This article is presented in recognition of the International Year of Crystallography and efforts to increase public awareness worldwide of the science of crystallography.

COLLEGE to CAREER

Explore Career Options in Crystallography

BY NANCY McGUIRE

Crystallography is the science that examines crystals, which can be found everywhere in nature—from salt to snowflakes to gemstones. The properties and inner structures of crystals help scientists to examine the arrangement of atoms in the solid state, and this knowledge is used in fields such as chemistry, physics, and biology.

What crystallographers do

Crystallographers use X-ray, neutron, and electron diffraction techniques to identify and characterize solid materials. They commonly bring in information from other analytical techniques, including X-ray fluorescence, spectroscopic techniques, microscopic imaging, and computer modeling and visualization, to construct detailed models of the atomic arrangements in solids. This provides valuable information on a material's chemical makeup, polymorphic form, defects or disorder, and electronic properties. It also sheds light on how solids perform under temperature, pressure, and stress conditions.

Crystal-growing specialists use a variety of techniques to produce crystalline forms of compounds for use in research or manufacturing. They may be experts in working with hard-to-crystallize materials, or they may grow crystals to exacting specifications for use in computer chips, solar cells, optical components, or pharmaceutical products.

Crystallography has become an important tool for studying structural biology. Proteins and other biological materials (including viruses) may be crystallized to aid in studying their structures and composition. Many important pharmaceuticals are administered in crystalline form, and detailed descriptions of their crystal structures provide evidence to verify claims in patents.

Instrument manufacturers hire crystallographers for customer sales and support functions, including instrument repair and helping customers with special projects. Staff crystallographers at the national laboratories develop and maintain leading-edge research instruments and software capabilities. They also assist visiting users in setting up and running experiments using specialized

Quick Facts

- **OPPORTUNITIES**

  Crystallography specialists may find opportunities working in instrument and software development, customer support for instrument manufacturing companies, user support at national laboratories, or working in crystal-growing laboratories.

  Historically, crystallographers have been associated with the geosciences, metallurgy, and ceramics engineering. However, the largest areas of demand today are in the medical and life sciences.

- **EDUCATION NEEDED**

  Laboratory technicians usually require a bachelor's degree in chemistry, biology, geology, physics, or a related field.

  Research positions usually require a Ph.D. and additional experience in a field of specialization (pharmaceuticals, structural biology, geosciences, materials science, physics, etc.). Research associates may have master's degrees and some experience.

  Customer and user support positions may require a graduate degree, depending on the nature and complexity of the service provided. These positions often require practical experience gained on the job, in addition to a strong academic foundation.

- **SALARIES**

  Jobs requiring undergraduate degrees range from $35,000 to $85,000 per year (2010).

  Jobs requiring graduate degrees range from $65,000 to $140,000 per year (2010).

- **LICENSES AND TRAINING**

  Licenses are not generally required for crystallography.

  Crystallographers must take safety training because their laboratory instruments produce X-rays, neutrons, or high-energy electrons. They wear one or more radiation dosimetry devices in the laboratory and must submit these devices for periodic checks to ensure that they have not been exposed to excessive amounts of ionizing radiation.

  Crystallographers working at government agencies or national laboratories may be required to undergo background checks or obtain security clearances on the basis of the nature of the work and the security requirements of the laboratory.

techniques, including synchrotron X-ray diffraction and neutron diffraction. Universities employ staff members to maintain and operate their research laboratories and to train students to use the instruments.

Crystallographers may develop instrumentation and software for collecting, analyzing, and visualizing data and for translating these data into crystal structure models. Some crystallographers maintain and develop archival databases at industrial and academic institutions, as well as some nonprofit organizations and government laboratories.

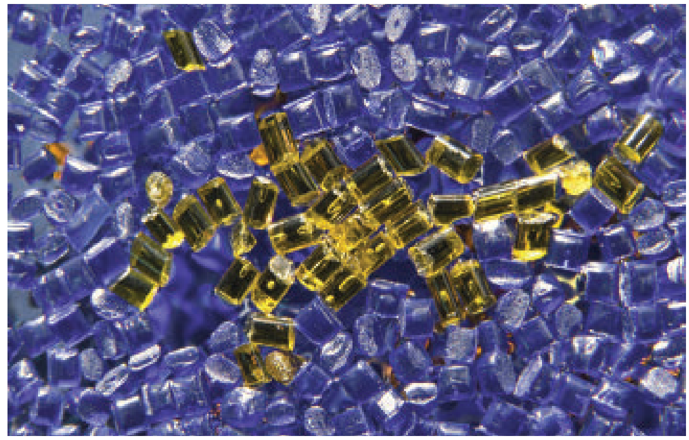
Service laboratories hire diffraction technicians to prepare and catalog samples, run the data collections, and prepare routine reports on the results. Technicians may also be called on to perform routine instrument maintenance and simple repairs.

Forensics laboratories use crystallography to investigate cases involving product adulteration or counterfeiting. They may identify minerals, metals, or other materials found at crime scenes. They may also identify corrosion products and other residues found at the site of an industrial accident to help verify the events leading up to the accident.

Workspace

Crystallographers generally work in laboratories. Because crystallography is a very computation-intensive specialization, crystallographers must be able to use, and train others on, proper data collection and analysis methods, software packages, and computer visualization capabilities. They may be systems administrators for the computing networks associated with their laboratories.

Crystal-growing labs may have controlled-environment



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devices, including glove boxes, furnaces, and cryogenic chambers. These spaces must be kept free from contaminants and unwanted sources of vibration or other factors that could damage the crystals as they grow.

Crystallographers in academic environments often teach courses in diffraction theory or provide individualized instruction on using the instruments and software. At national laboratories, crystallographers train visiting users, and they perform their own research and maintain custom-designed instruments, many of which are quite large.

Research crystallographers make presentations at conferences, and they may travel to specialized facilities to run experiments.

TECHNICAL SKILLS REQUIRED

Required skills vary according to specialization, but may include the following:

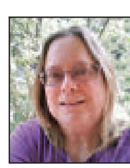
- **Problem-solving skills and an interest in solving basic and applied research problems**
- **Critical thinking and analytical skills to design experiments, troubleshoot processes, and analyze data collected**
- **Written and oral communication skills to explain findings and share results with scientists and nonscientists**
- **Computer skills, including familiarity with computer modeling and data analysis**
- **Skills in adapting and integrating computer software to solve new categories of problems**
- **Ability to visualize structures in three dimensions**
- **Crystal-growing capabilities**
- **Instrument maintenance, operation, and development**

Is this career a good fit for you?

Although computer hardware and software have evolved to the point where they perform much of the computation, a crystallographer must understand the underlying principles to set up the calculations properly and ensure that the results are meaningful and properly interpreted. Computers can create 3D models of crystal structures, but an ability to correlate these structures with properties of the material requires an ability to visualize and interpret these models. This requires patience and attention to detail.

Crystallographers must collaborate with experts in synthesis and in other analytical techniques, and often, they must have some degree of expertise across several disciplines. They may be required to develop novel sample configurations, adapt their instruments to new applications, or adapt and create new software capabilities to handle unusual or difficult problems.

Crystallographers, especially technicians, may serve a support function for chemical synthesis labs. They may work in commercial service labs or as a part of an in-house analytical team. This requires them to understand the problem that their customers or colleagues are trying to solve, and to devise a data collection and analysis procedure that provides useful and accurate results. iC



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Chemists in the Real World: Brian Toby, Ph.D.

SENIOR PHYSICIST/SECTION HEAD, ARGONNE NATIONAL LABORATORY

PH.D., PHYSICAL CHEMISTRY, CALIFORNIA INSTITUTE OF TECHNOLOGY

B.A., CHEMISTRY, RUTGERS, THE STATE UNIVERSITY OF NEW JERSEY-NEW BRUNSWICK

Brian Toby has worked for eight years at the Advanced Photon Source (APS), a synchrotron-type particle accelerator at Argonne National Laboratory that provides intense X-ray beams to a variety of specialized instruments. His current job title is Senior Physicist and Section Head for Scientific Software. He assists scientists at the synchrotron in automating their instruments, analyzing data, and doing instrument support. He spends much of his time developing a crystallographic data analysis software package, GSAS-II, that can be used with a variety of diffraction instruments and experimental setups. "I see my job as being a resource," he says.

Previously, as a group leader at Argonne, he headed up efforts to build a high-resolution powder diffractometer that is now the APS's most productive instrument, in terms of publications generated using data from the facility. This instrument is highly automated for high sample throughput, so that scientists can mail their samples to the lab and receive their results online, after the data have been reviewed for quality by an Argonne staffer. Toby has done considerable work on automating processes, which enables scientists to spend more time productively, rather than doing repetitive tasks.

Toby learned crystallography as a chemistry undergraduate and then studied surface science in graduate school, receiving his doctorate in physical chemistry in 1986. He landed his first job after graduate school through an on-campus recruiting program. Two companies interviewed him, and one of those companies offered him his choice of jobs in two different locations. Since then, he has worked in industry and academia, before going into government laboratory work.

Please describe your typical day on the job.

My typical day starts by clearing my e-mail inbox. With that out of the way, I then pick up a task I want to work on for the day, which may be writing or editing a paper, putting together a talk, analyzing some data, or adding a feature to some data analysis code. Once in a while I collect data, but I try to give the pleasure of that to my collaborators.

At least a few times each year, I go to universities and conferences to give seminars, or to professional workshops and give tutorials. I have a website where I archive recordings of my tutorials, but eventually, I would like to replace that with a MOOC (massive open online course) where students can interact to help each other solve problems.

What apps/software/instrumentation/tools can't you live without?

I use the Beamline 11 BM High Resolution X-ray powder diffraction instrument at Argonne to collect data; it is the best resource of its type in the United States. For data analysis, I use the GSAS/EXPGUI and GSAS-II diffraction software packages and the Python programming language. I use the Emacs text editor for writing code, and EndNote for writing papers. I love working on a Mac so that I can alternate between typing Unix commands and the Mac GUI (graphical user interface) features.

How many hours do you work in a typical week?

I probably work 30–45 hours per week in the office and 10–30 more at home. Previously, I had a role with way too many tasks — until I was replaced by four people. For now, my work pace is largely self-driven, but I always have more things I want to do than energy to get them done.

Is there anything else you would like to mention about your career?

I spent two stints in industrial labs, with a non-tenure track university job in between, before starting the first of my two government research jobs. Prevailing wisdom is that does not happen. A lot of people think that once you go into industry, you never leave, but this was not true in my case.

What is your work environment like?

I have a private office; I once turned down a job because scientists were housed in an "open office" environment. I think for a living, and distraction would kill my productivity. I can get quite a bit done with just my laptop while traveling, but many tasks need a really quiet place where I can concentrate. Multiple computer monitors are also great to have.

What essential habit do you have now that you wish you'd started much earlier?

I wish that, when I was a student, it had been possible to receive journal tables of contents by e-mail. I read them for many journals and follow up on a small number of articles. Some I skim, others I look at more carefully. It took me too long to learn that time spent on calendar keeping (meetings, deadlines, etc.) is never wasted.

What is your favorite ACS resource?

The ACS journals and their free e-mail contents/ASAP service. Also, I attended and gave a presentation at an especially well-organized symposium at the ACS national meeting earlier this year. I made some good new professional connections, and I got to speak with a number of old friends. iC