Actanced Light Sources

Tools of Discovery and Innovation

Published by LAAAMP, Lightsources for Africa, the Americas, Asia and Middle East Project

Advanced Light Sources and Crystallography

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The Crab Nebula is the remnant of a supernova explosion that was observed on Earth in AD 1054. The Crab is about 6,500 light years from the Earth. Energetic electrons from the explosion follow curved paths caused by the strong magnetic field in the nebula and emit synchrotron light, just as do advanced light sources here on Earth.

What are advanced light sources? What is crystallography?

Not all light is visible. In science and technology the word **light** applies generally to electromagnetic **radiation**. Most wavelengths of light are not visible.

Light sources generate radio, microwave, infrared, visible, ultraviolet, X-ray and gamma-ray light.

Advanced light sources are much more intense than conventional sources, such as light bulbs and traditional lasers.





Different wavelengths of light compared to sizes of various objects. To see an object we need light with a wavelength that is equal to or less than the size of the object.

The smallest object we can see with visible light is a bacterium. To see the details of the constituents of a cell, *e.g.* proteins, we need a shorter wavelength such as X-rays.

Crystallography is the science that examines the arrangement of atoms in solids. There is a close connection between the science of Crystallography and much of the work done at Advanced Light Source Facilities.

Well-focused X-ray beams, generated by advanced synchrotron radiation facilities, yielded high-resolution diffraction data from crystals of ribosomes, the cellular nano-machines that translate the genetic code into proteins.

Ada Yonath, 2009 Nobel Prize in Chemistry

Why care about advanced light sources?

OBSERVING MATTER and decoding its secrets are at the heart of humanity's quest to understand the world around us. Advanced light sources offer unique tools to expand the boundaries of scientific investigations into new materials and living matter. As centres for fundamental and applied research, light sources play a key role in stimulating innovation and enhancing industrial competitiveness.

Advanced light sources are revolutionising a myriad of fundamental, applied and industrial sciences, including agriculture, archaeology, biology, biomedicine, chemistry, cultural heritage studies, engineering, energy, environmental science, forensic science, geology, materials science, nanotechnology, new drugs, palaeontology and physics. Advanced light sources are *the* ultimate means of characterising materials in our age. They open insights to micro- and nano-structures of manufactured materials that are not possible to obtain in any other way. Industry recognises this, and is an increasing user of advanced light sources to support research and innovation in product development.

These facilities have major impacts on the education and training of graduate students, our future scientists.





Advanced light sources are key to research frontiers in many disciplines and industries — sometimes addressing current scientific, commercial and educational needs of a particular country or region. Thousands of graduate students in biology, chemistry, environmental, materials and

medical sciences, and other disciplines have done world-class research for their Ph.D. theses at light sources around the world. Providing such a resource was a major motivation for many countries to start their light sources in the mid-1980s.







The National Synchrotron Light Source II (NSLS-II) (photo) at Brookhaven National Laboratory in the United States is one of the world's newest and brightest light sources, serving up to 6,000 users per year.

How does a light source work?

A CCELERATION is a change in speed or direction of motion. When they are accelerated all electrically charged particles emit radiation, which we call light.

When they are accelerated, protons and electrons can emit light. But electrons emit vastly more than protons. That is why all advanced light sources use electrons.

There are two major types of advanced light sources: **circular**, doughnut-shaped electron storage rings called synchrotrons or synchrotron light sources, and **linear**, free-electron lasers (FELs).

Each synchrotron radiation facility is different and has somewhat different capabilities. However, in general, the facility is like a chain composed of links.

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Each link in the chain accelerates the electrons further and injects them into the next link in the chain. Details below are for the medium-energy Diamond ring.

CIRCULAR. When an electron beam passes between the north and south poles of a magnet, its path is curved. It changes direction and emits light. The electrons can be stored and circulate in a ring for periods of up to a day. As the electrons turn they emit electromagnetic radiation, both visible and invisible, from very long wavelengths (infrared) to very short wavelengths (X-rays). Since the

radiation is emitted tangentially to the ring, many beam lines can be constructed, and scientists can take data simultaneously.







Electron gun. Electrons "evaporate" from a hot surface and are accelerated to 90,000 electron volts (90 keV) of energy. A linac (linear accelerator) is the first of 3 particle accelerators in this chain; electrons are accelerated from 90 keV to 100 million electron volts (100 MeV). Booster. Bending magnets curve the electrons around a circle, and a radio-frequency source accelerates them to 3 GeV (3 giga or billion electron volts) before being transferred into the storage ring. The storage ring consists of straight sections angled together to form a closed loop approximately 600 m in circumference. It is filled every 10 minutes with a new batch of electrons. At some facilities it is filled every few hours. Beamlines operating simultaneously carry different wavelengths of light to the user groups.

Introduction



LCLS, The Linac Coherent Light Source at Stanford University's SLAC National Accelerator Laboratory in California, one of the world's first linear free-electron lasers.

LINEAR. Making light from electron beams.

Conventional lasers make their extraordinarily useful light by jiggling electrons bound in atoms. Accelerator-driven free-electron lasers (FELs) make light by using magnets called undulators to jiggle electrons that are freed from atoms. The pulses from a FEL are a thousand times shorter than those from a storage ring and many times more intense. This has opened up exciting new possibilities for research in many diverse fields. A disadvantage of FELs is the comparatively small number of beamlines that can be operated simultaneously.

Brilliance

When comparing light sources, an important measure of quality called brilliance, also known as brightness, takes into account the number of photons produced per second, how fast the beam spreads out, the beam size and the spread in frequencies or wavelengths in the beam. X-ray beams from advanced light sources are many orders of magnitude more brilliant than from conventional X-ray tubes. An **undulator** is an "insertion device" because it is "inserted" into the accelerator track. It is used in both circular and linear advanced light sources and is a periodic magnetic structure with the north and south poles of the magnets alternating in orientation. The undulator stimulates highly brilliant, forward-directed synchrotron radiation emission by forcing a charged particle beam to perform wiggles (accelerations), or undulations, as it passes through the device.



Research at an advanced light source facility



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Diagram of Diamond Light Source, UK, specifying the typical area of research of each beamline.

Beamlines in the Experimental Hall at the Photon Factory, KEK, Japan.

The ambiance of working at science and technology frontiers

A group of scientists, usually from a university, but sometimes an industry or government laboratory, and often in a collaboration among several institutions, will write a proposal. They will describe the study, specify which beamline they want to use and how many hours of beam time they require. A committee appointed by the facility Director chooses the best science, usually without regard to institution or country.

Often the group is led by a Professor with post-doctoral scientists and doctoral students. Most facilities have on-site housing, a cafeteria, a library, and a computing centre. They are unique hubs for training and education and the interactions between groups is part of the experience.



Education and outreach

A SUCCESSFUL outreach programme is the International Union of Crystallography IUCr-UNESCO OpenLab programme. OpenLabs is a network of operational crystallography laboratories based in different countries worldwide, mainly in Africa, South and Central America and Southeast Asia and is aimed at allowing access to knowledge gained from crystallography in all parts of the world. Funds from LAAAMP are used for additional OpenLabs.





IUCr-UNESCO OpenLab, Rabat. Morocco, May 2014.

This OpenLab was run with the formula of the travelling lab: a portable diffractometer was moved through different locations in the country (Rabat, El Jadida and Agadir) and at each stop it served as the basis for a crystallographic school, including tutorials about the use of the instrument and related software.

TO LEARN MORE

http://www.iucr.org

IUCr-UNESCO OpenLab in Uruguay, July 2014. Students at the microscope are preparing crystals

for an X-ray diffraction measurement while other students in the room analyse data from a previous experiment.

Applications to nanomaterials

TANO is the prefix for one-billionth. A nanometre (**nm**) is one-billionth of a metre. A nanosecond (nsec) is one-billionth of a second. A convenient way to remember the duration of a nsec, is that a signal travelling in a wire or piece of fibre optic 30 cm long takes about one nsec to go from one end to the other.

Protein molecules are a few nanometres in size (page 1) and the soft X-ray beams from advanced light sources have wavelengths of a few nm's so this is an ideal match for basic studies of protein molecules.

Nanotechnology and nanomaterials are general terms for the design and creation of materials whose use depends on structure at the nanoscale, generally 100 nanometres or less. They include devices or systems made by manipulating individual atoms or molecules, as well as materials which contain very small structures. Nanomaterials may have different physical and chemical properties than the same materials in bulk form. The number of products produced by nanotechnology or containing nanomaterials is increasing. Current applications include healthcare (in targeted drug delivery, regenerative medicine, and diagnostics), electronics, cosmetics, textiles, information technology and environmental protection. Nanomaterials appear in a range of products, including food packaging, wound dressings and food supplements.







Nanowire images from Dr. Öztürk

Özgül Öztürk doing powder X-ray diffraction measurements to study the effect of doping on semiconductor nanowires. The work was done at the European Synchrotron Radiation Facility in Grenoble. Dr. Öztürk chairs the LAAAMP Middle East Regional Committee as well as the SESAME Users' Committee.



Elettra Sincrotrone in Trieste, Italy, is an international research centre serving science and industry. The centre hosts two advanced light sources: FERMI, a free-electron laser, and Elettra, a storage ring. The light produced is transferred to over 30 experimental stations specializing in many fields, including chemistry, microscopy, materials science, electronics and information technology.

The International Atomic Energy Agency (IAEA) and Elettra jointly built and operate an XRF beamline and End Station. This provides research and advanced training opportunities for scientists from developing countries, and creates links between these scientists and existing large research groups.

The invention and development of FELs has opened a fantastic new window into fundamental research. The extremely short duration pulses from a FEL, only 30 femtoseconds in length (one femtosecond is one millionth of a nanosec!) allow a movie to be made of fundamental molecular processes as they occur.

Sunlight-driven photosynthesis is the energy source of all green plants. The Linac Coherent Light Source (LCLS) at Stanford University produced a "molecular movie" of a bacterial molecular complex that catalyses photosynthesis as it splits water into hydrogen and oxygen. A deeper understanding of photosynthesis could aid the development of better solar cells and might advance the quest for artificial photosynthesis.

Structural biology

Powerful tools to study the biology of diseases

MALARIA

Using the Advanced Photon Source at Argonne National Laboratory, researchers from the University of Texas Southwestern Medical Center contribute to the fight against malaria, a disease that kills millions. They study how a protein in the mosquito immune system operates against the parasite that causes malaria.



Thanks to Richard Baxter and Johann Deisenhofer for providing the image.

ZIKA

Z IKA virus is spread by daytime-active Aedes mosquitos and has become a world-wide scourge. Below is a digitally-colourised image of Zika virus particles (coloured blue) about 40 nm in diameter. Scientists at the Brazilian Synchrotron Light Laboratory are researching methods to combat Zika.



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Courtesy Centers for Disease Control and Prevention, U.S. Department of Health and Human Services

© Adobe Stocl



Courtesy National Synchrotron Light Source, Brookhaven National Laboratory

HIV/AIDS

Globally, about 35 million people are living with HIV, which constantly adapts and mutates creating challenges for researchers. Scientists armed with clear light source images of the HIV virus and its constituent proteins are learning how the body can combat the virus with the ultimate aim of producing more effective antiviral drugs.

LASSA

Perseverance pays off in the fight against the deadly Lassa virus at the Stanford Synchrotron Radiation Lightsource. Investigation revealed the first-ever image of its elusive viral protein. An antibody from a human survivor (light blue or turquoise) is shown inactivating the Lassa virus surface protein. The work shows how to engineer vaccine strategies to elicit protective immune responses.





Ebola, a viral hemorrhagic fever of humans and other primates, caused by Ebola virus, spreads by direct contact with body fluids of an infected human or other animal. The largest outbreak to date was the epidemic in West Africa from December 2013 to January 2016. It was declared no longer an emergency in March 2016. Another outbreak in Africa began in May 2017 in the Democratic Republic of the Congo. Scientists armed with data from advanced light sources will help to defeat Ebola.

Source: PureLife Pulse. PureLife is a manufacturer of health and safety products

Foot-and-mouth disease



Courtesy Diamond Light Source

SCIENTISTS at Diamond Light Source and Oxford University have produced a vaccine for foot-and-mouth disease, which is caused by a virus. The 2001 outbreak in the UK caused the deaths of over 7 million livestock. Globally it remains one of the most economically devastating diseases in livestock. It is endemic to central Africa and some parts of the Middle East and Asia. The image shows the the virus lifecycle.

Applications to energy

THE modern world consumes ever increasing amounts of energy. Current reserves of fossil fuels are limited. One of the greatest challenges in the 21st century is providing the world's population with the energy it needs without significantly raising the concentration of greenhouse gases in the atmosphere. A significant fraction will have to come from solar cells taking advantage of the sunlight bathing our planet. Organic photovoltaics show great promise for providing cost-effective and lightweight solar panels. Development of new energy sources and improving the efficiency and exploitation of existing systems requires detailed understanding of both structure and behaviour at the fundamental microscopic level. This is an area where the powerful X-ray beams of a synchrotron radiation source play a major role.

Research at many light source facilities is aimed at understanding and improving the multilayer materials that compose an organic solar cell. One such effort is at the Molecular Sciences Research Center at the University of Puerto Rico, which is leading the LAAAMP effort to advance light source and crystallographic sciences in the Caribbean.



PEDOT AI IN AI PET foil

Courtesy Kivirus at English Wikipedia

An organic solar cell or plastic solar cell uses organic electronics, a branch of electronics that deals with conductive organic polymers or small organic molecules, for light absorption and charge transport to produce electricity from sunlight by the photovoltaic effect. The symbols on the diagram are abbreviations for the compounds used. Advantages are flexibility and low cost. Advanced light sources are used for some of the development of these solar panels.

Large arrays of solar panels are becoming more and more common

Applications

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Study of materials under extreme conditions

THE STUDY of the effects of pressure and temperature on material properties is fundamental. These studies are relevant to many problems in condensed matter physics and chemistry, Earth and planetary sciences, and materials science and technology.

In particular, high-pressure and high-temperature research is vitally important for studying the composition, thermal state and properties inside the Earth and other planets. Rocks and plausible mantle materials are subjected to appropriate pressure and temperature conditions and their properties measured. These data, together with geophysical and geochemical observations, are indispensable for the understanding and modelling of planetary interiors.

Synchrotron radiation is powerful and can penetrate the highly absorbing walls of the pressure vessels in which the samples are contained.

Furthermore the high brilliance beams are ideal for micron-sized foci needed to probe the very small samples required for high-pressure studies.

Some of these studies have been conducted by a group from the University of Johannesburg using the beams at the ESRF, the European Synchrotron Radiation Facility in Grenoble, France. In 2013, South Africa became a Scientific Associate Member of the ESRF.

~ 5.0 mm

2,4 mm

7,0 mm



Cross section of the Earth's interior. The lower mantle extends from a depth of 660 km to a depth of 2,800 km. The pressures are in units of GPa (giga Pascals; one GPa is roughly 10,000 times atmospheric pressure at sea level.)

Nature Geosci,

Parker et al.,

Kan

van

Courtesy M.

Mechanical cell for exposing materials under high pressure to the beam.

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Applications to forensic science

Synchrotron radiation provides a tool to study trace evidence: glass, gunshot residues, pigments and biological samples such as human hair. Imaging can be done at high resolution and sensitivity. The ability to tune energy gives powerful chemical identification and mapping through X-ray absorption

spectroscopy. These techniques are particularly suitable for small sample sizes.

Hair Analysis. Trace-level components of blood supply become incorporated into the growing hair cells in the hair bulb. As the hair grows each segment of growth shifts outwards, producing a timeline of the individual's blood concentrations. The hair may tell us a great deal, such as dietary intake, exposure to pollutants, effects of disease, and profiles relating to ingestion of drugs including performance enhancing drugs.

ADVANCED LIGHT SOURCE NEWS

CRIMES NEW AND OLD RE-EXAMINED. ADVANCES MADE IN IDENTIFYING ENVIRONMENTAL CONTAMINANTS



Where does mercury contamination in our bodies come from?

Mercury, a potent neurotoxin, can accumulate over the years. An international team including the European Synchrotron Radiation Facility in Grenoble has developed new capabilities that identify the source of mercury in human hair.

Where did the arsenic that killed four people in Japan in 1988 come from?

X-Ray fluorescence using beams at SPring-8 and the KEK photon factory in Japan, has been used to shed new light on this famous case where people were poisoned from eating arsenic-tainted curry. The alleged murderer has been sentenced to death.



How did Phar Lap, the famous Australian race horse die in 1932?



Phar Lap died suddenly in suspicious circumstances. Hair analysis using the Australian Synchrotron at first indicated murder by arsenic poisoning and created worldwide headlines, but later analysis proved the horse died of colic.

Was Agnes Sorel, the first official royal mistress of France poisoned?

The ESRF has gone back in time to study the sudden death of the beautiful mistress of King Charles VII in the XV century. Hair analysis shows incredibly high mercury levels.



What are the white spots in the famous Munch painting "The Scream?"



Were they bird droppings? Analysis using PETRA III, the advanced light source in Hamburg ruled that out and instead confirmed it was beeswax used to consolidate flaking paint.

Applications

Palaeontology Research on ancient fossils



Skull of a 200-million-year-old fanged dinosaur. The fossil was scanned with X-rays at ESRF, using a beam 100 billion times more powerful than those used in hospitals. This allowed the research team from the Evolutionary Studies Institute at The University of Witwatersrand (Wits) in South Africa to peek "inside" it for the very first time.

The ESRF is supported by 22 partner nations, of which 13 are Members and 9 are Scientific Associates. Not limited to European nations, the ESRF's most recent affiliate is South Africa.

Palaeontology

Palaeontologists use fossils to study life throughout geologic time. Both animal and plant fossils are collected, observed, described, and classified. Palaeontologists

use fossils to learn more about what the Earth was like in the past and how environments changed over time. Fossils help us learn about evolution of species. Important research in palaeontology is done at advanced light sources.



The interior of a one-centimetre-long fossilised egg. The eggs were found in northeastern Thailand and turned out to be 125 million years old. Using microtomography imaging to scrutinise the hidden embryonic skeletons preserved in the egg, the team now knows the egg layer's true identity—an anguimorph lizard, a category that includes Komodo dragons.

Archaeology Research on ancient materials

Virtually reconstructed dentition of a Neanderthal child. Synchrotron virtual histology reveals precise developmental information that is recorded in the form of tiny growth tracks inside the teeth.



Archaeology

Archaeology is the study of human activity through the recovery and analysis of material culture. The archaeological record consists of artifacts, architecture, biofacts, and cultural landscapes. Archaeologists study human prehistory and history, from the development of the



Restored in 1831, the **Temple of the Emerald Buddha** was redecorated with fine patterns of very thin coloured glass mirrors. The mirrors resemble natural gems more than ordinary mirrors. Unfortunately, this fine art of mirror decoration has disappeared for almost 150 years. The ultimate goal of exposing the glass mirrors to the beam at the Synchrotron Light Research Institute in Thailand was to quantify chemical composition and trace transition metals, and thus successfully enable restoration to their previous grandeur.

first stone tools at Lomekwi in East Africa 3.3 million years ago up until recent decades. Archaeology is a field distinct from palaeontology. Archaeology is particularly important for learning about prehistoric societies, for whom there may be no written records. Important research in archaeology is done at advanced light sources.



Reference: W. Klysubon *et al.*, "Characterization of the Ancient Decorative Mirrors from the Grand Palace Bangkok by SR-Based techniques", Trends of Synchrotron Radiation Applications in Cultural Heritage, Forensics and Materials Science, *IAEA TECDOC*, No. 1803, p. 86-92, 2016.

Applications

High technology centres feed industry

THE microscopic and nanoscopic structures of materials are directly related to their macro-scale properties and to their optimisation for modern day manufacturing processes and recycling.

One of the major users of advanced light source facilities is the pharmaceutical industry to obtain knowledge of the three-dimensional structure of protein targets and protein complexes.

Herceptin – used to treat advanced breast cancer – benefited from synchrotron experiments. Using synchrotron light in the infrared range, pioneering research is underway into developing new cancer therapies that can be tailored to the individual patient.





Duminsani Kama is adjusting a microcrystal to be irradiated by a powerful short laser pulse. He is working on beamline ID09 at the ESRF and is wearing special eye protection. The catalyst's photo-chemical activation will be induced, and then the re-equilibrium will be studied with X-ray crystallography.

Hester Esna du Plessis is carrying out a high resolution X-ray diffraction experiment for catalyst characterisation.



ourtesy ESRF

The impact of advanced light sources on science and society in developing countries

D RAZIL is a model for establishing a D synchrotron radiation facility in a developing country. It designed its first synchrotron light source, called UVX, in 1985 and launched in 1997. Initially, it was difficult to convince key parties of the benefits from having such a facility in one's own country. At its opening, researchers submitted only a few proposals, but the number of proposals grew quickly by orders of magnitude. Brazil is now internationally recognised for the quality of its research, particularly in structural biology, and currently is constructing a new light source called Sirius.

Similar experiences in South Korea and Taiwan led each of these countries to invest hundreds of millions of dollars in new light sources. These are examples of how excellent scientific research centres can improve local scientific and private enterprise opportunities. Dozens of mid-career diaspora scientists have returned home when they realised they can do world class research at an advanced light sources in their own countries.

UVX





SESAME, Synchrotron light for Experimental Science and Applications in the Middle East, is an advanced light source facility in Allan, Jordan, near the capital of Amman, established under the auspices of UNESCO and closely modeled on CERN. This advanced synchrotron serves a wide spectrum of disciplines including biology and medical sciences, materials science, physics, chemistry and archaeology.

Beginning operations in 2017. The **SESAME** member countries are Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestinian Authority and Turkey.

The European Union is an active supporter of **SESAME**, providing support via its Research Framework Programmes with projects such as CESSAMag* and OPEN SESAME**.



The IAEA has supported the development of **SESAME** through its Technical Cooperation program, *e.g.*, by providing training for personnel and experts for the project, as well as procuring radiation equipment.

* CERN-EC Support for SESAME Magnets.

** Supported by Europe's Horizon 2020 programme, OPEN SESAME provides staff training and capacity building among Middle East researchers for optimal use of a modern light source facility.

SESAME combines capacity building with peace building through science and is a model project for other regions.

Scientists from different countries work together to advance human knowledge.

Jobs and careers at advanced light sources

ESIGNING, building, maintaining, operating and using these complex machines require an enormous range of scientific, engineering, technological and industrial skills. There are career opportunities both at these facilities themselves and with the many scientific user groups that do experiments there. They are unique centres of education for young technicians, engineers and scientists.

There are encounters among researchers from different groups studying different disciplines. There are budding friendships between researchers from different countries, universities and institutions. Encounters take place in the cafeteria, the library, the computing centre and at presentations of scientific results. This is part of the excitement of working at such a facility.

University of Saskatchewan bioarchaeologist Dr. Angela Lieverse conducts research on a rare skull from the Bronze Age at the Canadian Light Source.





Installing a new narrowband terahertz system as part of an accelerator improvement program by a group of scientists, technicians and engineers at DELTA, the advanced light source in Dortmund, Germany.



Mary Upton (X-ray Science Division, Advanced Photon Source, Argonne National Laboratory) aligning a high-resolution monochromator in preparation for a resonant inelastic X-ray scattering experiment.

Future

THE international research community is collaborating to construct ever more intense sources to address the most challenging questions in living and condensed matter sciences. X-rays were used to determine the double helical structure of DNA by Rosalind Franklin to revolutionise biology. It must have taken Franklin weeks to get this pattern using conventional X-ray tubes in 1952. This can now be done in seconds. In order to understand and deal with health problems associated with thousands of proteins, the detailed structure of these proteins must be determined. This is a main job of light sources and they are used to study viruses. Biomedical, environmental, human heritage issues and concerns are local, which is why so many light sources are needed. Although there are more than 50 light sources and hundreds of beamlines, the user communities have grown faster requiring light sources for their fundamental, applied and industrial research. There is often a wait of months or years to get access, thus the need for more light sources, especially in developing countries.

These new endeavours will face challenges. But they share with SESAME the goals of building regional capacity and promoting understanding, friendship and peace, bringing together scientists from different countries and ethnicities to perform world class science.

Sekazi K. Mtingwa and Herman WINICK. "SESAME and beyond," Editorial. Science Magazine, May 20, 2017



MAX IV Laboratory, Swedish National Synchrotron, inaugurated 2016.



The High Energy Photon Source (HEPS) will be built in China.

Courtesy Roger Eriksor



X-ray diffraction pattern of DNA by Rosalind Franklin in 1952.

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Tools of Discovery and Innovation



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