QUANTUM PHYSICS

THE ULTIMATE X-RAY MACHINE

What started as a "Star Wars" idea for a 1980s-era antimissile weapon is now a microscope of unprecedented power, able to create exotic forms of matter found nowhere else in the universe

By Nora Berrah and Philip H. Bucksbaum

Photographs by Spencer Lowell

VACUUM CHAMBER (*horizontal structure studded with blue-rimmed ports*) houses specially designed mirrors to focus the world's most powerful x-ray beam to the width of a dust grain.

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AN atom, molecule or speck of dust placed at the focus of the world's most powerful x-ray laser doesn't stand a chance. The illuminated matter reaches a temperature in excess of one million kelvins, as hot as the solar corona, in less than a trillionth of a second. Atoms of, for example, neon subjected to such extreme radiation rapidly lose all 10 of their electrons, and once they have lost their protective cloak of electrons, they explode away from neighboring atoms. For physicists, the trail of destruction holds a peculiar fascination.

What makes the process astonishing is that the laser boils away the atoms' electrons from the inside out. The electrons, which surround the nucleus of the atom in onionlike orbital shells, do not all react uniformly to the x-ray beam. The outer shells are nearly transparent to x-rays, so the inner shell takes the brunt of the radiation, much as coffee in a microwave oven is heated long before the cup that holds it. The two electrons in that shell shoot off, leaving empty space in their wake; the atom is hollow. Within a few femtoseconds (quadrillionths of a second), other electrons get sucked in to replace the lost ones, and the cycle of core-hole formation and vacancy filling continues until no electrons are left. This process occurs for molecules as well as solid matter.

The resulting exotic state of matter lasts only a few femtoseconds. In solids, it decays into an ionized state—a plasma—called warm dense matter, which is normally found only in extreme settings such as nuclear fusion reactions and the cores of giant planets. The brief but extreme environment at the focus of an x-ray laser beam has no parallels on Earth.

The x-ray laser itself is as remarkable as the exotic phenomena it reveals. Known as the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory, it evokes memories of the 1980s-era "Star Wars" missile-defense system, whose advocates proposed wielding x-ray lasers to shoot down ballistic missiles and satellites, although this real-world x-ray laser owes much more to the great atom smashers developed at about the same time. The device repurposes one of the nation's premier atom smashers, the SLAC linear accelerator, operated by Stanford University for the U.S. Department of Energy. This machine produced many of the discoveries and the Nobel Prizes that kept the U.S. at

IN BRIEF

X-ray lasers have long been a staple of science fiction, but the first one employed for scientific use began operation at Stanford University as a Department of Energy Office of Science facility only four years ago. Known as the Linac Coherent Light Source (LCLS), it is powered by the world's longest linear particle accelerator at the SLAC National Accelerator Laboratory.

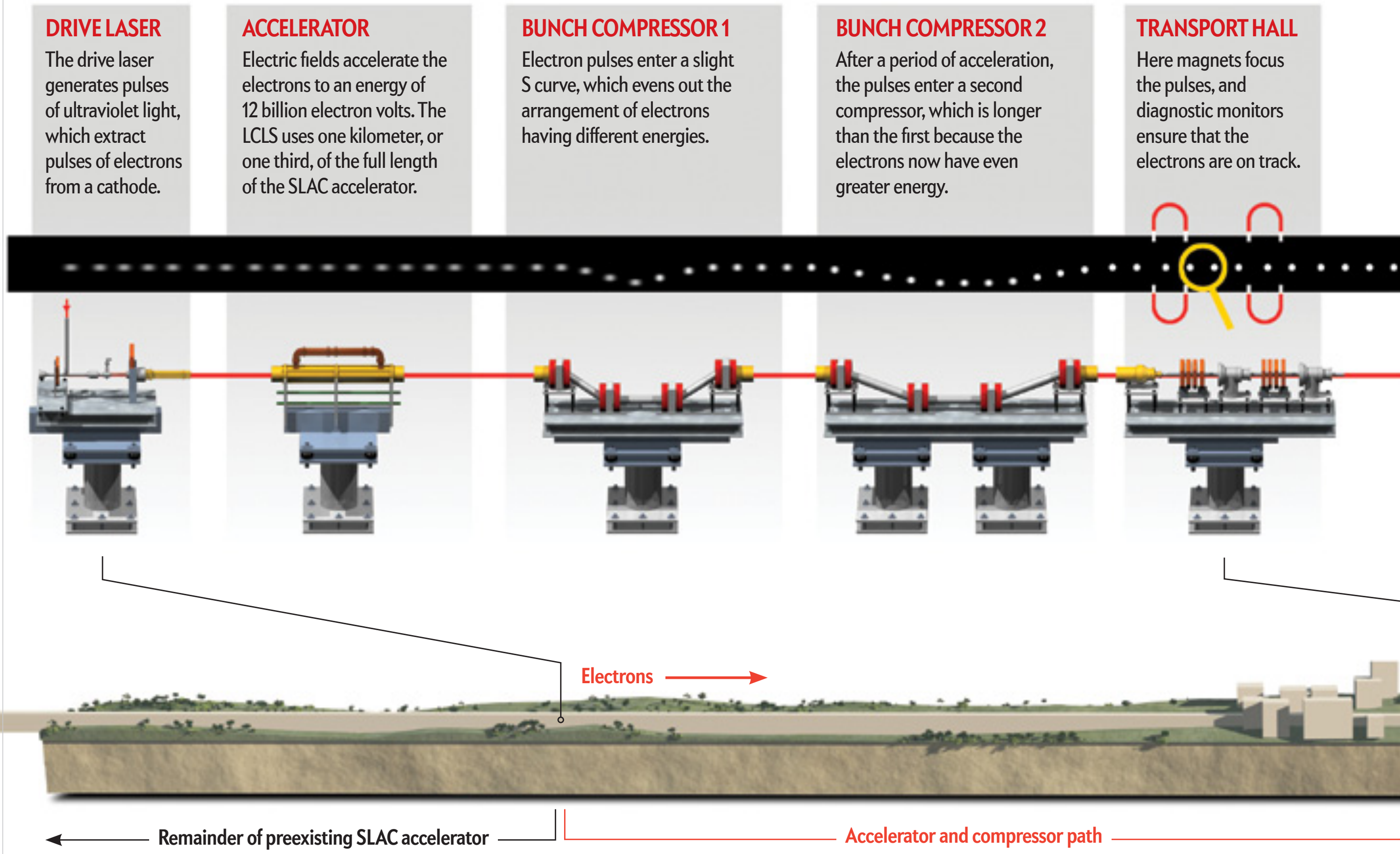
Exotic states of matter that occur nowhere else in the universe have been created by subjecting atoms, molecules and solids to high-intensity x-ray pulses.

Acting as a kind of strobe light, the laser has frozen the motion of atoms, captured high-speed images of proteins and viruses, and recorded physical and chemical transformations that take less than a trillionth of a second.

X-RAY LASER BEAM shoots down a pipe connecting the two experimental halls of the Linac Coherent Light Source.

Anatomy of the X-ray Laser

The LCLS is the closest to a starship laser blaster that earthlings have yet to create. It is powered by a linear particle accelerator, a gigantic version of the electron guns inside old-style TV sets, that fires electrons at near light speed. The heart of the contraption is the undulator, which



the forefront of elementary particle physics for decades. Since its recommissioning as the LCLS x-ray laser in October 2009, it has been to atomic and plasma physics, chemistry, condensed matter physics and biology what the Large Hadron Collider at CERN near Geneva is to elementary particle physics: a way to smash the building blocks of nature with tremendous amounts of energy, creating new forms of matter such as hollow atoms or simply zooming in on the quantum realm like a powerful, high-speed microscope. The LCLS's x-ray pulses can be so short (a few femtoseconds) that they freeze the motion of atoms, allowing physicists to observe chemical reactions in progress. The pulses are also very bright, letting us image proteins and other biological molecules that have been very difficult to study using other x-ray sources.

SHADOWS OF ATOMS

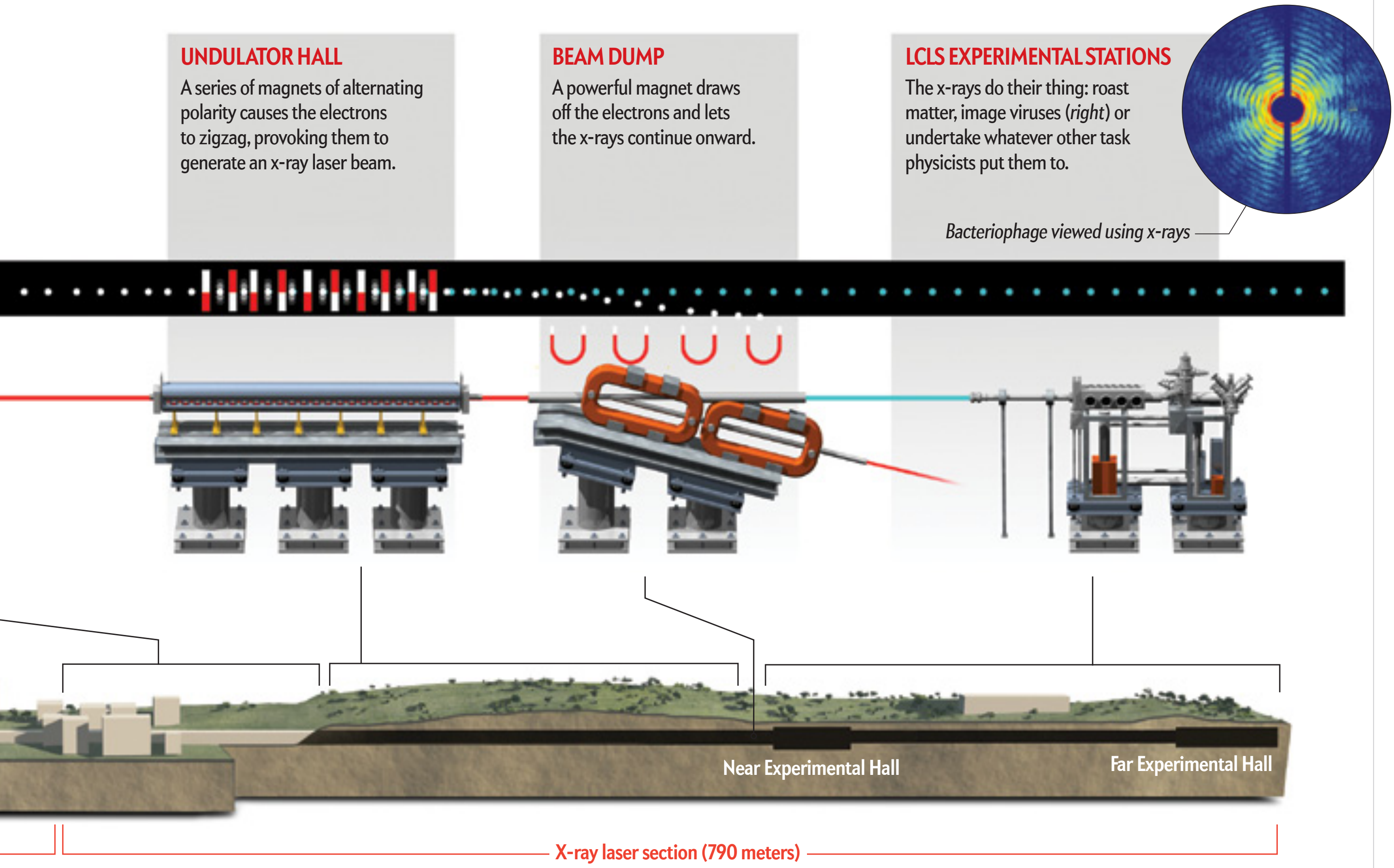
THE X-RAY LASER FUSES two of the main tools used by today's experimental physicists: synchrotron light sources and ultrafast lasers. Synchrotrons are racetrack particle accelerators. Electrons circling through them throw off x-rays, which enter instruments arrayed around the circumference of the machines like pinwheel spokes. One of us (Berrah) has spent a career using synchrotron x-rays to study the deep interior of atoms, molecules and nanosystems. X-ray light is ideal for this purpose. Its wavelengths are atomic-size, so atoms cast a shadow in an x-ray beam. In addition, x-rays can be tuned to pick out specific kinds of atoms—say, only those of iron—and show where they sit in a solid or in a large molecule such as hemoglobin. (Iron is responsible for the red color of our blood.)

What x-rays from synchrotrons cannot do, however, is trace out atomic motion inside a molecule or a solid. All we see is a dim blur; the pulses are not short enough or bright enough. A synchrotron source can image molecules only if they are arrayed in crystals, where local forces hold millions of them in precise ranks like identical soldiers at attention.

Lasers, for their part, are far brighter because they produce coherent light: the electromagnetic field in a laser is not choppy like the surface of a rough sea but smoothly oscillates with controlled regularity. Coherence means that lasers can concentrate enormous energy into a tiny spot and can switch on and off in as little as one femtosecond. One of us (Bucksbaum) uses ultra-

Illustration by Don Foley

causes the electrons to zigzag; whenever electrons change direction, they emit radiation—in this case, x-rays. Because the electrons are moving nearly as fast as the x-rays they produce, the process feeds on itself and produces an unusually pure and intense beam.



STEPHAN KASSEMEYER *Max Planck Institute for Medical Research (bacteriophage)*

fast optical laser pulses as a strobe light to study the motion of atoms and the steps in chemical reactions.

Conventional lasers, however, operate at visible and near-visible wavelengths, more than 1,000 times longer than the wavelength needed to resolve individual atoms. Just as weather radar can see a rainstorm but not resolve the raindrops, conventional lasers can see how collections of atoms are moving but cannot resolve those atoms. To cast a sharp shadow, the wavelength of the light must be at least as small as the object under observation. For that, we need an x-ray laser.

In short, the x-ray laser overcomes the drawbacks that existing tools pose for imaging matter on the tiniest scales. Yet making such a device is no easy task.

DEATH RAYS

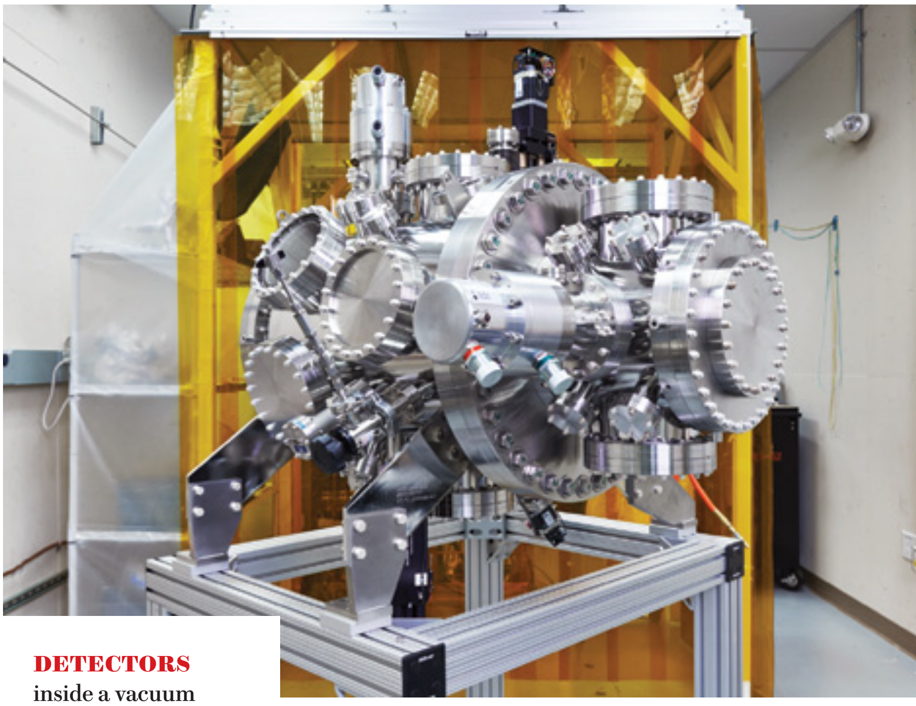
AT ONE TIME, THE IDEA OF BUILDING an x-ray laser seemed outlandish, given that making any laser is challenging. Standard lasers work because atoms are like miniature batteries: they can absorb, store and release small amounts of energy in the form of photons, or particles of light. Typically they release their energy spontaneously, but early in the 20th century Albert Einstein discovered a way to trigger the release, a process known as stimulated emission. If you cause an atom to absorb a certain amount of energy and hit it with a photon having the same amount of energy, the atom can release the originally absorbed energy—producing a clone of the photon. The two photons (the original one and its clone) go forth to trigger the release of energy from a pair of other atoms, and so on, building up a clone army in an exponential chain reaction. Laser beams are the result.

Even when conditions are right, though, atoms do not always clone photons. The probability that a given atom will emit a photon when hit by another is rather small, and the atom has a greater chance of releasing its energy spontaneously before that happens. Conventional lasers overcome this limitation by pumping in energy to prime the atoms and by using mirrors to send the cloned light surging back and forth, picking up new recruits. In a typical helium-neon laser used in supermarket price scanners, a continuous stream of electrons collides with atoms in the gas, and light is recycled 200 times by bouncing back and forth between mirrors.

For an x-ray laser, every step of this process becomes much more difficult. An x-ray photon may contain 1,000 times more energy than an optical photon, so each atom must absorb 1,000 times more energy. The atoms do not hold on to their energy for long. Moreover, x-ray mirrors are hard to come by. Although these impediments are not fundamental, it takes an enormous input of energy to create the lasing conditions.

In fact, the first x-ray laser got its energy from an underground nuclear bomb test. It was built for a secret project, code-named Excalibur, carried out by Lawrence Livermore National Laboratory east of San Francisco. The project is still classified, although quite a bit of information about it has been made public. The device was a component of former president Ronald Reagan's Strategic Defense Initiative, nicknamed "Stars Wars," in the 1980s and was meant to act as a death ray to shoot down missiles and satellites.

During the same decade, Lawrence Livermore also built the first nonnuclear laboratory-scale version of an x-ray laser, with energy supplied by powerful optical lasers that had been designed to test properties of nuclear weapons. These were not practical research instruments, though, and the possibility that x-ray lasers would ever be used routinely for science applications seemed remote.



DETECTORS **inside a vacuum chamber can make ultrahigh-resolution images of proteins and cells.**

NOT SLAC-ING OFF

THE BREAKTHROUGH that finally enabled investigators to develop x-ray lasers for civilian use came from another Bay Area institution, using a device intended for a different purpose entirely. In the 1960s Stanford built the world's longest electron accelerator, a three-kilometer building that, viewed from space, resembles a needle pointing from the mountains to the heart of the university's campus. The SLAC linac, as the machine is called, accelerates dense bunches of electrons to velocities extremely close to the speed of light (within one centimeter per second). The machine led to three Nobel Prizes for experimental discoveries in particle physics.

It did, however, reach the end of its useful life, and particle physicists now make their discoveries at the Large Hadron Collider. A decade ago Stanford and SLAC's parent agency—the Department of Energy's Office of Science—decided to turn part of the aging machine into an x-ray laser. SLAC outfitted the accelerator with the same device used to produce x-rays at modern synchrotrons: an undulator.

Undulators consist of a series of magnets that generate alternating magnetic fields. Electrons moving through undulators wiggle and emit x-rays. In synchrotrons, which are closed loops, once the electrons leave the undulator, their paths are bent in an arc. That way the particles get out of the way of the x-rays, which are channeled to experimental stations. The electrons keep going around the racetrack, emitting a burst of x-rays each time they pass through the undulator.

The SLAC accelerator, however, is a straight line, and the undulator is unusually long (130 meters). The electrons move along the same path as the photons and at nearly the same speed. The result is a subatomic demolition derby. The electrons cannot get out of the way of the x-ray photons they have emitted, so the photons sideswipe them again and again. In so doing, the photons induce the electrons to emit clone x-ray photons through the process of stimulated emission.

Mirrors are not needed to bounce the light back and forth through the electrons, because they travel together. All it takes to produce the laser is an intense beam of fast electrons and a space big enough to house a long undulator. And SLAC possesses both. If everything is lined up nearly perfectly, voilà, an extraordinarily bright x-ray beam. At the end of the line, the electrons are diverted, and the photons enter the experimental stations. The system is known technically as a free-electron laser.

Though not a gun for "Star Wars," the LCLS is still a formidable device. Its peak focused intensity, 10^{18} watts per square centimeter, is billions of times greater than synchrotron light sources. The laser can cut through steel. Its oscillating electromagnetic field can be 1,000 times stronger than the fields that bind atoms to one another in molecules.

THE HEART OF THE MATTER

THE DEMAND FOR THE LASER is so great that it can accommodate fewer than one in four research proposals to use it. The on-site staff scientists work with large visiting teams of students, postdocs and senior scientists in intense marathons, 12 hours a day for five days. Every microsecond counts.

The research made possible by x-ray lasers is broad. To offer a taste of what is possible, we focus here on two scientific problems that particularly interest us: how matter behaves under extreme conditions and what can be learned from the ultrafast imaging of molecules. These two problems are intimately connected to fundamental processes studied in atomic, molecular and optical physics, our field of expertise.

When the LCLS creates hollow atoms in molecules and solids, it takes advantage of the tendency of electrons from the outer

SCIENTIFIC AMERICAN ONLINE Watch an animation of powerful x-ray beams blasting hapless atoms at ScientificAmerican.com/jan2014/x-ray-lasers

Staff scientists work with large visiting teams in intense marathons, 12 hours a day for five days. Every microsecond counts.

shells of an atom to fall in to replace those that have been lost from the inner shells. This phenomenon, called Auger relaxation, takes a few femtoseconds. Therefore, if we shine a one-femtosecond x-ray pulse on the system, no outer electrons will have time to drop into the hollow inner-shell spots. Under these conditions, the hollow atoms will be transparent to any additional x-ray photons even if they are extremely intense. We have detected this hollow transparency at the LCLS not only for atoms but also for molecules and larger samples of material.

Theory suggests that inside giant planets such as Jupiter, temperatures reach 20,000 kelvins—four times hotter than the surface of the sun. Hydrogen and helium, the planet's main constituents, presumably take on exotic solid phases with extreme densities and structures. Yet little is known about the specifics. Even the strength of the material, its compression in response to pressure, is not easy to measure and not well understood from basic principles. So far research in this domain has relied heavily on theoretical models. Experiments that can validate the models have been scarce.

Some of the first experiments done at the LCLS attempted to re-create these hostile conditions. The laser's colossal intensity can heat matter with dizzying speed, producing unusual effects. For instance, we observed for the first time how multiple x-rays can gang-tackle molecules made of many atoms to liberate electrons that are strongly bound to atomic nuclei, a process called multiphoton absorption. The high photon density can also strip multiple electrons out of a single atom, molecules or solids, hollowing them out as described earlier, in a process known as sequential absorption. Bright x-rays can, in addition, rapidly break all the bonds in molecules that are expected to reside inside giant planets, including water, methane and ammonia. Measurements of matter in extreme conditions have helped determine the equation of state—the formula that governs the density, temperature and pressure—in cores of giant planets and during meteor impacts.

EXPLODING PROTEINS

THE SECOND LINE OF RESEARCH—exploiting the laser as an x-ray high-speed camera to image molecules and record movies of physical, chemical and biological dynamics—is filling in a serious gap in our knowledge. Researchers know distressingly little about the structure of many biological molecules—in particular, membrane proteins and large macromolecular complexes. The standard technique, crystallography, starts by growing a crystal that is large enough and perfect enough to diffract a beam of synchrotron x-rays. The resulting pattern reveals the structure of the molecule. The drawback is that x-rays readily damage the molecules they are probing. To compensate, researchers must prepare large crystals, yet many molecules of interest, including membrane proteins, are very difficult to crystallize. The synchrotron technique is also slow and thus unable to observe transient phenomena that occur on the femtosecond chemical timescale.

At first glance, the LCLS seems exactly the wrong tool for the job. Because it is billions of times more intense than synchrotron light sources, fragile materials such as proteins or noncrystalline systems cannot survive even one pulse of its x-rays before they explode and turn into a very hot soup of plasma. Ironically, that destructive intensity is just what we need. Because the pulse is so short and bright, it can capture an image faster than the molecule is able to blow up. Consequently, although the laser obliterates the sample, it captures a clear image of the molecule just before its demise.

This concept, called diffraction before destruction, is already beginning to pay off. Scientists have used femtosecond crystallography to record diffraction patterns of nanocrystals, proteins and viruses [*see box on pages 68 and 69*]. Recent work has mapped out the structure of proteins involved in sleeping sickness, a fatal disease caused by protozoan parasites.

Now that the LCLS has pioneered the technology, laboratories in Europe and Asia are also planning or building their own free-electron x-ray lasers. This new generation of machines will be more stable and provide better control of the beam. One particularly important goal is to make the x-ray pulses even shorter. With pulses as short as 0.1 femtosecond (100 attoseconds, or quintillionths of a second), we might begin to observe the motion not just of atoms but also of electrons within atoms and molecules. New devices could even allow us to control this motion. The dream of making movies showing how chemical bonds break and new ones form is within our reach. SA

MORE TO EXPLORE

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