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Lawrence Livermore National Laboratory
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Science & Technology REVIEW

November 1996

Lawrence
Livermore
National
Laboratory

Conflict Simulations

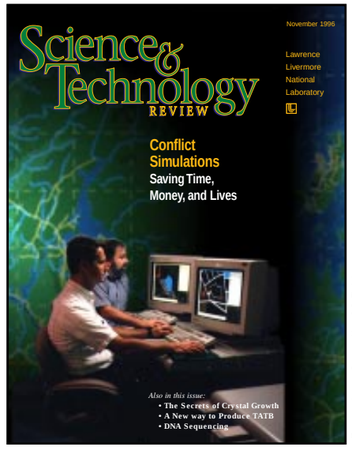
Saving Time, Money, and Lives

Also in this issue:

- **The Secrets of Crystal Growth**
- **A New way to Produce TATB**
- **DNA Sequencing**

About the Cover

Since the early 1970s, Lawrence Livermore scientists have been developing interactive computer programs to simulate conflict situations for military training and planning. Today, these highly complex simulation models are used not only for battlefield exercises but also for security purposes (such as planning the Presidential Inauguration), disaster relief, hostage rescues, and drug interdictions, to name but a few. Pictured on this month's cover are Hal Brand (foreground) and Gary Friedman working with the Joint Tactical Simulation model developed in the Laboratory's Conflict Simulation Laboratory. *S&TR*'s report on recent developments in computerized conflict simulation technology and their contributions to national safety and security begins on p. 4.



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About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. Science & Technology Review is published ten times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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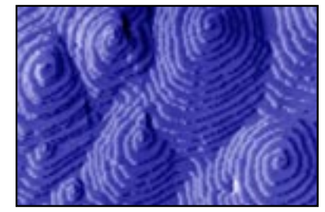

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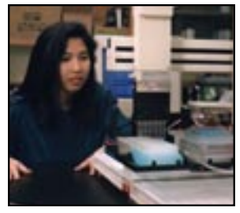

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Laboratory prepares for CTB implementation

The challenges of implementing the Comprehensive Test Ban Treaty will require major contributions from Lawrence Livermore and other Department of Energy Defense Program facilities, says Livermore Director Bruce Tarter.

In a statement following President Clinton's signing of the CTB Treaty at the United Nations on September 24, Tarter pointed out that the Laboratory takes "very seriously the importance of a successful Stockpile Stewardship Management Program to make certain that the nation's nuclear deterrent is safe, secure, and reliable." He also said Lawrence Livermore intends "to remain at the cutting edge in the enhancement of monitoring technologies in support of verification."

Observing that the scientific challenges are considerable, Tarter said "they will require us to apply a very wide range of technical skills to sustained, difficult, large-scale tasks important to all Americans. This is the sort of national effort at which Livermore has always excelled, the kind of bold program that defines us as a Laboratory."

Tarter noted that Lawrence Livermore personnel had spent "many thousands of hours"—at the Laboratory, in Washington, D.C., and in Geneva supporting efforts by the U.S. government to bring the CTB Treaty negotiations to completion. Said the Director: "Many key challenges during the negotiations were overcome with the help of experts and technologies from LLNL."

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Lab gets $6.2 million for environmental cleanup R&D

The Department of Energy awarded $6.2 million to the Laboratory during the summer under DOE's Environmental Management Science Program, designed for basic research that stimulates development of innovative environmental cleanup technologies. The $6.2 million funds five separate Lawrence Livermore projects:

- $1.6 million goes to an effort to use accelerator mass spectrometry to investigate the geochemical factors influencing the migration of radioactive elements through the soil.
- $1.3 million funds the development of computer codes for integrating various geophysical data, such as seismic or electromagnetic data, to produce as accurate a picture as possible of underground contamination.
- $1.2 million will be spent to develop techniques for tracking the motion and chemistry of contaminants as they flow downward to the watertable.
- $1 million is earmarked for a companion project to the above, aimed at developing electromagnetic imaging methods to diagnose contaminants beneath the earth.
- $1.1 million funds a study of the mechanism of movement of toxic metals found underground.

Lab recipients of the DOE funds anticipate that their projects will spawn new environmental research collaborations with other national laboratories and universities, as well as expand existing collaborations.

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Lab conference looks at peacekeeping technology

Policymakers, United Nations military commanders, and national laboratory scientists met at Lawrence Livermore recently to explore how technology could aid international peacekeeping operations. Of particular interest to military commanders and policymakers were mine removal, sensor, and antisniper technologies.

Titled "Meeting the Challenges of International Peace Operations: Assessing the Contributions of Technology," the two-day event in September was the inaugural conference for the Laboratory's Center for Global Security Research, established to better connect the Laboratory to the policy community.

Said Robert Andrews, the Laboratory's former associate director for Nonproliferation, Arms Control, and International Security, who led the effort to create the center: "Peacekeeping forces are used for many different purposes. The Laboratory can play an important role because of the technology we have here."

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Carrano elected VP of Human Genome Organization

Tony Carrano, the Laboratory's associate director for Biology and Biotechnology, has been elected vice president of the international Human Genome Organization (HUGO). As vice president, Carrano heads up America's branch of the organization, which represents North, Central, and South America.

Internationally, HUGO represents nearly 1,000 members from 50 countries who are involved in the global effort to map and sequence all of the human DNA. Carrano, director of the Laboratory's Human Genome Center, is one of 18 members of HUGO's international council.

The Laboratory has been involved in the Human Genome Project since 1986. In 1991, it received official designation as a Human Genome Center. Lab researchers focused much of their early work on mapping chromosome 19, which represents only 2% of the human DNA. Since early 1995, Lab researchers have broadened their scope to include the entire human genome. (See a related article beginning on p. 24 of this issue of *S&TR*.)

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(continued on page 28)

Countering Terrorism with Computers

IN an increasingly complex post–Cold War world, the challenge of countering terrorism against the public and military stands side by side with the need to maintain the security of thousands of nuclear weapons and fissile material parts. To meet this challenge, Lawrence Livermore and other national security laboratories are relying more and more on their computational power. Just as our nuclear weapon designers have turned increasingly to computers to ensure the safety and reliability of the nuclear stockpile, so our experts in nonproliferation and arms control are investing in computer simulation to respond to crises. Moreover, as described in the article on conflict simulation beginning on p. 4 of this issue of *Science & Technology Review*, they are able to respond *before* the crises happen, thus creating a better chance of prevention.

In fact, Livermore's Conflict Simulation Laboratory is developing a computer simulation to address an extremely important preventable crisis related to stockpile security—a program to help prevent the theft of nuclear weapons from U.S. or foreign stockpiles. Detailed simulations are being used to train security forces to deal with potential terrorist attacks.

A key advantage of computer simulations is that they provide "mini-exercises." Because they do not involve the time-consuming and cumbersome deployment of troops and equipment in the field, they are a cost-effective way to assess a wide range of "what-if" scenarios. They can provide realism and, if necessary, allow a scenario to be dissected and then rerun quickly to assess how different assumptions would affect the result.

In dealing with nonproliferation and arms control for over 25 years, the Laboratory has assembled in the Nonproliferation, Arms Control, and International Security (NAI) Directorate a broad range of programs to analyze intelligence information, respond to emergencies, design sensors to monitor treaties, support international negotiations, and evaluate weapon effects. These endeavors are all benefiting from the computer revolution. Intelligence analysts are challenged to digest huge amounts of information to find the elusive combination of evidence that would indicate a secret nuclear, biological, or chemical weapons project somewhere in the world. Emergency response experts have a similar data-sifting challenge in working with law enforcement authorities to separate real weapon-blackmail messages from hoaxes. In designing instruments to monitor suspect facilities and to detect intruders at weapon storage sites, our sensor designers are developing information systems with local processing to interpret simultaneous signals from nuclear, optical, magnetic, chemical, motion, and other sources; the system sends the analyses to a home base through global communication networks. And, as described in this issue's feature article, computer simulation of a battlefield requires numerous types of military equipment and soldiers in real-world deployments with dozens of characteristics such as location, speed, and fighting capabilities, as well as quantifying how each element degrades during the course of the battle.

Almost all of the Laboratory's directorates are involved in responding to the nation's new and highly complex nonproliferation and arms control challenges—countering both nuclear smuggling and nuclear, biological, and chemical weapon terrorism, while promoting international cooperation in protecting nuclear material. To perform these tasks in the future, Laboratory organizations will become increasingly reliant on our growing computational power and expertise. In particular, NAI will rely on increasingly powerful and sophisticated computerized conflict and crisis simulations to prevent weapons proliferation and terrorism before they happen and to counter them when they do.

■ Wayne Shotts is Associate Director of the Nonproliferation, Arms Control, and International Security (NAI) Directorate.

Simulations to Save Time, Money, and Lives

Simulating a battle, hostage rescue—or Presidential inauguration—on-screen before it happens saves time and money and may save lives.

INAUGURATION Day is fast approaching, and the Secret Service is planning the protection of the President. He will be taking the oath of office, speaking before a huge crowd, and walking or riding down wide streets lined with people. Planning such an event has always been a major undertaking, but it is complicated today by the growth of terrorist activities. The Secret Service must make many decisions—how large a security force to use, where individuals should be located, where temporary fences or other barricades should be constructed, the likeliest sources of sniper fire and other attacks, and to which nearby buildings should access be restricted.

In April 1996, the Secret Service contacted Lawrence Livermore National Laboratory's Conflict Simulation Laboratory asking to use their JTS (Joint Tactical Simulation) system for inaugural planning. By portraying various scenarios using JTS, the Secret Service can watch each scenario unfold on-screen and quickly analyze security tactics and options, rehearse the event so that there will be few surprises, and train its officers and other leaders to conduct the operation effectively.

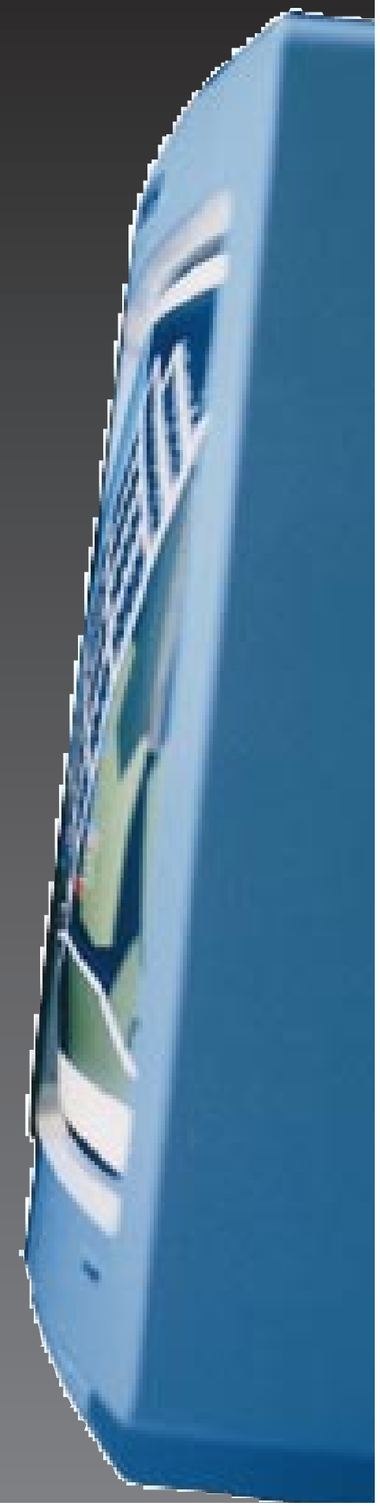
JTS and other computerized conflict simulation systems were originally designed for the military for battlefield exercises. After these programs became popular, organizations responsible for site security, disaster relief, and hostage rescues recognized their usefulness. More recently, state and local governments have become interested in using simulations to plan police raids, drug interdictions, fire fighting, crowd control, and prison riot control.

LLNL's Pioneering Work

Well into the 1970s, the principal tool for simulating battle and conducting "what-if" scenarios was the "sand table." This was a large surface dotted with tiny trees, rivers, and towns where model tanks, soldiers, and other accoutrements of battle could be deployed and moved about to simulate military maneuvers. Sand was often used to form the terrain, hence the term. But sand tables were an imperfect way to portray war games because they were an open system—both sides could see each other. Lines of sight were determined by running a piece of string between two points, and decisions about the outcome of a conflict were decided by tossing dice.

Livermore's involvement in combat simulation was born in 1973 when Laboratory scientists began studying the battlefield utility of recently developed tactical nuclear weapons. They needed something better than a sand table to graphically portray potential uses of these weapons and the ramifications of their use. Out of this need came Janus, a two-sided, interactive, conflict simulation program named for the Roman god of portals who had two faces to look in two directions at once. Written in FORTRAN and running on 16-bit computers, Janus was one of the first simulation programs to feature player input and output using an interactive graphical user interface. Scientists and battle planners finally had a realistic, digitized battlefield map with movable, changeable icons. (For reference, Janus was developed at about the time that "Pong," the first interactive computer game, became popular.)

An early version of Janus was transferred to the Army in 1983 while Livermore continued to refine it. In the mid-1980s, 32-bit microprocessors were adopted and the design was modified to support asynchronous operations, a more flexible programming system that allows a program to be interrupted and/or extended. Incorporating high-resolution graphics, distributed processing, and real-time play, Janus could be used for combat and tactical processes from the squad to brigade level. In 1991, the Army took over full responsibility for Janus.



On December 20, 1989, 20,000 U.S. troops invaded Panama and overthrew the dictatorship of General Manuel Noriega. Prior to the invasion, the U.S. Army used Janus as an operational planning tool. During a full day of simulations, it became clear that the planned placement of one platoon prior to the outbreak of hostilities caused a delay in arriving at a company's fire support position, so the platoon's position was changed. A later poll of battalion and company leaders revealed that the war games may have saved lives during the invasion and ensuing battle—a significant accomplishment for the first known use of a computerized, interactive, force-on-force war game prior to an actual battle.[1]

Why Use a Simulation?

The experience with the Panama invasion makes clear the benefit of conflict simulations prior to a battle. But multisided, interactive simulations allow fast, cost-effective planning, evaluation, and training for almost any endeavor that involves multiple persons or agencies working together for a common goal. Simulations can assist with resource allocation and scheduling, coordination in and between agencies, management decision-making, procurement planning, and tactics. Simulations of a conflict are also valuable tools for apprising staff and others of the current situation while the event is under way. Simulations of what actually occurred are also frequently used for after-the-fact analysis of an event.

For military training, simulations are particularly useful now because military organizations can afford fewer training hours and smaller expenditures during field exercises. As the military moves into nontraditional missions such as large-scale evacuations, peacekeeping, and famine relief, simulations help to train military leaders without a large investment.

These simulation programs are not intended to train individual soldiers or other participants in a conflict; rather, they train the mission leaders. By participating in different scenarios, leaders learn how to respond to a wide variety of situations.

The sides in a two-sided "game" are generally referred to as the Red Team and the Blue Team. This game is taking place in the facilities of the Conflict Simulation Laboratory at Lawrence Livermore.

JTS Is State of the Art

Livermore's Conflict Simulation Laboratory (CSL) was established in 1974 to develop simulation programs such as Janus. After Janus attracted the attention of the Army, the CSL was asked by several other organizations to expand upon Janus's capabilities.

For the Department of Energy, the CSL developed a system to evaluate the effectiveness of site security and to train security personnel. Over the next several years, various iterations of this system, for the U.S. Air Force Security Police Agency, the Berlin Brigade, and U.S. Army Europe, were created and ultimately merged in the single system known today as the Joint Tactical Simulation (JTS) model, which is being used by the Secret Service for inaugural planning. JTS simulates conflict in both urban and suburban environments and in building interiors.

JTS is constantly being updated to incorporate new features, and new versions of the system are released about every six months. The latest release was delivered in September 1996.

JTS can be applied to a battalion-level battle as well as to the defense of an individual building or site—in other words, JTS can be used to plan a large engagement or the rescue of a single hostage. The design is compatible with modern conflict simulation standards, including the Distributed Interactive Simulation protocol, that allow interaction with other simulations, human instrumentation systems, and a variety of vehicle and aircraft simulators.

JTS is used today by military and DOE organizations for security assessments of U.S. and NATO military bases and DOE sites. It is also used by the Army in Europe for large-scale combat modeling and leadership training. In advance of U.S. involvement in Somalia, the Army used JTS to analyze terrain at the Mogadishu

In the mid-1970s, a program developer at the Conflict Simulation Laboratory runs an early, very simple conflict simulation.

An early version of the Janus simulation program from the late 1970s used a graphics digitizer board.

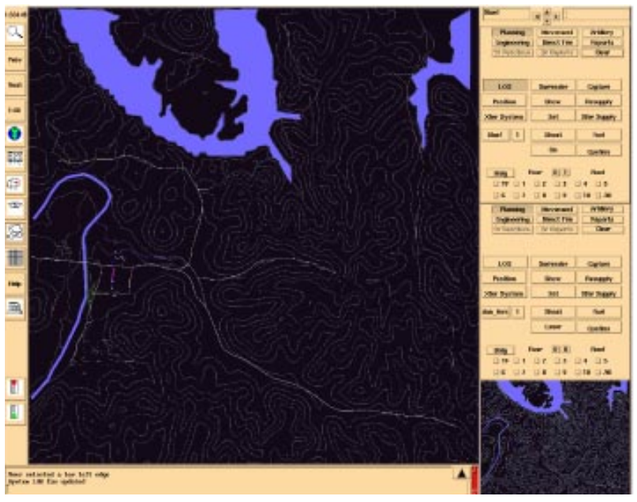
airport in order to select appropriate guard tower heights, identify the least vulnerable areas for civilian shelters, optimize sniper placement, and find the safest take-off and landing paths at the airport. In 1995, prior to our present involvement in Bosnia, the Army used JTS to run "what-if" scenarios for sending troops overland to Sarajevo from the sea. They identified bottlenecks in the mountainous terrain and simulated probable ambush locations.

JTS is an entity-level simulation, which means that it explicitly models an individual howitzer, plane, ship, or soldier. It can handle force sizes from 2 entities to 2,000.

JTS is one of the few programs to simulate night and adverse weather operations, with area lights and spotlights that can be turned on and off as needs require. Terrain features such as buildings, roads, rivers, fences, and vegetation can be modeled down to the nearest 10 centimeters. Underwater obstacles and river currents can also be modeled.

JTS is also rare in that it addresses direct-fire fratricide, the killing of friendly forces by directly firing on them, usually with small weapons. (This contrasts with indirect-fire fratricide, which occurs when large-weapons fire is aimed at an area about which the shooter has minimal information. Many simulation models address indirect-fire fratricide.) Even with the best of information about where enemy and friendly forces are located, direct-fire fratricide does happen in the confusion of battle. But it has traditionally been difficult to model because of its sensitivity and lack of available data. With JTS, the user may establish how and where direct-fire fratricide might occur through a simulation.

A strategic planning exercise in Central America coordinated by the U.S. Southern Command involved soldiers from several countries. They are shown using the Joint Conflict Model (JCM) developed at Lawrence Livermore. (For more information on JCM, see "Modern Technology for Advanced Military Training," *Energy & Technology Review*, UCRL-52000-95-3 [March 1995], pp. 22–24.)



A 10-square-kilometer view using the Joint Tactical Simulation (JTS), Livermore's most recent contribution to advanced conflict simulation modeling.

Using JTS

A JTS simulation session might involve as few as 2 terminals or as many as 40, each viewing a different part of a battlefield. There can be as many as ten sides represented in the conflict simulation, each represented by a set of workstations networked together. A conflict is usually thought of as having two sides, but civilians and other players may be treated as one or more neutral sides.

The JTS system database stores extremely detailed information on every facet of a conflict—weapons, munitions, sensors, groups of soldiers, types of missions, observers, vehicles, security systems, and others. For example, the database stores approximately 150 pieces of data on a typical engineering squad, including the time it takes the squad to get into and out of trucks, the types and numbers of weapons available to the squad, and the time it takes the squad to dig foxholes, penetrate wire barriers and rubble, and perform other engineering tasks. User organizations construct this huge database, and they may add and modify information as needed.

For a particular simulation, its planners select appropriate people, weapons, vehicles, etc., from this database. For analysis of security at an embassy, the numbers selected might be relatively small. Operational planning before the Panama invasion would have required the database to include thousands of soldiers in various configurations, as well as large numbers and many types of weapons, munitions, vehicles, tanks, helicopters, planes, and the like.

Before the start of a battle scenario, planners decide the parameters: they decide the location, the weather, the local civilian situation, when and how the battle will begin, and the makeup of the various sides; they select initial routes and speeds for vehicles and people; they determine where, when, and what kind of reinforcements will be dropped off. An almost infinite number of variations are possible. Later, when the scenario is being played out, these variables may be changed as requirements demand.

JTS allows for a simulation area as large as 6 degrees of latitude and longitude, the equivalent of 660 by 660 kilometers. Any user may view the entire playing field during a scenario, although each player can only view forces that have been acquired by the assets he or she controls. A high-level mission leader may choose to view the entire playing field, while a lower level player responsible for maneuvering specific forces will likely zoom in for a more detailed view of a smaller area.

The workstation screens show such features as topography, vegetation, built-up areas, roads, rivers, ocean depths, building floor plans. Vegetation appears on the screen in various colors,

(a)

(b)

Two views of an Air Force weapons storage facility using JTS. (a) A 1-square-kilometer view of the entire facility. Terrorists attacking the base are shown in red, and the blue figures are the defending Air Force Security Police. (b) Kim Lohman works with a view of just part of the facility showing lines of sight for one of the terrorists.

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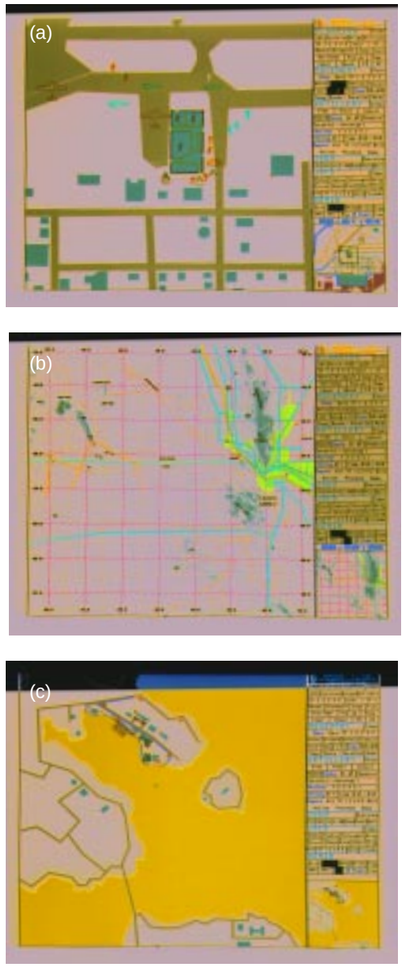


Several applications of the Security Exercise Evaluation System, a precursor to JTS, are shown: (a) an airport security exercise, (b) a drug interdiction training exercise, and (c) a harbor protection exercise involving both the Navy and the Coast Guard.

differentiated not by type but by penetrability, visibility, and ease of movement, which are what matter to a person or vehicle trying to move around on the ground or to a plane flying overhead trying to see those people and vehicles.

Lines of sight are constantly being determined as soldiers and vehicles move on and over the terrain. As an aircraft or other vehicle moves over long distances or comes into the area of another friendly player's forces, its tactical control may be transferred from one terminal to another. Intelligence reports pass back and forth between terminals by telephone or other real-world communications media as users report that an enemy tank unit has appeared or that a company in their area is being fired upon.

In a small-scale simulation (of a hostage rescue, for example), the locale might be a city with low-rise and high-rise areas; an airport; a river; many narrow, winding streets; and numerous bridges, in addition to an unfriendly civilian population. During the scenario, a user might zoom in on a multistory building and see individual soldiers and civilians moving around inside it.

JCATS Innovations

The Conflict Simulation Laboratory is currently developing for the Joint Chiefs of Staff a new, more broadly useful simulation system known as the Joint Conflict and Tactical Simulation (JCATS). More detailed than JTS, JCATS increases the number of entities that can be handled in a simulation from 2,000 to 60,000. The first version of JCATS is due to be released in 1997.

JCATS will incorporate a unique experimental feature that allows a user to "aggregate" entities into a group to be moved, viewed, and controlled as one icon and then "deaggregate" the group back to the entity level for detailed operations. A user will thus be able to manage a large number of entities on the battlefield and play a very detailed, high-resolution game in specific areas without high-end computers or large numbers of players.

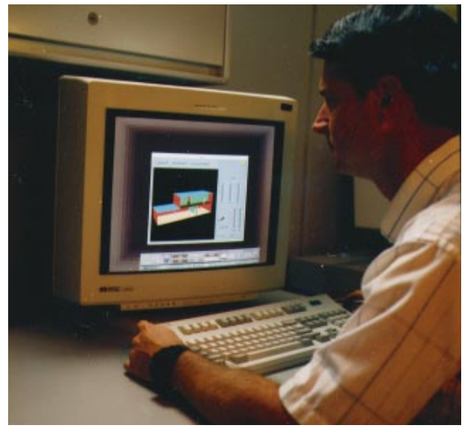
This aggregation/deaggregation feature will help to control the cost of training exercises, but it is requiring the CSL to meet a major challenge. When a unit has been aggregated to include a variety of unlike entities such as riflemen, scouts, tanks, trucks, and other vehicles, how does the unit behave? The aggregated unit "inherits" some behaviors from its component parts, but other behaviors change when individuals become part of a group. For example, the group moves at the speed of the slowest individual, and there is little truly independent behavior in a group. These and other changes in behavior are being considered when defining aggregated unit behavior.

JCATS simulations include more realistic graphics, especially for visualizing activity inside a multistory building or on complex terrain. Users will get a three-dimensional look at activity inside a building without significantly slowing down computer processing.

JCATS will be the only entity-level model to show detailed, high-resolution amphibious operations and other aspects of sea-coast warfare, a particularly useful feature for the U.S. Marine Corps and the Navy.

Another unique feature will be the establishment of a "matrix of relationships" among the various players in a simulation. In a multisided conflict, there can be friends, enemies, and neutral players. A group of "friends" may form a coalition and function as a single "side." But at some point during a simulation, the coalition may break down, causing a former friend to become a neutral player or even an enemy. There may also be guerrilla troops who are on one side during part of the scenario and then defect to another side. JCATS will be able to accommodate these fluid relationships.

Military personnel will be able to use JCATS as a training tool while working at their own real-world equipment rather than at a computer terminal. For example, simulation data will be fed into shipboard equipment, and sailors and officers will respond to it as though it were the real thing. While JTS and other programs have been used in conjunction with vehicle and flight simulators, this use of a simulation program with real equipment will be a first.



Hal Brand uses the experimental three-dimensional building editor for the Conflict Simulation Laboratory's newest program, the Joint Conflict and Tactical Simulation (JCATS). This program is under development and due for release in 1997.

Future Work for the CSL

Livermore's Conflict Simulation Laboratory now has over 20 years of experience in developing and deploying systems such as JTS and JCATS, working closely with the relevant branches of the military during all phases of each project. Upon its release next year, JCATS will be the cornerstone of the Joint Chiefs of Staff's battalion, brigade, and lower-level training programs until the Joint Chiefs bring the Joint Simulation System (JSIMS) on line in 2003. Lawrence Livermore will likely be a technical advisor for the development of JSIMS.

The CSL has already begun working on additions to JCATS that will appear in later versions of the model. In particular, the CSL aims to fill a major gap in modern conflict models, which is that none accurately models the impacts of information warfare. The capability to handle information warfare attacks is a significant challenge because communications and control systems are currently implicit in simulation programs and assumed to be perfect. This new modeling capability will include an interface with operational command, control, computers, communications, and intelligence (C4I) systems. Other changes will include increasing the size of simulated scenarios and adding an ability to develop a software architecture in the future to take advantage of new computer networking and computing technologies as they arise.

After its release, JCATS will be used as a test bed for JSIMS concepts and will be integrated into the JSIMS architecture. Through these activities, the CSL staff will continue to stay in the forefront of conflict simulation technology.

Key Words: conflict simulation, Janus, Joint Conflict and Tactical Simulation (JCATS), Joint Tactical Simulation (JTS).

Reference

1. *Evaluating the Use of Janus as an Operational Planning Tool in Operation Just Cause*, The Titan Corporation, Olympia, Washington, June 1991. (Subcontract B098749).

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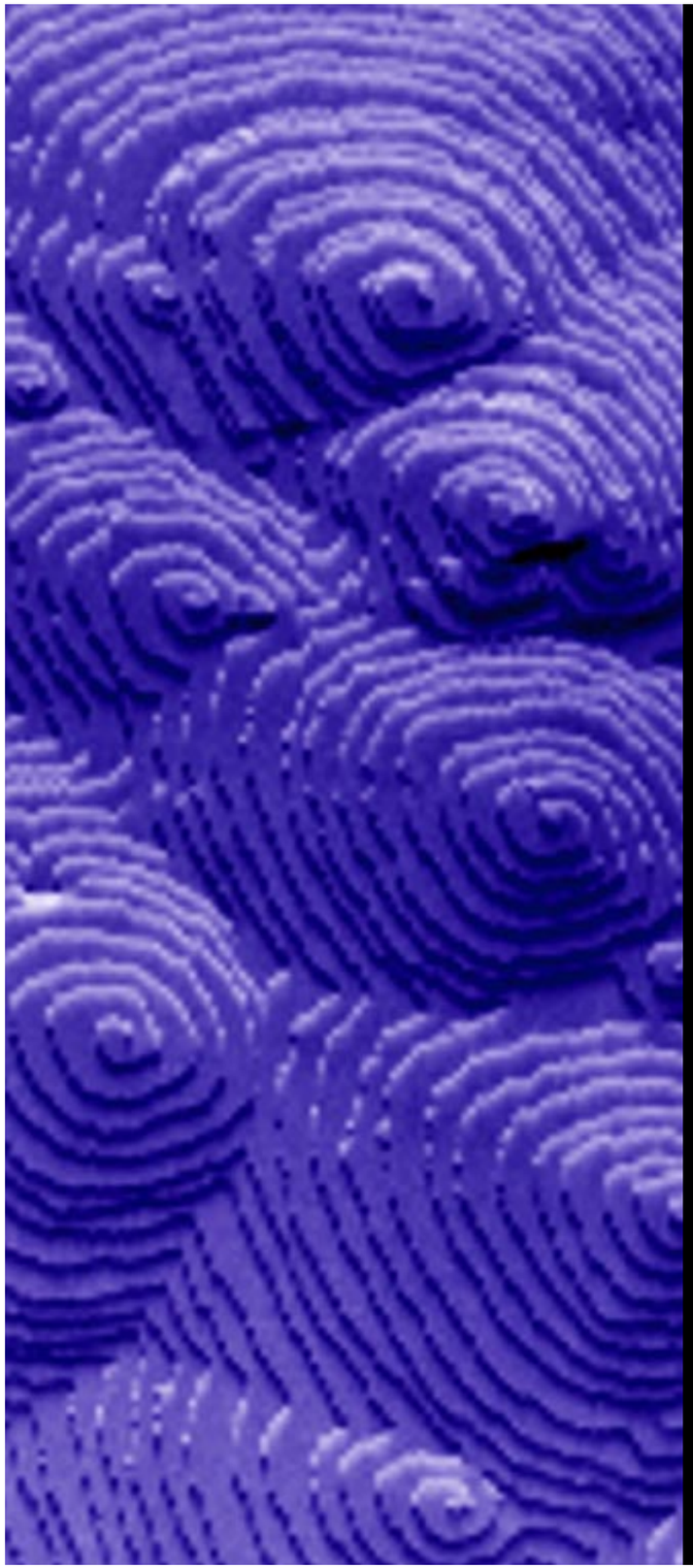
About the Scientist

DIANA E. SACKETT joined the Laboratory as a computer scientist in 1975 after having received a B.S. in mathematics from Occidental College in 1974 and an M.S. in mathematics from Stanford in 1975. She has worked on a variety of scientific and engineering computing projects since coming to Lawrence Livermore. She is currently the Associate Division Leader for Modeling and Simulation in D Division and is head of the Conflict Simulation Laboratory.



The Secrets of Crystal Growth

Using the powerful atomic-force microscope, Laboratory researchers are discovering the complex growth mechanisms and three-dimensional structures of solution-based crystals. The results portend a new generation of products, ranging from life-saving pharmaceuticals to new manmade materials.

THE crystallized forms of a world of materials—from viruses to semiconductors—hold the secrets to their shapes and functions. With the advent of the powerful atomic-force microscope (AFM), Lawrence Livermore researchers have begun elucidating the growth mechanisms and three-dimensional structures of widely different solution-based crystals on the nanometer (billionth-of-a-meter) scale.

The detailed images reveal, in unprecedented clarity, the complex world of crystal growth, including mechanisms never before seen or even postulated. The results portend a new generation of products, ranging from life-saving pharmaceuticals to new optical materials.

Leading the Lawrence Livermore effort to unravel the mysteries of crystal growth are physicist James De Yoreo and his crystal development team in the Laboratory's Chemistry and Materials Science and Laser Programs Directorates. De Yoreo and his colleagues received an R&D 100 Award in 1994 for developing a process that produces very high quality KDP (potassium dihydrogen phosphate) crystals for inertial confinement fusion lasers.[1] Using this process, which is dramatically faster than traditional methods, they announced in May 1996 that their process had, in only 27 days, produced a KDP crystal measuring 44 centimeters across. Under standard growing conditions, such an accomplishment would have taken up to 15 months.

In 1994, De Yoreo and his colleague Terry Land began using one of the seven AFMs on the Livermore site to explore the growth mechanisms of crystals in a way never before possible. "The AFM has given us the opportunity to study at the nanometer level the physics of crystal growth and how it is affected by impurities, defects, and solution conditions," according to De Yoreo. (See the box, p. 14, for a description of the three-dimensional, atomic-level resolving power of the AFM and the box, p. 15, for a discussion of how crystals grow.)

Research with the AFM is a vital element of LLNL's longstanding crystal growth and characterization effort, born out of the Laser Programs' requirement for large, ultrapure crystals grown from tiny seeds. This work is also part of a much larger Laboratory program to characterize materials on the atomic level, recognized by several R&D 100 Awards to LLNL researchers in the area of nanotechnology. This research offers significant potential payoffs to virtually every major program at Livermore.

Avenues of Research

Much of the crystal development team's AFM work has centered on the need to better understand KDP crystal growth because of its direct impact on the National Ignition Facility (NIF), a planned laser facility essential for the Department of Energy's Stockpile Stewardship and Management Program. High-power lasers like the Laboratory's Nova laser use KDP crystals for optical switching and frequency conversion of the initial infrared light to ultraviolet light. Some 600 plates of KDP approximately 40 centimeters in diameter and 1 centimeter thick will be employed in the forthcoming NIF.[2]

How the AFM Works

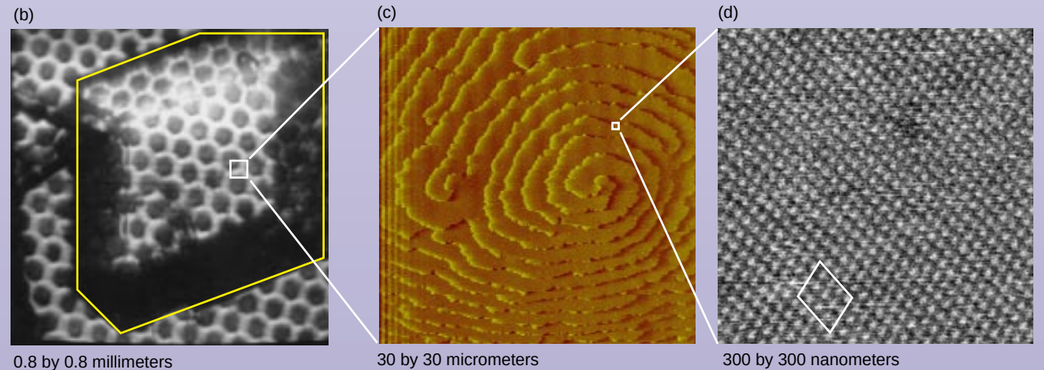
Lawrence Livermore researchers probing the dynamics of crystal growth use an atomic-force microscope (AFM), a recent descendant of the scanning tunneling microscope (STM). Developed in 1981, the STM has become so important to materials scientists that its inventors were awarded the Nobel Prize in Physics in 1986. In 1987, a Lawrence Livermore–Lawrence Berkeley team used the STM to create the first images ever produced of native DNA.*

Many researchers have turned to the AFM, an instrument ideally suited to imaging nonconductive samples such as crystals in solution. The AFM is similar to the STM in that both instruments use an extremely sharp tip to sense the atomic shape of a sample as well as a computer to record the path of the tip and slowly build up a three-dimensional image. The only difference between the two is that the STM electron tunneling tip is replaced by a mechanical tip, and the detection of the STM's minute tunneling current is replaced by the detection of the minute deflection of the AFM's cantilever.

In practice, the AFM tip is positioned at the end of an extremely thin cantilever beam and "touches" the sample with a force of only one ten-millionth of a gram, too weak to budge even one atom. As the tip is repelled or attracted to the sample surface, the cantilever beam deflects. A laser shining on the very end of the cantilever captures the magnitude of the deflection. The sample is oscillating left to right and front to back, and a plot of the laser deflection versus sample position provides the resolution of the peaks and depressions that constitute the topography of the surface. Images take only 20 to 30 seconds to complete.

Just as with a light microscope, researchers can vary the level of magnification of an STM or AFM image. The greater the movement of the sample, the larger the area being imaged. The broad magnifying range is shown below. Here a crystal of the plant protein canavalin is seen in its entirety, then further enlarged to a 30- by 30-micrometer close-up of a growth mound, and then enlarged still further to reveal its three-dimensional molecular lattice.

The AFM can be adapted to sense a range of forces including attractive or repulsive, interatomic, electrostatic, and magnetic forces. This ability allows the AFM to be used on insulating surfaces and in liquids, feats the STM cannot do. Thus, the instrument is ideal for following the dynamics of solution-based crystal growth.



(a) The atomic-force microscope reveals, in ever-increasing magnification (b through d), the complexity of solution-based crystals. In (b) a canavalin protein crystal (within the yellow box) is shown on top of a hexagonal grid. (c) shows growth sources on the crystal's face. Each step is one molecule in height. In (d) the rhombohedral structure of the underlying lattice, outlined by the solid box, defines the macroscopic rhombohedral form seen in (a).

* "Scanning Tunneling Microscopy: Opening a New Era of Materials Engineering," *Science & Technology Review*, UCRL-52000-95-8 (August 1995), pp. 4–11.

The crystal team's research has also focused on the growth of solution-based crystals of biological macromolecules such as proteins and viruses. Slow growth rates, large diameters, and great complexity in composition, structure, and surface make biological macromolecular crystals ideal systems to study with the AFM. The team reasoned that the images might reveal entirely new growth mechanisms not seen in inorganic crystals.

An enhanced understanding of crystal growth of biological macromolecules is likely to advance rational drug design, the technique of using powerful computers to literally design, in three dimensions, molecules that will precisely bind to key sites on proteins and enzymes to trigger or block a biochemical action. Designing new drugs in this fashion is dependent upon using x-ray diffraction to reveal the three-dimensional structure of complex macromolecules. In this technique an x-ray beam is scattered by a crystal of the material of interest, a diffraction pattern is recorded, and the data are transformed into a three-dimensional structure by computer.

However, this technique has been limited by problems encountered in obtaining high-quality crystals large enough to yield precise structural information. In fact, crystallization has become the rate-limiting step in most structure analyses because little is known of the growth mechanisms of the crystals and the orientation and bonding of the molecules in the crystalline lattice. Even less is understood about the role of defects either as a promoter or a limiting factor in crystal growth. Using the AFM to study crystal growth is sure to improve the quality of x-ray diffractions and, hence, help hasten the arrival of new pharmaceuticals.

Biomineralization Revolution

In a similar light, the knowledge gained by the research team will advance the understanding of biomineralization, a process used by a wide variety of organisms from bacteria to humans to synthesize inorganic complexes such as bones, shells, teeth, and even magnetic material. These inorganic complexes are true "nanostructured" composite materials and their physical properties are often superior to manmade materials.

"Biomineralization research represents a revolution in materials processing," De Yoreo says. Understanding the process, however, again requires the ability to investigate crystal growth at nanometer scale.

Most researchers have studied the growth of crystal surfaces by molecular beam epitaxy or chemical vapor deposition, two processes used in the electronics industry. However, these processes are not representative of the liquid environments in which most crystals are grown. Such environments are characterized by varying levels of supersaturation (the driving force of crystal growth studies), where, because

How Crystals Grow—A Short Primer

Watching crystals grow with an atomic-force microscope reveals a frantic world of molecules continually bonding and dissolving, attaching occasionally to the surface of a large crystal seed in one of many ways, and then perhaps joining together as part of a growing structure of spiraling mounds, spreading layers, and small islands.

In the simplest form of crystal growth, molecules land on the surface of a growing seed and become weakly adsorbed. They may join together to form small, two-dimensional islands and spread outward in a layer (called a "step") one molecule thick, with other islands forming and growing on top. In this dynamic growth process, molecules continually adsorb and dissolve from islands.

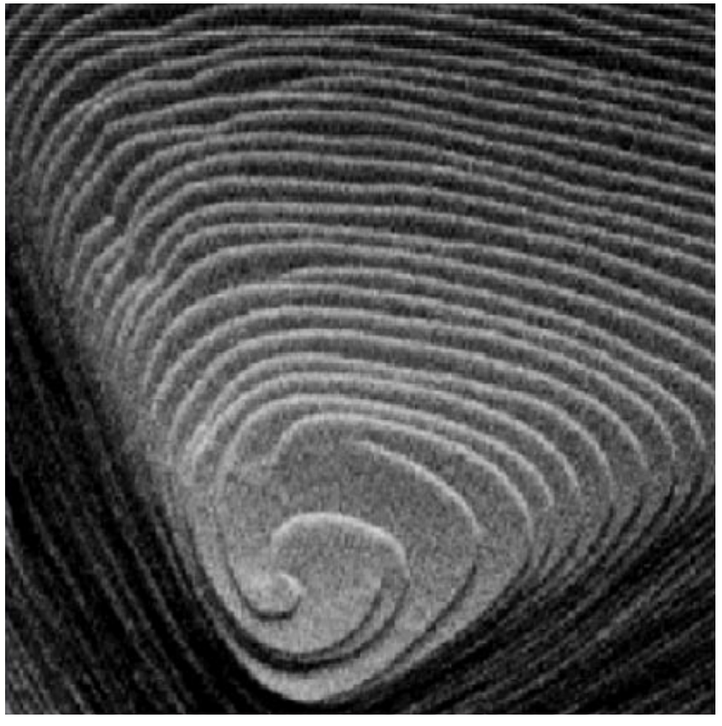
As the step edges advance, single molecules may diffuse from islands in the vicinity of the outer edge of a step or from solution and be "captured" by that edge. In this way the edge acts as a "sink" to diffusing molecules. It should be remembered, however, that molecules have complex shapes that prevent them from bonding in every orientation. For example, a molecule may have to diffuse to the edge of a step many times until it has the correct orientation for incorporation.

Continuous spiraling steps are formed by screw dislocations, actual breaks in the crystal's structure often caused by impurities or from the applied stress of two blocks of crystals that meet up and do not match. Such "screw" dislocations create spiraling, multilayered mounds called vicinal hillocks.

Two other growth phenomena are easily seen with the AFM. The first, three-dimensional growth, consists of small clusters of molecules falling out of solution onto the surface of a growing crystal face, meshing perfectly with the underlying structure. The second consists of the incorporation of sizable "microcrystals" that fall onto the growing crystal surface and create misaligned lattices.

In the dynamic world of crystal growth, all of the growth features described above may occur simultaneously. Which growth processes predominate are determined by the size and shape of the molecule, the physical properties of the material, supersaturation levels, pH, the kind and quantities of impurities present in solution, and defects that may form in the crystal's structure.

Figure 1. At low supersaturation levels, many crystals grow on dislocations (formed by stress inside the crystal lattice) that produce spiraling mounds called vicinal hillocks. Vicinal hillocks on a crystal of KDP (potassium dihydrogen phosphate) are shown here.



8 by 8 micrometers

of increased temperature and pressure, most molecules are dissolved beyond the saturation point and then permitted to precipitate out of solution onto the seed crystal.

Given the dearth of research in high-resolution, solution-based crystal growth, some basic questions need to be answered: What are the dominant growth mechanisms and how do they vary with different supersaturation levels? What are the kinetic factors that control the rate at which crystals grow? And how do impurities and defects affect growth?

To answer those questions, De Yoreo and Land at Livermore and Alex Malkin and Yuri Kuznetsov from the University of California at Riverside have been using AFMs to examine in unprecedented detail the growth of crystals of the plant protein canavalin, the satellite tobacco mosaic virus (STMV), and KDP. Their experiments involve growing the crystals under supersaturated conditions until about 3 to 5 seed crystals in a volume of 3 microliters are produced. The crystals are then transferred to the 50-microliter fluid cell of an AFM. As the crystals grow, supersaturation levels and pH are varied and dozens of images recorded.

Prized Protein Images

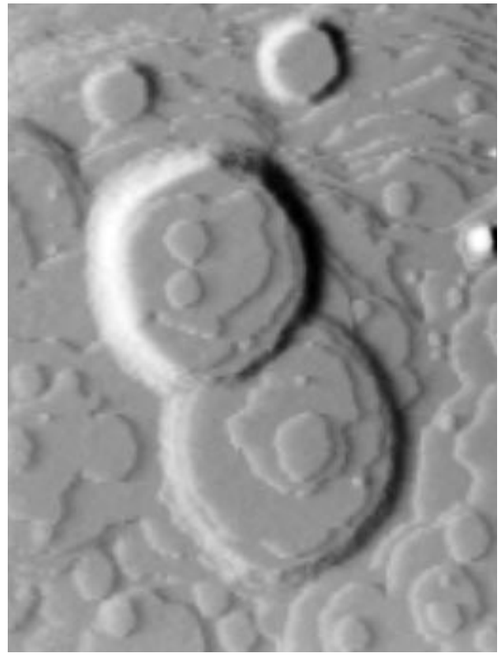
The macromolecule canavalin, the storage protein of the jack bean, was chosen for study because the UC Riverside collaborators know its structure well and can prepare very pure solutions of its crystallizable form. The AFM images (Figure 1 and those on p. 12) show that at low supersaturated levels, the crystals grow by formation of dislocations (formed by stress inside the crystal lattice) and simple diffusion of single canavalin molecules onto the growing spiral layers caused by the dislocations. (See the box on p. 15 for a general discussion of how crystals grow.) The dislocations produce polygonal spiral mounds called vicinal hillocks that appear in several variations: simple hillocks with individual dislocation sources one or two layers high, complex ones with many interacting dislocations, and left- or right-handed hillocks.

As supersaturation increases, two-dimensional growth sets in, seen in the appearance of small islands rising from the surface (Figure 2). At the highest supersaturation levels, another growth source, first discovered at Livermore during STMV studies, is seen: the adsorption of small, three-dimensional

clusters containing 50 to 500 molecules. The most remarkable feature of this so-called three-dimensional growth is that upon adsorption, the molecular clusters reorient so that the cluster lattice merges with the lattice of the larger crystal to which they adsorb, without creating defects or discontinuities. The multilayer islands in Figure 2 are examples of such clusters.

At very high magnification, the images show that the crystal surface supports a dynamic population of small clusters (25 to 50 nanometer in diameter) of 7 to 30 canavalin molecules. While some of the smaller clusters adsorb onto the surface but then dissolve rapidly, others are stable and are incorporated into the advancing steps (or layers) formed by the dislocations.

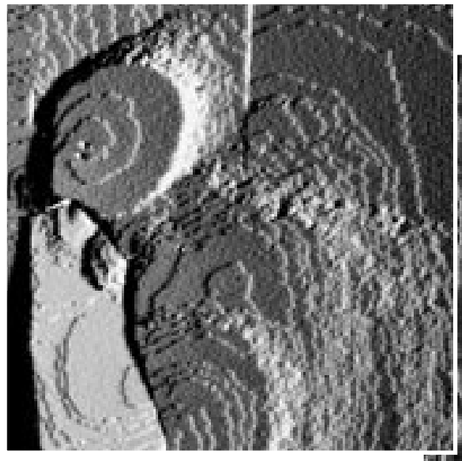
At typical supersaturation levels used in protein crystal growth, a new defect generation mechanism, never before reported, was discovered: the incorporation of sizable "microcrystals" much larger than the clusters (Figure 3). When these microcrystals fall onto the



33 by 58 micrometers

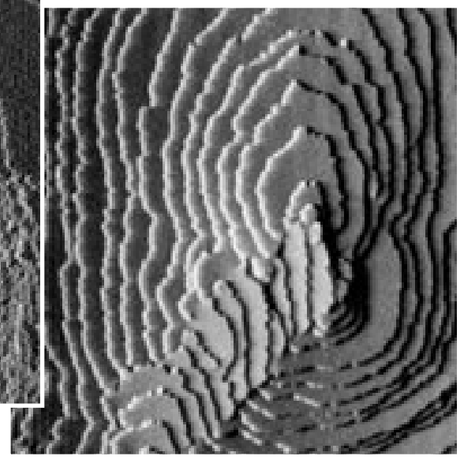
Figure 2. As supersaturation increases, two-dimensional growth of canavalin crystals sets in, seen in the appearance of small islands rising from the surface.

(a)



50 by 50 micrometers

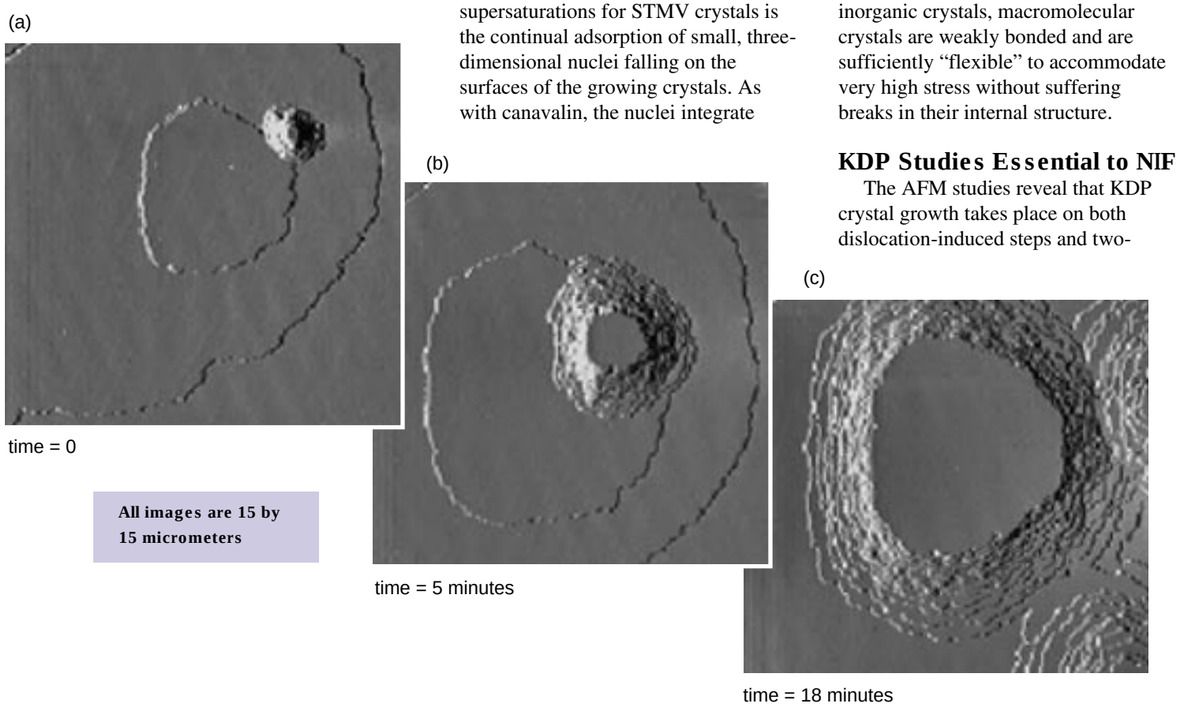
(b)



27 by 27 micrometers

Figure 3. At high supersaturation levels, microcrystals fall onto the growing surface of canavalin crystals and are incorporated into the main crystal, resulting in misaligned and distorted lattices. Shown are (a) crystal being incorporated and (b) defect remaining after incorporation.

Figure 4. (a) Once adsorbed, three-dimensional nuclei grow by (b) lateral spreading and formation of two-dimensional islands on their faces. (c) These islands coalesce in the formation of "stacks" consisting of a few to tens of layers projected above the larger crystal surface.



growing crystal surface, they result in misaligned and distorted lattices. Such defects should significantly impair the ability of crystallographers to resolve molecular structure through x-ray diffraction techniques.

Viruses Prove Good Models

Because of their relatively large size, near-spherical shapes, and simple packing geometries, viruses provide especially good models for investigation of macromolecular crystallization. The research team used an AFM to conduct the first nanometer-scale crystal growth study of STMV. The virus was chosen because past studies have determined its structure and have shown it to be easily crystallized under a wide range of conditions.

The AFM images reveal that the dominant growth mechanism at all supersaturations for STMV crystals is the continual adsorption of small, three-dimensional nuclei falling on the surfaces of the growing crystals. As with canavalin, the nuclei integrate remarkably well with the underlying structure. Livermore crystal researchers believe that this integration suggests that the underlying lattice either "guides" the adsorbing nuclei into preferred orientations as they arrive or that subsequent reorientation by diffusion ultimately produces the correct alignment.

Once adsorbed, the three-dimensional nuclei spread laterally and are accompanied by the formation of two-dimensional islands on their tops. These islands coalesce in the formation of "stacks" consisting of a few to tens of layers projected above the larger crystal surface. Such stacks serve as the growth centers for the entire crystal (Figure 4).

No screw dislocations are observed on STMV crystals during their growth. De Yoreo conjectures that no dislocations occur because, unlike inorganic crystals, macromolecular crystals are weakly bonded and are sufficiently "flexible" to accommodate very high stress without suffering breaks in their internal structure.

KDP Studies Essential to NIF

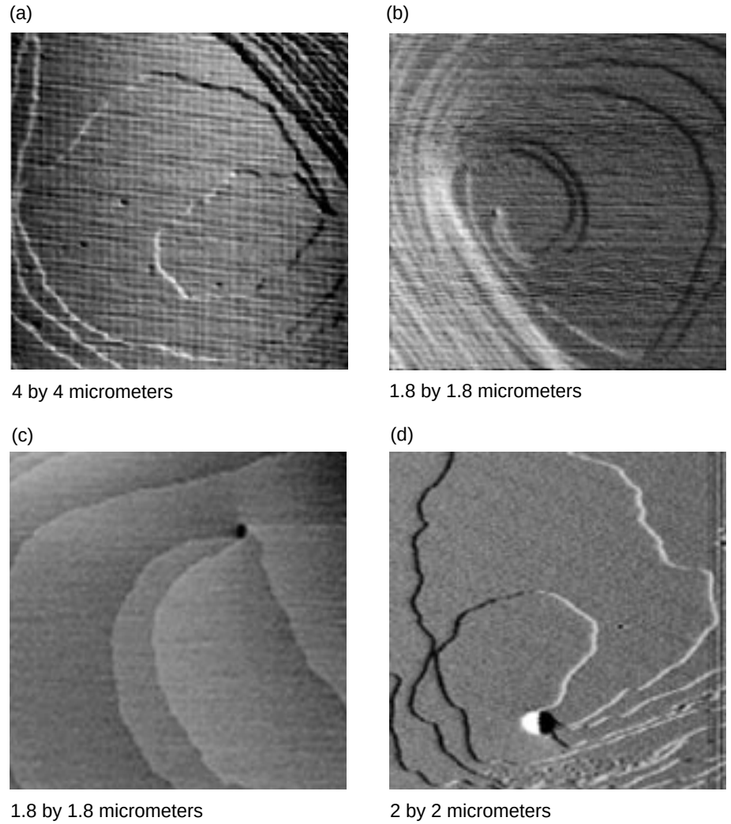
The AFM studies reveal that KDP crystal growth takes place on both dislocation-induced steps and two-dimensional islands. In addition, numerous two-dimensional islands appear on the "terraces" (spaces between layers) formed by dislocations. As with canavalin, the dislocations are caused by stresses in the crystal's "stiff" lattice and produce growth hillocks whose triangular shapes reflect the crystal symmetry (Figure 1). However, because the KDP lattice is much stiffer, the region near the dislocations is highly stressed and unstable. As a result, it exhibits hollow channels full of solution at the dislocation cores (Figure 5). These hollow cores (1 to 50 nanometers in diameter) are a result of stresses near the dislocations. Using the AFM to investigate the details of the dislocation structure has allowed Livermore researchers to show for the first time that core radii are one of the primary determining factors in hillock size and growth rate.

The diffusion and incorporation kinetics of single KDP molecules is 1,000 times faster than seen in canavalin; indeed, typical KDP growth rates—about 100 molecular layers per second—make it impossible to access a wide range of experimental conditions. The crystal research team believes that the disparity in growth rates occurs either because KDP is much smaller and therefore more mobile than canavalin or because KDP molecules have a higher probability of having the proper molecular orientation for direct incorporation into the crystal, as opposed to more geometrically complex biological macromolecules.

First-ever images also show how impurities cause growing layers to exhibit discontinuous motion because they become "pinned." In a dynamic, repeating process, steps encounter impurities, seemingly stop, then grow around the impurities, and once again encounter other impurities. One series of images shows how an adsorbed particle (impurity) is displaced upward as growing steps move through it.

The Laboratory's crystal development team plans additional experiments with various concentrations of known impurities to further understand how they are incorporated in the KDP crystal and how they influence growth. Such experiments are important because despite dramatic gains in growth speed and quality, the number of defects in KDP crystals caused by impurities is still unacceptably high for laser scientists planning the optical systems of NIF. When an intense laser beam strikes a defect in the KDP crystal,

Figure 5. Stresses in the KDP crystal's "stiff" lattice produce growth hillocks with hollow channels full of solution. The size of the channel increases rapidly with the size of the dislocation from (a) one step where no core is observable to (b) two, (c) three, and (d) four steps.



tiny cracks appear in the crystal that grow with each laser shot. Eventually the damage significantly disrupts the laser beam quality by distorting the laser light and reducing its energy.

Future areas of study also include growing several crystallized proteins, among them human insulin, whose use depends on a better understanding of how they grow and dissolve in solution. The crystal development team is also planning to study biomineralization in more detail, in particular the growth characteristics of the essential calcium carbonate mineral that forms the skeletal tissue of most organisms. The study should shed light on how living organisms produce crystalline materials, thereby pointing the way for new, nanostructured materials for industry.

By understanding and then controlling the crystallization process at the molecular level, complex microstructures can be synthesized that will affect many disciplines and technologies, says De Yoreo. "There's a revolution on the horizon in materials and materials processing, but to get there we need to acquire the scientific underpinnings of crystal growth," he says. Thanks to the AFM, that day is rapidly approaching.

Key Words: atomic-force microscope (AFM), protein crystallography, crystals, KDP (potassium dihydrogen phosphate), National Ignition Facility (NIF), scanning tunneling microscope (STM), stockpile stewardship.

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1. "Growing High-Quality KDP Crystals Quickly," *Energy & Technology Review*, UCRL-52000-94-11 (November 1994), pp. 3–5.
2. The December 1994 issue of *Energy & Technology Review*, UCRL-52000-94-12, is dedicated to a complete description of NIF and its planned uses.

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About the Scientists

JAMES DE YOREO joined Lawrence Livermore National Laboratory in 1989 as a physicist in the Chemistry and Materials Science Directorate. He received his B.S. from Colby College and his M.S. and Ph.D. from Cornell University. He is currently the leader of the Laboratory's crystal development team and has done extensive research in crystal growth physics and applications. In 1994, he shared an R&D 100 Award for the development of a rapid growth process for KDP (potassium dihydrogen phosphate) laser crystals with colleagues at the Laboratory and at Moscow State University in Russia. He has written numerous articles on organic and inorganic crystal growth and is co-holder of one existing and one pending U.S. patent related to crystal growth.

TERRY LAND received both her B.S. in chemistry (1988) and her Ph.D. in physical chemistry (1992) from the University of California, Irvine. She joined the Laboratory's Chemistry and Materials Science Directorate in 1992. Her primary area of academic and professional research has been the fundamental growth mechanisms of solution-grown inorganic and macromolecular biological crystals using advanced techniques such as scanning tunneling and atomic-force microscopy. She has co-written over 20 scholarly articles and has been a presenter and invited speaker at meetings and conferences in the U.S. and Europe on the mechanisms and techniques of crystal growth.

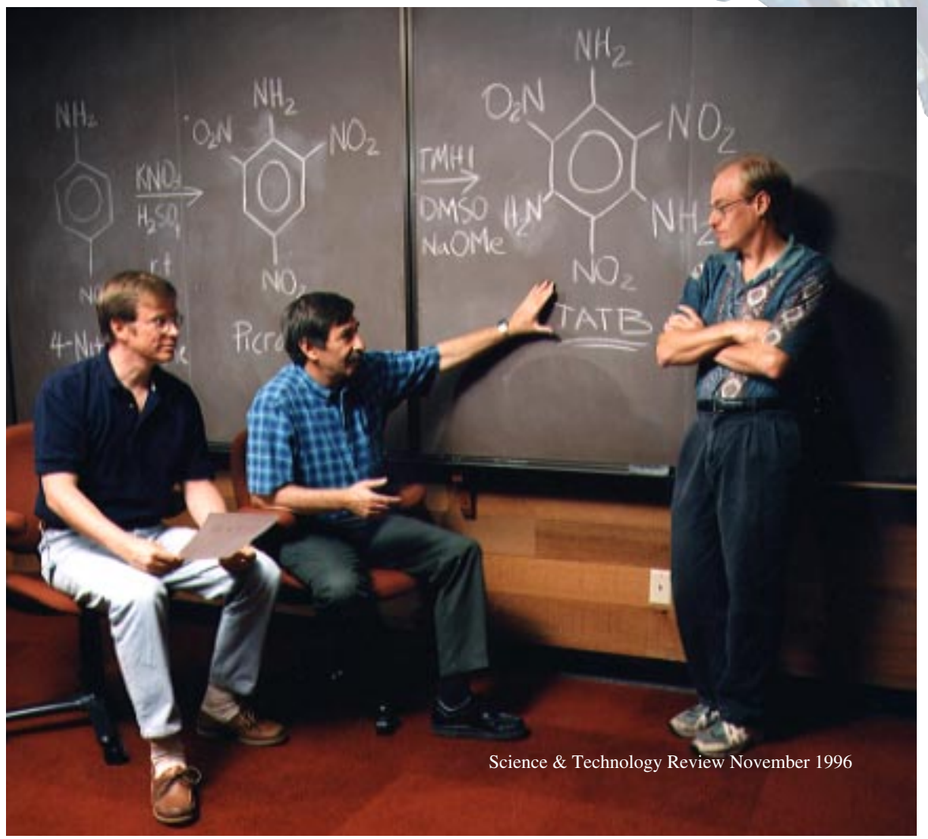
Addressing a Cold War Legacy with a New Way to Produce TATB

ONE of the most important accomplishments made by weapons laboratories' chemists in the past two decades has been the formulation of powerful conventional high explosives that are remarkably insensitive to high temperatures, shock, and impact. These insensitive high explosives (IHEs) significantly improve the safety and survivability of munitions, weapons, and personnel. The Department of Energy's most important IHE for use in modern nuclear warheads is TATB (triamino-trinitrobenzene) because its resistance to heat and physical shock is greater than that of any other known material of comparable energy.

The Department of Energy currently maintains an estimated five-year supply of TATB for its Stockpile Stewardship and Management Program (see the August 1996 *Science & Technology Review*, pp. 6–15), which is designed to ensure the safety, security, and reliability of the U.S. nuclear stockpile. The Department of Defense is also studying the possible use of TATB as an insensitive booster material, because even with its safety characteristics, a given amount of that explosive has more power than an equivalent volume of TNT.

In addition to its military uses, TATB has been proposed for use as a reagent in the manufacturing of components for liquid crystal computer displays. There is also interest in employing the explosive in the civilian sector for deep oil well explorations where heat-insensitive explosives are required.

Despite its broad potential, the high cost of manufacturing TATB has limited its use. Several years ago, TATB produced on an industrial scale in the U.S. was priced at $90 to $250 per kilogram. Today it is available to customers outside DOE for



Rob Schmidt (left), Alex Mitchell, and Phil Pagoria discuss the chemistry of the method for synthesizing TATB (triamino-trinitrobenzene) developed at Livermore. Their method lowers the cost and production time of this insensitive high explosive and increases the environmental friendliness of the manufacturing process. (The reaction scheme on the board appears also in the figure on p. 23.)

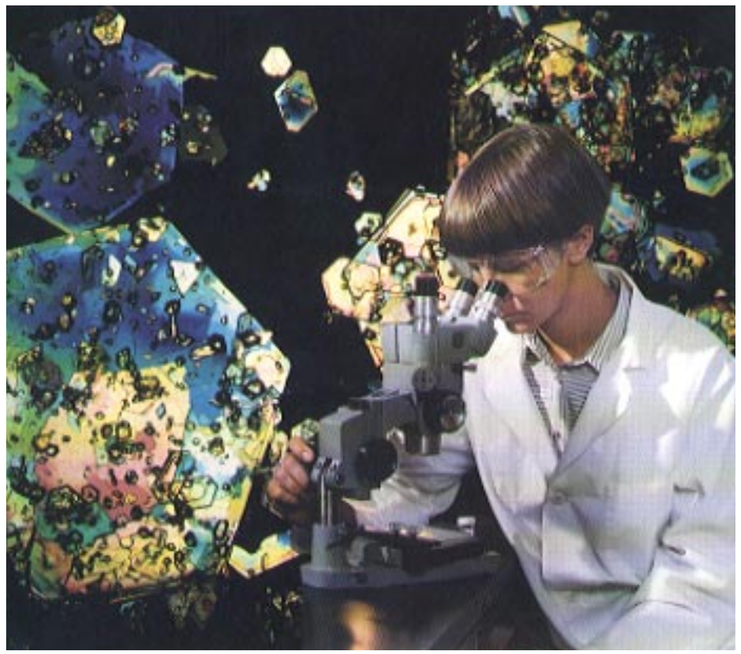
about $200 per kilogram. In response to a need for a more economical product, chemists at Lawrence Livermore have developed a flexible and convenient means of synthesizing TATB as well as DATB (diamino-trinitrobenzene), a closely related but less well known IHE developed by the U.S. Navy. The initial phase of this work was funded by the Department of Defense (U.S. Navy) to explore the chemical conversion of surplus energetic materials to higher value products as an alternative to detonation.

The Lawrence Livermore process—also called the VNS (vicarious nucleophilic substitution) process—should be able to produce TATB for less than $90 a kilogram on an industrial scale in about 40% less manufacturing time. The process also offers significant advantages over the current method of synthesis in environmental friendliness, for example, by avoiding chlorinated starting materials. What's more, the process uses either inexpensive, commercially available chemicals or surplus energetic materials from both the former Soviet Union (UDMH, a rocket propellant) and the U.S. (Explosive D, a high explosive).

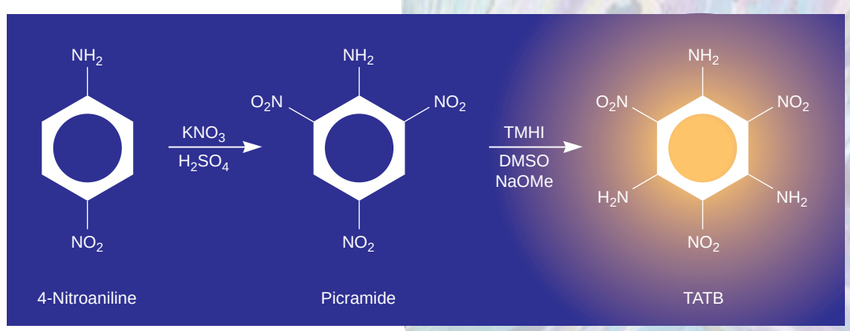
By using UDMH (*uns*-dimethylhydrazine) and Explosive D (ammonium picrate), this process disposes of energetic materials left over as a legacy of the Cold War in an environmentally responsible manner. It allows the use of surplus energetic materials as unique feedstocks to make more valuable materials such as higher value explosives or other products. Indeed, the new chemistry is also applicable to the synthesis of chemicals that are important intermediates in the preparation of numerous pharmaceutical and agricultural chemicals.

Current Process Produces Impurities

The currently accepted method for manufacturing TATB in the U.S. involves a reaction sequence that starts with the relatively expensive and domestically unavailable chlorinated compound TCB (trichlorobenzene). Elevated temperatures of 150°C are required for two of the reaction steps leading to TATB. The major impurity produced is ammonium chloride; in addition there are low levels of chlorinated reaction side-products.



Fran Foltz examines crystals of TATB (triamino-trinitrobenzene) under a microscope. The background photograph shows TATB crystals at high magnification.



The process of synthesizing TATB (triamino-trinitrobenzene) from picramide using TMHI (trimethylhydrazinium iodide) as expressed in this reaction scheme may result in a large decrease in the cost of TATB.

The VNS process is more environmentally friendly than the current synthesis. It employs mild reaction conditions and eliminates the need for chlorinated starting materials. The latter characteristic is especially important in light of the growing movement to eliminate chlorinated compounds from the industrial sector altogether because of their possible adverse environmental effects.

The VNS process depends on two key materials, TMHI (trimethylhydrazinium iodide) and picramide (trinitroaniline), which can be obtained from either inexpensive starting compounds or surplus energetic materials available from demilitarization activities. TMHI can be prepared directly from hydrazine and methyl iodide, or it can be synthesized by reacting UDMH with methyl iodide. Some 30,000 metric tons of UDMH rocket propellant are located in the former Soviet Union, where they await disposal in a safe and environmentally responsible manner.

Two U.S. companies have received congressional funding to demilitarize UDMH in Russia using a chemical process that produces lower value products (ammonia and dimethylamine). In contrast, the VNS process converts UVMH to TMHI, which will be used for the production of higher value products such as TATB.

TMHI reacts with picramide in the presence of a strong base to give TATB at a yield of over 95%. Picramide may be obtained from low-cost, domestically available nitroaniline. Or, as in the synthesis of TMHI, picramide may be synthesized from a surplus munition, in this case, Explosive D. Several million kilograms of Explosive D are available for disposal in the U.S.

New Process to Increase TATB Availability

The availability of relatively inexpensive TATB using the improved synthesis will facilitate its use, both for military and civilian applications. At the same time, the VNS process provides a new avenue for disposing of large quantities of energetic materials that are a legacy of the Cold War. The process reflects a new perspective within both the Department of Defense and the Department of Energy—treating surplus energetic materials as assets to be recycled whenever possible.

This new approach to the synthesis of TATB and other insensitive energetic materials is still in the development stage. Over the next year, the synthesis will progress from the 10-gram scale at the Laboratory's state-of-the-art High Explosives Applications Facility to the kilogram-pilot-plant scale at Site 300. During this stage, the necessary performance and sensitivity tests will be conducted to qualify the synthesis in terms of ease of use, purity, particle size, and cost. The process will also be evaluated for environmental friendliness and waste reduction. At the conclusion of the study, the technology will be ready for transfer to an industrial partner for commercial scale-up.

Key Words: insensitive high explosives (IHE), stockpile stewardship, TATB (triamino-trinitrobenzene).

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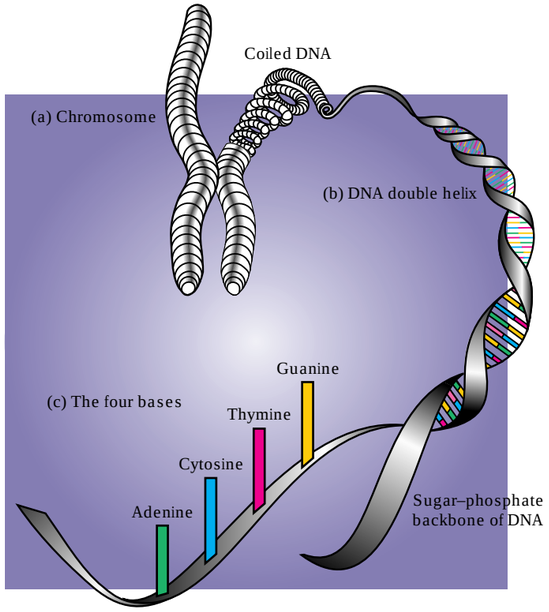
DNA Sequencing
The Next Step in the Search for Genes

FOR Lawrence Livermore researchers involved in the Human Genome Project, gene hunting is like standing in front of a mountain, shovel in hand, and knowing somewhere, amongst tons of rock, is the motherlode.

The search has been going on for years, but it has accelerated recently to a new level, noted Linda Ashworth, a Lawrence Livermore biomedical scientist working in the Laboratory's Human Genome Center. "In 1992, about 80% of our effort was devoted to generating road maps for specific chromosomes or regions on a chromosome.[1] Now, about 70% of our effort goes towards sequencing DNA and furthering sequencing technology."

Sequencing involves determining the exact order of the individual chemical building blocks, or bases, that form DNA. The four chemical bases—commonly abbreviated as A, G, C, and T—bind together to create base pairs that are the "business end" of the DNA molecule. (See figure at right.)

After researchers sequence a piece of DNA, they search for the special strings of sequence that form genes. The ultimate goal of the worldwide Human Genome Project is to find all the genes in the DNA sequence and develop tools for using this information in the study of human biology and medicine. Major benefits will be a better understanding of and treatments for genetic diseases.



The basics of genetics. Each cell in the human body (except red blood cells) contains 23 pairs of chromosomes. Chromosomes are inherited: each parent contributes one chromosome per pair to their children. (a) Each chromosome is made up of a tightly coiled strand of DNA. The current research lies in the details of the DNA structure, which, in its uncoiled state reveals (b) the familiar "double helix" shape. If we picture DNA as a twisted ladder, the sides, made of sugar and phosphate molecules, are connected by (c) rungs made of chemicals called "bases." DNA has four bases—adenine (A), thymine (T), guanine (G), and cytosine (C)—that form interlocking pairs. The order of the bases along the length of the ladder is called the DNA sequence. The hunt for genes is focused on reading the order of the bases for each DNA strand and determining which parts of the sequence constitute genes.

To the Hunt

It is a hunt of gigantic magnitude, a bit like chopping away at Mount Everest with a pick and shovel. Genes range in size from 1,000 base pairs (bp) to over 1,000,000 bp. The smallest human chromosome (21) contains approximately 45 million bp; the largest (chromosome 1) has approximately 250 million. The entire human genome contains about 3 billion bp. As of mid-August 1996, about half of one percent of the human genome had been sequenced worldwide in 15,000 bp chunks or longer. "Maybe six times that amount has been sequenced in smaller pieces, which are useful for diagnostic purposes," according to Jane Lamerdin, one of the Center's researchers.

To put things in perspective, there are perhaps 100,000 human genes scattered throughout the chromosomes, interspersed with non-gene material. "Chromosome 19, the one we're focusing on here at Livermore, has about 2% of the total DNA, so we're estimating as many as 2,000 genes," said Ashworth. "We have a handle on about 400, so there are a lot left to find." (See the box, next page.)

High Technology to the Rescue

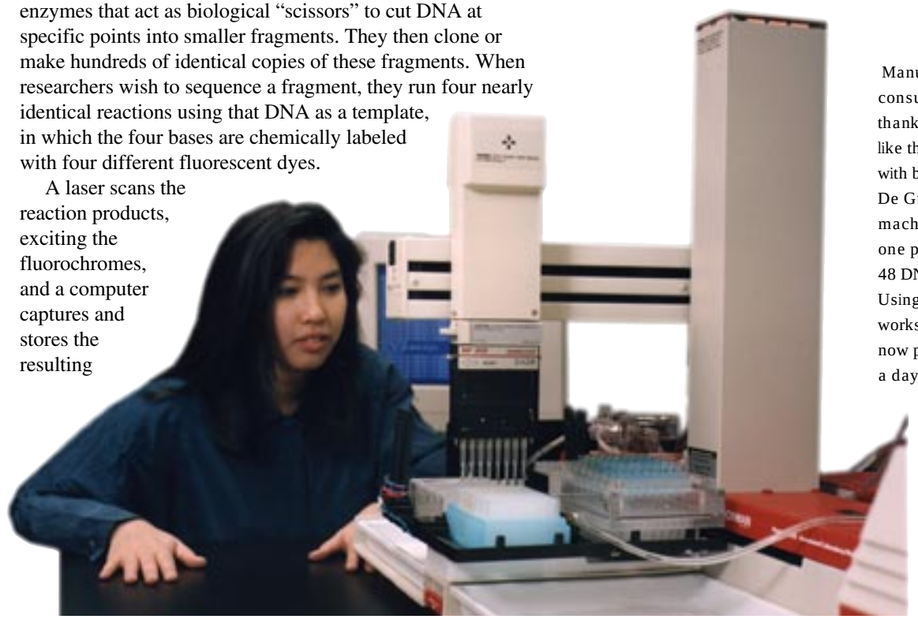
What has made it possible to even contemplate sequencing the entire genome are advances in genetic-engineering technologies in the past decade.

Not so long ago, sequencing 40,000 bp was considered a worthy multiyear thesis project for a Ph.D. student. Livermore's Center now sequences this amount in less than a week using the Center's integrated system that sequences and tracks the DNA fragments being studied.

The best of current technology allows researchers to sequence about 1,000 bp along a stretch of a piece of DNA. Most facilities only sequence in 300-bp chunks. The Laboratory's Genome Center currently sequences about 700 to 800 bp along the DNA. "We're entering the era of production sequencing," said Lamerdin. "A lot of the up-front work has been automated. There's no more manual pipetting, for instance. We have robots to do that." (See the photo below.)

To sequence a section of DNA, researchers first use special enzymes that act as biological "scissors" to cut DNA at specific points into smaller fragments. They then clone or make hundreds of identical copies of these fragments. When researchers wish to sequence a fragment, they run four nearly identical reactions using that DNA as a template, in which the four bases are chemically labeled with four different fluorescent dyes.

A laser scans the reaction products, exciting the fluorochromes, and a computer captures and stores the resulting fluorescent signals. (See the photo on p. 26.) Software automatically determines the order of bases from the four-color data. The Center has 13 of these sequencing machines, each capable of reading more than 25,000 bases a day. Additional software actually hunts for particular A, G, C, and T combinations that mark the beginnings and endings of genes.



Manual pipetting is a time-consuming task of the past, thanks to automated workstations like the one pictured at the left with biomedical scientist Maria De Guzman. Before these machines were available, it took one person all day to process 48 DNA samples for sequencing. Using the Genome Center's three workstations, one person can now process up to 1,000 samples a day.

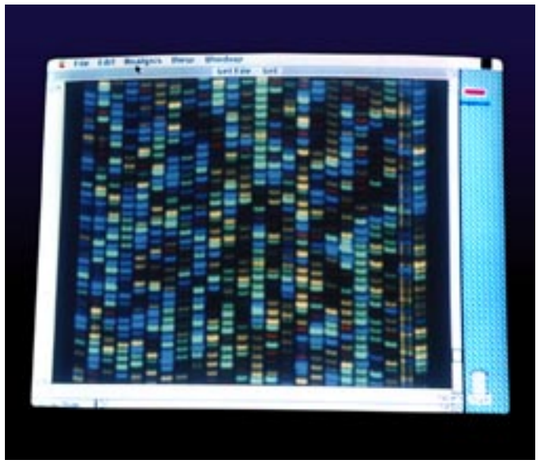
Genes at Livermore

The difference between weapons testing and gene hunting may seem enormous, but their connection relates to how the study of biology became an integral part of the Laboratory's work. Livermore's first biomedical program was chartered in 1963 to study the radiation dose to humans of isotopes in the environment; a natural extension was to explore how radiation and chemicals interact with human genetic material to produce cancers, mutations, and other adverse biological effects.

In the last 20 years, advances in microbiology, biochemistry, genetics, and bioengineering gave rise to the field of biotechnology. Recent advances in genetic-engineering technologies then made it possible to examine and sequence DNA faster and more efficiently than ever imagined. The Laboratory was well positioned to take advantage of this new field, which combines the disciplines of biology, genetics, engineering, and computer science. Pulling from other Laboratory organizations, the Biology and Biotechnology Research Program called on engineers, physicists, and computer scientists to join biologists to help solve the mystery of the human genome.

In 1987, researchers at Lawrence Livermore began studying all of chromosome 19. This project grew out of research on three genes, each involved in the repair of DNA damaged by radiation or chemicals. As the Laboratory became known worldwide for its work on this chromosome, other researchers, hunting for genes thought to be somewhere on this chromosome, contacted the Laboratory and international collaborations were formed. Such collaborations discovered, for example, the genes for myotonic dystrophy (a late-onset genetic disease causing muscle atrophy) and a form of dwarfism called pseudoachondroplasia.

In 1990, the Department of Energy and the National Institutes of Health formed the joint Human Genome Project. The long-term goal of this 15-year project is to decipher the DNA of the entire human genome. Three DOE national laboratories—Lawrence Livermore, Los Alamos, and Lawrence Berkeley—are DOE centers for this project, while NIH supports eight facilities involved in this work.



Livermore's Human Genome Center has 13 sequencing machines, each capable of reading more than 25,000 bases a day. This image shows one form of their output, where each color in the vertical bands or "sequencing ladders" corresponds to one of the four DNA bases. Using the following translator, blue = C; green = A; yellow = G; red = T, you can trace a sequence ladder vertically and read a small portion of the genetic code.

A relational database, developed by Lawrence Livermore computer scientists, keeps track of where each clone is, what has been done to it, who did it, when they did it, and what has yet to be done. "When the sequencing was someone's thesis project, the individual usually kept track of progress in a notebook," explained Lamerdin. "But in this kind of high-throughput environment, we need computers to track the progress of all these pieces and also to help us make decisions. Computational support is a critical element in the success of this project."

After Sequencing

Determining the human genome sequence and finding the genes is really just a first step. "Knowing the bases that make up a gene and where it's located on a chromosome doesn't tell you what the gene *does*," noted Ashworth. "After sequencing, we still need to determine what proteins the genes produce, and what those proteins do in the cell."

Why bother? First and foremost, genes and their proteins hold the key to unlocking the mysteries of inherited diseases. Once the genetic code for a disease is broken, gene and drug therapies can follow. For example, the gene for cystic fibrosis was discovered four years ago, and while we are still a long way off from "fixing" the gene defect that causes this disease, unraveling the gene's secrets has allowed private industry to deal with one of the major symptoms of cystic fibrosis.

"So, the sequence is really a starting point," said Ashworth. "We still need to know the structure and function of the protein produced by the gene, and how that protein interacts in the environment of the cell. The sequence, you might say, is the detailed map we need to help us find the buried treasure."

Future *S&TR* highlights will discuss the Center's work on the next-generation sequencing machine and a collaboration to uncover the gene involved in one form of inherited kidney disease.

Key Words: chromosome, DNA sequencing, gene, Human Genome Project.

Reference

1. "The Human Genome Project," *Energy & Technology Review*, UCRL-52000-92-4/5 (April/May 1992), pp. 29–62.

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The Human Genome Center's Internet home page is available at http://www.llnl.gov/bbrp/genome/genome.html. The Department of Energy's "Primer on Molecular Genetics" is available on the Internet at http://www.gdb.org/Dan/DOE/intro.html.

Patents and Awards

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
John W. Elmer Dennis W. O'Brien	**Electron Beam Machining Using Rotating and Shaped Beam Power Distribution** U.S. Patent 5,534,677 July 9, 1996	An apparatus and method for electron beam (EB) machining (drilling, cutting, and welding) that uses conventional EB guns, power supplies, and welding machine technology without the need for fast bias pulsing technology. A magnetic lensing (EB optics) system and electronic controls are used to concurrently bend, focus, shape, scan, and rotate the beam to protect the EB gun, to create a desired effective power-density distribution, and to rotate or scan this shaped beam in a controlled way.
Mark Bowers Allen Hankla	**Phase and Birefringence Aberration Correction** U.S. Patent 5,535,049 July 9, 1996	A four-wave mixing phase conjugate mirror that corrects phase aberrations of a coherent electromagnetic beam and birefringence induced upon that beam. The stimulated Brillouin scattering phase conjugation technique is augmented to include Brillouin-enhanced four-wave mixing. A seed beam is generated by a main oscillator that arrives at the phase conjugate cell before the signal beams in order to initiate the Brillouin effect. The signal beam being amplified through the amplifier chain is split into two perpendicularly polarized beams.
Craig J. Rivers Roanne A. Lee Glenn E. Jones	**Electrically Shielded Enclosure with Magnetically Retained Removable Cover** U.S. Patent 5,534,663 July 9, 1996	An enclosure having electrical components and an easily removable shielded cover with magnetic securement means to secure the cover to the enclosure in a manner that provides an electrical seal between the cover and the enclosure to prevent the passage of electromagnetic radiation through the joint between the cover and the enclosure. The magnetic securement means are provided on the surface of the enclosure surrounding the opening and facing the cover, and ferromagnetic means are provided on the surface of the cover facing the magnetic securement means.
Troy W. Barbee, Jr. Timothy Weihs	**Ignitable Heterogeneous Stratified Structure for the Propagation of an Internal Exothermic Chemical Reaction along an Expanding Wavefront and Method of Making Same** U.S. Patent 5,538,795 July 23, 1996	A multilayer structure with a selectable propagating reaction front velocity (V), a reaction initiation temperature attained by application of external energy, and an amount of energy delivered by a reaction of alternating unreacted layers of the multilayer structure. Because V is selectable and controllable, a variety of different applications for the multilayer structures are possible, including their use as ignitors, in joining applications, in fabrication of new materials, as smart materials, and in medical applications and devices.
Chi Y. Fu	**Process for Forming Synapses in Neural Networks and Resistor Therefor** U.S. Patent 5,538,915 July 23, 1996	A customizable neural network where one or more resistors form each synapse. All the resistors in the synaptic array are identical, thus simplifying the processing issues. Doped, amorphous silicon is used as the resistor material to create extremely high resistances occupying very small spaces. Connected in series with each resistor in the array is at least one severable conductor whose uppermost layer has a lower reflectivity of laser energy than typical metal conductors at a desired laser wavelength.

Awards

James "Buddy" Swingle recently received the **Intelligence Community Seal Medallion** from Central Intelligence Agency Director John Deutch during a ceremony at CIA headquarters in Langley, Virginia. Swingle, who is executive secretary and acting chairman of the Joint Atomic Energy Intelligence Committee, was cited for his "sustained superior performance" in producing foreign nuclear intelligence reports that "provided significant assistance to the intelligence and policy communities." Swingle has been at Livermore since 1972, working on a variety of high-energy laser and nuclear weapons programs. He joined the Nonproliferation, Arms Control, and International Security Directorate in 1990 and was recently named leader of Z Division.

Lawrence Livermore's **Storm Water Management Program** has received the U.S. Environmental Protection Agency's 1996 **National Storm Water Control Program Excellence Award** in the industrial category. The award recognizes the Laboratory's efforts to curb water pollution through improved storm water control. Representatives from the Storm Water Management Program, a part of the Environmental Protection Department in the Laboratory's Plant Operations Directorate traveled to Dallas, Texas, in early October to receive the award at the Annual Water Environment Federation Conference.

Three teams of Laboratory employees are recipients of **Hammer Awards** for the Department of Energy. They are: the **Life Cycle Asset Management** (LCAM) team from the Plant Engineering Department, a part of the Plant Operations Directorate; the **Directives Reengineering Group**, out of the Office of Scientific and Technical Information in the Director's Office; and the **Performance Management Team**, working out of the Office of Policy, also in the Director's Office. The Hammer Awards were created by Vice President Al Gore to recognize special achievements in the efforts to reinvent government by improving customer service, cutting red tape, empowering employees, or getting back to basics.

(*continued from page 2*)

Researchers discover ice that resists melting

While performing studies of methane clatrate, a material viewed as a potential energy source, scientists produced a mysterious phenomenon—ice that does not liquefy when heated well beyond its usual melting temperature.The energy stored in methane clathrate deposits on Earth has been estimated at twice that in all conventional hydrocarbon deposits of oil, gas, and coal.

The discovery occurred while researchers—Bill Durham of Lawrence Livermore and Laura Stern and Stephen Kirby of the U.S. Geological Survey—were experimenting with a new method for synthesizing methane clathrate, a solid compound of water and methane occurring on Earth and possibly on the icy moons of the outer solar system. Clathrate refers to the compound's porous lattice–work structure.

In a project funded by NASA, the team mixed fine, granular ice and cold, pressurized methane gas in a constant-volume reaction vessel that was slowly heated under strictly regulated conditions. Curiously, the scientists found that the ice did not liquefy as predicted when the melting temperature was reached and surpassed. Clathrate was formed only after many hours, with the temperatures inside the reaction vessel reaching above 50˚F before the last of the ice was consumed (the researchers never did see melting) as part of the process.

The three scientists concluded that a kind of "chemical armoring effect" accompanying clathrate formation suppresses the melting of the ice. They are hopeful that their new method of producing methane clathrates will pave the way for further experimentation and a better understanding of this phenomenon. Their findings were published in the September 27 issue of *Science* magazine.

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Lab-IBM making progress with new supercomputer

Lawrence Livermore and IBM are moving ahead on a $93 million project to build the world's fastest supercomputer. The production model of the 3-trillion-calculations-per-second supercomputer is scheduled for demonstration in December 1998.

In September, Lawrence Livermore took delivery from IBM of the first 512 processors, which make up two separate systems that operate at 136 billion calculations per second, contain 67 billion bytes of memory, and include 2.5 trillion bytes of storage.

The supercomputer is based on the IBM RS/6000 SP* line of processors that allows a building block approach to high-performance computing with clusters of shared-memory processors. Although the 512 processors are far fewer than the 4,096 that eventually will make up the production model, they possess computing power more than all that previously delivered to the Laboratory in its 45-year history, according to Mark Seager, who led the Livermore acquisition team.

The supercomputer is being installed as part of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI), a ten-year, $1 billion program designed to eventually deliver 100-trillion-calculations-per-second computing capability. The award of Blue–Pacific—as the Livermore machine is known—was announced by President Clinton at a White House event on July 26.

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Magmatic CO_2 may be key to volcano vitality

What is a volcano's potential for eruption? Two Lawrence Livermore researchers believe work they performed in the Cascade Volcanic Range in northern California and Oregon may point to a new method for determining how vital or dormant a volcano is.

Timothy Rose and M. Lee Davisson say the relative amount of magmatic carbon dioxide observed at different volcanoes may someday provide a means of monitoring a volcano's level of activity. Their work is discussed in a paper published in the September 6, 1996, issue of *Science*.

In a study to assess the presence of magmatic carbon dioxide from volcanoes, the pair measured carbon-14 in groundwater samples from 40 different springs and creeks located in the Cascade Range. The absence of carbon-14 in the water samples is an indicator that magmatic carbon dioxide came from deep within the earth. (Because it has a half-life of over 5,000 years, carbon-14 is used as a means of determining the age of objects.)

"There's no question it's a substantial leap from identifying carbon isotope tracers in groundwater to actually calibrating the amounts of gas to determine the degree of danger a volcano poses," said Rose. "But it's an intriguing phenomenon and worth further investigation."

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*IBM trademark

Abstracts

Simulations to Save Time, Money, and Lives

The Laboratory's Conflict Simulation Laboratory (CSL) has been developing computerized programs to simulate combat and other conflicts since 1974. All branches of the military use these systems for training purposes and to prepare for operations as diverse as the 1989 invasion of Panama and peacekeeping in Somalia. The CSL is presently continuing development of the Joint Tactical Simulation (JTS) and recently began work on the Joint Conflict and Tactical Simulation (JCATS) program for the Joint Chiefs of Staff. The Army is still using the CSL's first model, Janus.

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The Secrets of Crystal Growth

Lawrence Livermore researchers are using the atomic-force microscope (AFM) to elucidate the growth mechanisms and three-dimensional structures of widely different solution-based crystals on the nanometer (billionth-of-a-meter) scale. Much of the AFM work has been in support of the Laser Programs' need to better understand KDP (potassium dihydrogen phosphate) crystal growth because of its direct impact on advanced lasers such as the National Ignition Facility. A second avenue of research has focused on the growth of solution-based crystals of biological macromolecules, specifically the protein canavalin and the satellite tobacco mosaic virus. The AFM images have revealed how solution-based crystals grow and how they are affected by impurities, defects, and solution conditions. The results are likely to affect many disciplines and technologies, from pharmaceuticals to materials synthesis.

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