of how materials grow.

### How Mysteries of Cell Membranes and Electrical Signals Were Solved at CHESS

*ROD MACKINNON, 2003 Nobel Prize in Chemistry*



In 1998, to much surprise, Rod MacKinnon and his colleagues determined the three-dimensional structure of a membrane pore that allows cells to control their intake of potassium ions. By determining the structure of the potassium pore, or channel, MacKinnon and

his colleagues at the Rockefeller University solved a riddle that has perplexed biophysicists for decades: how does a potassium channel admit millions of potassium ions per second, while blocking the flow of smaller diameter sodium ions? He also explained, in molecular detail, the mechanism of potassium flow. Without the flow of potassium and sodium ions in nerves and muscle, neurons could not generate the electrical signals that are involved in the sense of touch or in keeping our hearts rhythmically beating.

**Robert E. Thorne, Physics, and his research group does x-ray diffraction to study defects in protein crystals, as well as x-ray fluorescence to recover ancient inscriptions carved into stones from 1,800 to 2,400 years ago. His group has also invented microfabricated tools that will improve protein crystallography on ultrasmall specimens.**



Matthew Miller

### Lots of Science Done Here

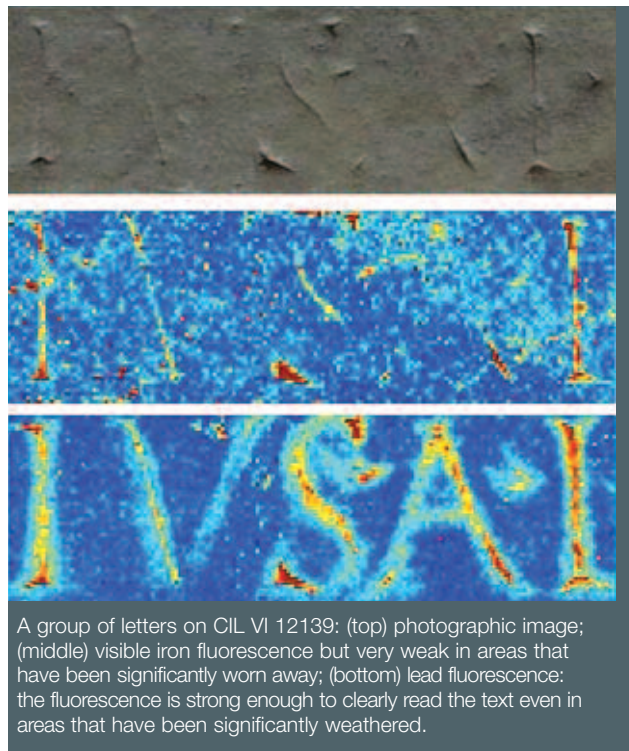
Lois Pollack, Applied and Engineering Physics, and her research group devised clever ways to study how complex biological macromolecules fold into exquisite three-dimensional

shapes. They expect that protein folding plays a critical role in biological function and specificity. Matthew P. Miller, Mechanical and Aerospace Engineering, focuses on properties and processing of engineering materials—primarily metallic alloys. His research group recently built a large apparatus to stretch metal bars while taking high-resolution x-ray diffraction patterns that sense changes in stresses and strains. They can resolve changes to the hundredth of a percent. Robert E. Thorne, Physics, and his research group does x-ray diffraction to study defects in protein crystals, as well as x-ray fluorescence to recover ancient inscriptions carved into stones from 1,800 to 2,400 years ago. His group has also invented microfabricated tools that will improve protein crystallography on ultrasmall specimens (see Economic Development on page 104). These are only a few of the many projects that utilize CHESS on a regular basis.

### Citizen Science

Outreach activities at CHESS encompass a wide range of educational venues. The CHESS staff, collaborating with John Chiment of Simple Interest, an Ithaca-based organization founded by him, is building a “citizen science” x-ray apparatus that can characterize the mineral content of historical artifacts and “cherts,” pieces of flint that are the raw material of

arrowheads. Because x-rays excite local atoms in the stones to give off fluorescent light characteristic of their atomic composition, this tool can identify and distinguish elements such as copper and iron and help build a database of “fingerprints.” Citizens participate by collecting samples and sending them to



A group of letters on CIL VI 12139: (top) photographic image; (middle) visible iron fluorescence but very weak in areas that have been significantly worn away; (bottom) lead fluorescence: the fluorescence is strong enough to clearly read the text even in areas that have been significantly weathered.



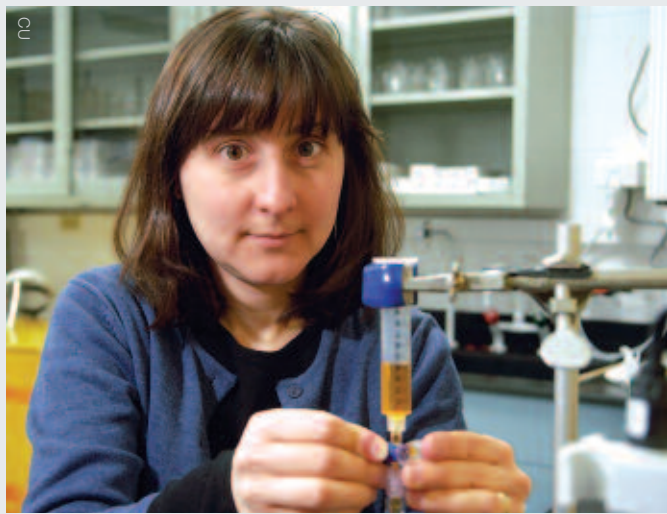
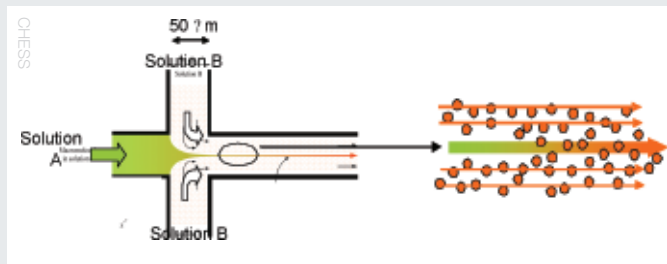
Richard Cerione with researchers  
Sandra Dias and Sebar Ramachandran

**MACCHESS, A NATIONAL INSTITUTES OF HEALTH-FUNDED GROUP THAT SUPPORTS PROTEIN CRYSTALLOGRAPHY AT CHESS, DEVELOPS TECHNIQUES, AND SUPPORTS VISITORS WHO BRING TINY PROTEIN CRYSTALS WITH HOPES OF BUILDING ATOMIC RESOLUTION IMAGES OF THEIR MOLECULES.**

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**Ultrafast Mixing Needed to See Protein Folding  
Lois Pollack, Applied and Engineering Physics**

Shown is a microfluidic mixer fabricated at the Cornell nanofabrication center that can be used to study protein folding. Mixing the protein solution (A) with a buffer solution (B) triggers the macromolecules to fold into a smaller size as they flow down the channel. Each position along the outlet channel corresponds to a fixed time after mixing. With an intense x-ray beam positioned at discrete positions, the scattering of the x-rays provides a direct measure of the size and shape of the macromolecules at discrete times during their folding process. CHESS x-rays have been instrumental in the development of this capability, which Pollack’s group now uses routinely to follow the folding of both proteins and large ribonucleic acids (RNAs) on time scales ranging from below 1/1000th to almost one full second.



CHESS for characterization. If x-ray fingerprints point to the true origin of the stone, and the object’s final destination is known, students can begin to visualize and document trading routes in early North America. The goal is to have a comprehensive fingerprint database that will provide scientific proof of the trade routes taken by individuals hundreds or thousands of years ago. Simple Interest is already conducting citizen science with its work on mastodon bones. The organization has its own journal that Cornell graduate students edit, overseeing the publication of the organization’s findings. Over 120,000 individuals have been involved in the bone artifact activity. This project could help scores of children do science and learn about x-rays and what they can do for historical studies.

*Donald H. Bilderback  
Associate Director, CHESS  
Applied and Engineering Physics*

**THE CHESS STAFF, COLLABORATING WITH JOHN CHIMENT OF SIMPLE INTEREST, AN ITHACA-BASED ORGANIZATION FOUNDED BY HIM, IS BUILDING A “CITIZEN SCIENCE” X-RAY APPARATUS THAT CAN CHARACTERIZE THE MINERAL CONTENT OF HISTORICAL ARTIFACTS AND “CHERTS,” PIECES OF FLINT THAT ARE THE RAW MATERIAL OF ARROWHEADS.**

**For more information:**

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