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PBX Properties
HE Crystals
Catacombs
Beryllium Texture

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Point of View

Richard Mah
Associate Director
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Job #1: Stockpile Stewardship

Stockpile Stewardship is the top priority for the nuclear weapons program at Los Alamos National Laboratory. As stewards of the nation's nuclear weapons stockpile, our focus is on maintaining high confidence in the safety, security, reliability, and performance of the warheads in the enduring stockpile.

Los Alamos is the Design Agency for five weapon systems in the enduring stockpile: B61, W76, W78, W80, and W88. The United States has not built a new nuclear weapon since 1989, and the design life of these warheads is limited. As warheads approach the end of their design life, the stewardship challenges increase. Currently, two Los Alamos systems, the B61 and the W76, are scheduled for refurbishment through Life Extension Programs (LEPs).

Weapons system refurbishment is managed under the Phase 6.X Process through the Project Officers Group (POG) and the Nuclear Weapons Council (NWC); Phase 6 of the acquisition process is Quantity Production and Stockpile. The Phase 6.X Process guidelines are based on the management framework for the nuclear weapon acquisition process that was established by DOE—in agreement with the DoD—and used for over 40 years to design and build the nation's nuclear arsenal. The 6.X phases are

- 6.1 Concept Assessment,
- 6.2 Feasibility Study and Option Down-Select,
- 6.2A Design Definition and Cost Study,
- 6.3 Development Engineering,
- 6.4 Production Engineering,
- 6.5 First Production, and
- 6.6 Full Production.

The B61 and the W76 are in Phase 6.3 of their LEP refurbishment schedules.

B61 LEP

The B61 is a family of strategic and tactical nuclear bombs. Modifications (Mods) 7 and 11, which are scheduled for refurbishment, are strategic bombs carried by the B-52 and the B-2 bombers. Mods 3, 4, and 10 are tactical bombs carried by the F-15 and the F-16 fighters. The B61 design incorporates insensitive high explosive and enhanced nuclear detonation safety features. Components being refurbished include the canned subassembly and associated seals, foams, pads, and cabling. These secondaries were built before 1970 for the B61-0/-1 and were originally designed for an 8-year life; however, an in-production process change later extended the estimated design life to 20 years.

Phase 6.2/6.2A life extension studies on the B61-7/-11 began in December 2000 and were completed in August 2002.

In November 2002, the NWC granted approval to proceed to Phase 6.3. These activities include completing the engineering development of the life extension options that were recommended as a result of the Phase 6.2/6.2A study and subsequent POG down-selection. Phase 6.3 also will require developing and providing complete engineering releases for various components and subsystems to the production facilities, in conjunction with concurrent engineering, to ensure that designs being developed can be produced.

Production engineering (Phase 6.4) is scheduled to begin in the first quarter of FY04, and the first production unit (Phase 6.5) is planned for 2006.

W76 LEP

The W76 is a strategic nuclear warhead that is carried in the Mark 4 (Mk4) reentry body on Trident I C4 and Trident II D5 submarine-launched ballistic missiles on Ohio-class submarines. The W76 design

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Quasi-Static Mechanical Properties Testing of Plastic-Bonded Explosives

In weapons applications, plastic-bonded explosive (PBX) components play a role in structure as well as performance, and it is very important to identify and understand PBX properties such as strength, ductility, and fracture propagation relative to the parameter space of their use. Various constitutive and micromechanical theories continue to be developed to model the complex properties and behaviors of PBX composites.

Mechanical properties measurements are used to aid in the evolution and validation of these modeling efforts. These PBX measurements are also used in stockpile surveillance activities as a means of evaluating the status of HE (high explosive) weapons components, and additionally, these measurements are used to characterize and certify new lots of stockpile-bound materials. Rigorous test methods are essential for providing integrity and statistical validity to these databases.

PBX formulations are typically 85–95 wt.% explosive crystals embedded in a 5–15 wt.% polymer matrix. PBX molding powders are pressed to high density (on the order of 98% of the theoretical maximum). This design results in an HE with enough cohesion and integrity to be precision machined for high-performance applications. Pressing parameters are adjusted to result in a specified weight of explosive per unit volume, so that each pressed charge has excellent and reproducible explosive performance.

As a class of materials, these highly filled polymers have nonlinear visco-elastic mechanical properties, and they are inherently difficult to accurately characterize and model. These properties are significantly affected by a myriad of parameters, including but not limited to temperature, strain rate, particle size and distribution, pressing density, relative humidity, long-term storage conditions, pedigree, lot-

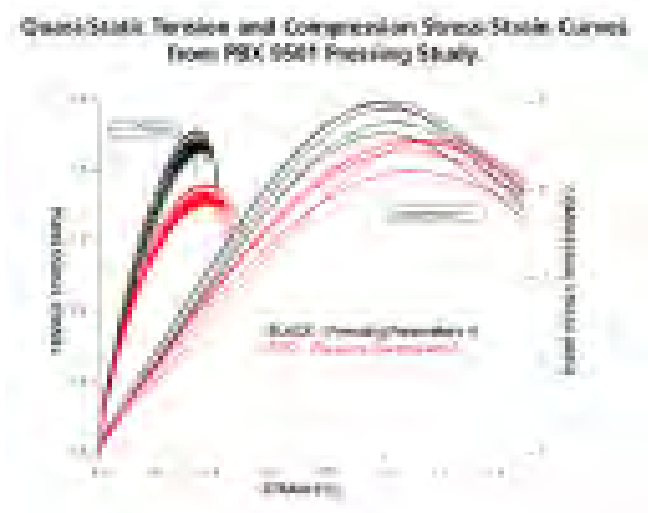
PBX materials have been tested to failure quasi-statically in uniaxial compression and tension under various conditions. Shown here is the Instron workstation and chamber, along with pre- and post-test compression (right) and tension (left) PBX 9502 specimens.

to-lot formulation differences, processing methods, thermal history, and polymer characteristics (molecular weight, etc.).

Most materials testing procedures are performed under standard procedures accepted and issued by the American Society for Testing and Materials (ASTM). Currently, there are no ASTM standards for testing HE. All HE mechanical properties tests are therefore modifications of ASTM standards developed and approved for other materials. HE test designs and methods continue to be modified and improved.

All HE mechanical properties tests are performed remotely behind a blast wall. Quasi-static tests are performed on an Instron workstation equipped with an environmental chamber to control the temperature and humidity of the testing environment. The operational temperatures of the envi- ronmental chamber can be varied over a range of approximately -54 to 95 °C, covering the stockpile-to-target (STS) temperature range of weapons applications. All tests are performed in strain rate control using strain-gage extensometers mounted directly on the specimen. With the current workstation and test design, the range of quasi-static strain rate operation is approximately 0.1 to 1e-6 s^{-1}. PBX materials have been tested to failure quasi-statically in uniaxial compression and tension under various conditions. Shear and fracture tests are being designed and performed in collaboration with MST-8 researchers, who have also measured high strain rate compression of PBX materials using the split-Hopkinson pressure bar and Taylor cylinder impact method.

In recent years, PBX uniaxial tensile and compressive properties have been quantified with respect to many interesting variables. We have investigated the effect on PBX 9501 of reducing the plasticizer concentration in the polymer binder and also the effect of decreasing the molecular weight of the long-chain polyester polyurethane used in the binder. We have explored the mechanical properties effects of changing the HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) explosive particle sizes and concentrations and changing the polymer matrix altogether. We have explored the



Uniaxial tension and compression stress-strain curves from the Set A (black) and Set B (red) charges (see Table 1 and discussion). The data shown were collected at 25 °C and 10% RH using strain rate control at 0.0001 s^{-1}. The tensile and compressive stress axes are on the left and right of the graph, respectively.

potential effects of machining parameters on PBX test specimens in a round-robin test matrix with other weapons-related facilities. The effects of virgin and recycled processing methods on the mechanical properties of PBX 9502 have also been evaluated.

A recent study in collaboration with ESA-WMM at Los Alamos investigated the role of the various hydrostatic pressing parameters in forming high-density parts from PBX 9501 molding powder. In total, 32 hemispherical charges were fabricated using a full permutation of six hydrostatic pressing parameters. Bulk densities were measured for all 32 charges, and density gradients were carefully measured in 5 select charges. Five other charges were chosen (from the remaining 27) for mechanical properties testing.

Table 1 gives the pressing parameters for two of the more interesting charges from this study. Note that these two charges have some of the same parameters and nearly identical bulk densities. Parameter Set A achieved density by using high powder temperature and short dwell times, while Parameter Set B achieved a similar density by using low powder temperature and long dwell

TABLE 1: Subset of Pressing Parameters in PBX 9501 Pressing Study							
Param. Set	Pressure (psi)	No. of Cycles	Temp. of Powder (°C)	Dwell Time (min)	Rest Time (min)	Sack Thickness (in.)	Bulk Density (g/cm^3)
A	20	5	95	2	1	1	1.8346
B	20	5	73	10	1	3	1.8347

times. (Data from the larger set of charges implied that the "sack thickness" parameter has little if any effect on the final charge density.)

While charges A and B possess nearly identical densities, their mechanical properties show some interesting differences. The average maximum tensile stress (left axis) of Set B is nearly 17% less than that of Set A, while the average Set B strain value (x-axis) at the maximum stress point is almost 12% larger than in Set A. The average Set B modulus E_{20} (slope of the stress-strain curve at 20% of the stress maximum) is 12% less than in Set A. In compression, the Set A and B differences show the same trends, but they are not as pronounced (Set B compressive strength is 8% lower, strain is 8% greater, and modulus E_{20} is 11% lower than Set A).

These data, along with a closer evaluation of the other mechanical properties data from this study, suggest to us that, with all other parameters held constant, the temperature of the molding powder (initially and through the pressing process) may be extremely important in determining the tensile properties of the charge. A higher molding powder temperature may allow better flow of the polymeric binder and a better "knitting" of the molding powder prills (or pellets), directly endowing the material with a higher tensile strength. Better flow appears to also result in higher charge densities (higher temperature had an effect similar to that of longer dwell times—see Table 1), and there is a known correla-tion of higher density with higher compressive strength; there may also be a small contribution to compressive strength arising directly from better binder flow and knitting at high temperatures.

Microscopy studies are under way to look for physical evidence to support these interpretations of the data. Further studies, on PBX and polymer alone, will explore the role of the binder and the importance of temperature in achieving desirable charge densities and mechanical properties in PBX composites.

Quasi-static mechanical properties measurements are used to evaluate the complex structural characteristics of PBX materials. These data are useful in HE model development, and the test methods provide a quantitative means of evaluating and certifying these materials in nuclear weapons applications. ✹

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Growing Crystals of Explosive Materials

We have restored the capability at the Laboratory to grow large crystals of explosive materials, a capability absent here for more than 20 years. Limited supplies of earlier-grown explosive crystals held in storage have been used to conduct early experiments and to supply samples to other laboratories. However, more and better explosive crystals are now needed for future work.

Many of the unknown properties of crystalline explosives are required as inputs for detailed constitutive modeling of plastic-bonded explosives used in weapons. Experiments designed to investigate crystal behavior also promise to help us understand the mechanisms of explosive initiation and detonation in shock-wave environments.

To meet the need for explosive crystals, we have set up a laboratory to grow, characterize, and prepare samples from crystals, performing all of the more hazardous operations remotely. We are capable now of routinely growing large crystals, cutting and polishing them, and characterizing their orientation and perfection by several methods, including Laue x-ray diffraction.

If you have ever tried to grow salt or sugar crystals at home, you know that it can be relatively easy to grow small crystals, but much more difficult to grow large, perfect crystals. Crystals are grown by saturating a solution with the material of interest and then changing the solubility by some means. The usual methods include evaporation and decreasing the temperature, although many other techniques can be used. Evaporation is easy to set up and does not require any special equipment but is difficult to control precisely. Decreasing the temperature of the solution is more controllable but requires equipment designed to decrease the temperature steadily.

The materials we are interested in include pentaerythritol tetranitrate (PETN), used in detonators; cyclotrimethylenetrinitramine (RDX), used in detonators and many mixed explosives; and cyclotetramethylenetetranitramine (HMX), used as the major constituent of PBX 9501 in weapons. Although crystals of PETN and RDX are relatively easy to grow, HMX is difficult to grow in large sizes and good quality. We have focused recently on HMX crystal growth because few of the available crystals offer the size and/or morphology that we need. Required sample sizes vary, but a sample intended for a shock-wave experiment needs to be about 1 cm square by a few millimeters thick; crystals weighing at least 10 g are needed to yield a sample of this size.

We have restored the capability to grow large crystals of explosive materials

Although HMX crystals of excellent quality are conveniently grown by evaporation from acetone, they tend to be flat, because growth is preferred on a specific face, and relatively small, because the solubility of HMX in acetone is relatively low. Despite these difficulties, we are now reliably producing HMX crystals of excellent quality from acetone. We have to start with at least 1 L of acetone to grow large crystals, but the process takes only about 3 weeks.

HMX crystals that offer a more favorable morphology for the cutting of particular faces are not expressed well in acetone. To grow such crystals, we tried using other solvents. Solvents with higher HMX solubilities and lower volatility, such as dimethyl sulfoxide (DMSO) and gamma-butyrolactone (γ-BL), are ideal for the growth of large crystals from smaller volumes of solvent by decreasing temperature. But these solvents present other problems. First, because it is difficult to measure solubility accurately, determining the right temperature at which to begin the temperature reduction and then drop in a "seed" crystal is tricky. Second, the solubility changes so rapidly with temperature that extremely accurate temperature control is necessary over very long times (up to 10 weeks). Finally, below certain temperatures, good solvents

have a tendency to form crystals, called "solvate crystals," with solvent molecules included at a nearly one-to-one ratio with explosive molecules.

We attempted temperature-reduction crystallizations from both γ-BL and DMSO. Crystals from γ-BL exhibit undesirable needle morphologies, while crystals from DMSO have more uniformly proportioned facets—exactly what we require. Whereas a larger temperature change during growth yields larger crystals, we have found that the solubility curve in DMSO is slightly too steep above 65 °C for temperature control precise enough to avoid rapid growth. Even with a gradual temperature reduction of 0.25 °C per day, there are typically regions of high solvent inclusion, termed "veiling," above 65 °C due to periods of rapid growth. To avoid veiling, we are growing HMX from DMSO by beginning temperature reduction below 65 °C. The crystals are smaller, but because of their excellent morphology, we can extract the samples we need.

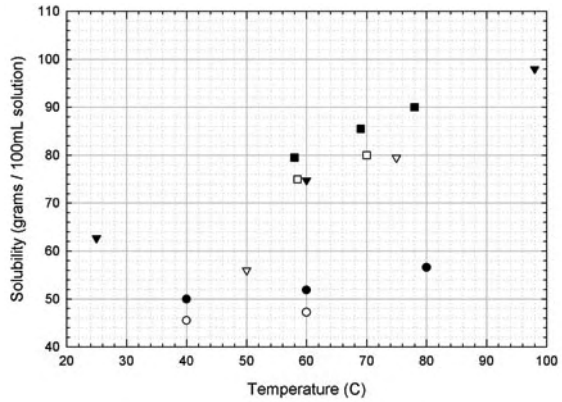
Now that we are able to reliably produce samples of PETN, RDX, and HMX crystals, we are performing experiments on them in our laboratory and in collaboration with others.

Over several years, Jerry Dick (DX-2) demonstrated that the shock sensitivity of PETN was extremely dependent on crystal orientation. This "anomalous" shock initiation behavior of PETN is thought to be due to "steric hindrance to shear" when impacted in the more sensitive directions. In short, when a single crystal is impacted, it must relieve stress. It does so by the coordinated slipping of molecules past each other in preferred directions. When a crystal is impacted in an insensitive direction, molecules are able to slide past each other with comparatively little resistance. Conversely, when a crystal is impacted in a sensitive direction, molecular sliding results in an entanglement that initiates reaction and detonation. In addition to impact sensitivity, elastic shock waves travel faster along the more sensitive direction.

An analysis of the slip behavior of HMX showed that, like PETN, there are directions in which stress relief through slip is difficult, suggesting that HMX has similarly anomalous shock initiation and elastic shock-wave behavior. In a set of experiments that is nearly complete, we have found that HMX shocked in different directions displays elastic shock-wave speeds nearly twice as fast in an orientation with sterically hindered slip as compared to orientations with unhindered slip. We suspect that this orientation will have a shock-initiation sensitivity that is more sensitive, and experiments are under way to test this hypothesis.

Our ability to prepare samples from these crystals has attracted collaborators. We are supplying samples to researchers for a number of experiments; a few examples follow. Researchers at Washington State University are performing gas-gun shock experiments on RDX crystals. Livermore researchers are performing isentropic compression experiments on HMX crystals using the Sandia Z-machine. Resonant ultrasound spectroscopy is being performed on HMX and RDX crystals (cut into parallelepipeds along principal faces) by two independent teams in the X and MST Divisions. These experiments will yield a complete set of elastic constants for RDX and HMX. The HERCULES team will explore laser-driven shock in HMX crystals (see the *Nuclear Weapons Journal,* January/February 2003, pp. 4–5), and researchers in C Division will investigate the spectra of explosive crystals in the THz regime.

Once the properties of explosive crystals have been measured accurately, we can begin to study the changes induced by introducing imperfections. There are a staggering number of possible experiments, in-



A plot of some of our data (open and closed squares) for HMX solubility in DMSO with data available in the literature (triangles). These large discrepancies in solubility as a function of temperature make it difficult to know the conditions at which to start the crystal growing process using this solvent. This problem is typical with many solvents.

cluding adjusting explosive powder properties by changing the solvent used for purification and studying the shock behavior of other crystal forms and even solvates.

A unique mechanical property of HMX offers an obvious starting point. When pressed, HMX undergoes a twinning process that is at first elastic and then plastic. As a result, some crystalline HMX in PBX 9501 is twinned. The polarized light microscopy image on p. 4 of the March/April issue of this journal shows parallel banding within crystals, indicating the presence of twinned crystals.) We plan to measure the stresses needed to cause this twinning and perform shock experiments on samples in which a known number of twins have been introduced.

The experiments being performed on explosive crystals grown in our laboratory will be both useful as inputs for modeling efforts and helpful in unraveling the mysteries of reaction initiation and detonation. ✹

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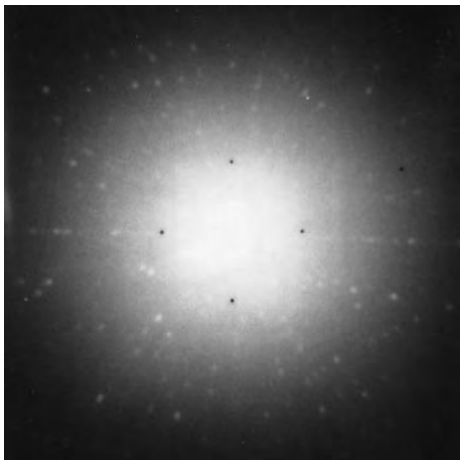
I acknowledge Jerry Dick, who began this work and continues to provide valuable insight, and A. Richard Martinez, who constructed the crystallization and characterization equipment and builds gas-gun experiments from the prepared crystal samples.

Four single crystals of HMX photographed on a 1-cm grid. The crystal on the right was grown from DMSO starting at 85 ˚C, and the other three were grown from acetone by slow evaporation at 30 ˚C. Note that the clarity of the acetone-grown crystals is much better and their birefringence (splitting of light into two components) causes an apparent doubling of the grid. The DMSO-grown crystal exhibits veiling defects, which cause opacity. Some of the parasite crystals nucleated at lower temperatures on the sides of this crystal are clear and free of defects. The bottom acetone-grown crystal has some cracks that were introduced by the temperature gradient caused by evaporation when the crystal was removed from the growth solution, illustrating how fragile these crystals are.

Two typical HMX crystals viewed from the same crystallographic direction. The one on the left was grown from acetone, and the one on the right was grown from DMSO. Both weigh about 15 g. Note that the acetone-grown crystal has a flatter shape than the DMSO-grown crystal.



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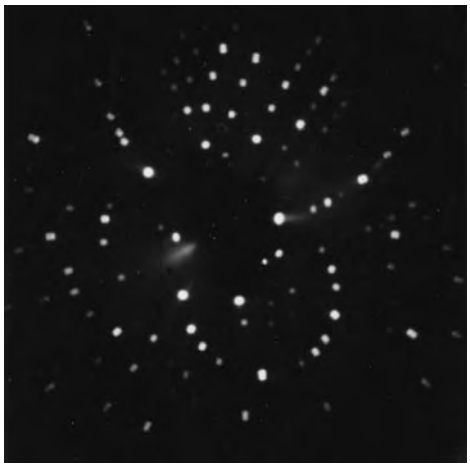


Ricardo Schwarz

Laue x-ray photos of a slab of HMX. In the reflection orientation (left), we are not able to get usable data even with very long exposure times (2 h). In the transmission orientation (right), we get excellent patterns at short exposure times (5 min). We can use these photos to measure the sample orientation very accurately and ensure that the crystal quality is high.

Assembly and Process Engineering Team

The 24 members of NMT-5's Assembly Team ensure that 22 processes are operational and war-reserve certified by focusing on maintaining production in three engineering capabilities: chemical operations, mechanical operations, and vacuum operations. To meet the deliverables associated with pit fabrication, we have trained at least three people to perform each operation.

Chemical Operations

Parts Cleaning: Work minimization is a primary focus for all cleaning operations. During processing, parts come in contact with several organic materials that must be removed from their surfaces prior to storage and additional processing. We clean those parts with trichloroethylene (TCE) as a solvent in an ultrasonic bath. To minimize the use of TCE without sacrificing quality, we developed a parts washer to extend the usability of the solvent. Unfortunately, there is no path forward for existing TCE waste; however, we are investigating filtration techniques to reduce the radioactive contamination of the waste stream to lower levels, which would allow other disposal techniques to be employed. Furthermore, distillation has been investigated as a means to reuse the existing TCE. Fourier transform infrared (FTIR) spectroscopic techniques have been established to monitor the cleanliness of the bath.

Density Determination: Density is used to verify the quality of the parts. By using Archimedes' Principle, we determine density by submerging the part and a standard in a liquid (bromobenzene) with well-characterized physical properties. Bromobenzene does not readily react with plutonium; however, during the process qualification, we determined that some side reactions take place over time. Because hydrogen bromide forms, we developed a test for determining the concentration in solution. Again, filtration techniques are being investigated to reduce the radioactive contamination of the waste stream. There is a high likelihood that the same FTIR techniques used with TCE can be used with bromobenzene to establish more precise cleanliness requirements for the bath.

Electrochemical Marking: We use electrochemical marking to place a serial mark on the final unit. Using an etching solution in conjunction with an electrical power supply unit enables a permanent mark to be placed in the desired location. This extremely flexible system allows a variety of marks to be made on a variety of materials. The primary concern with the marking process is the quality and consistency of the mark, which is ensured through operator training and ensuring the etching and cleaning solutions are thoroughly removed from the pit surface. Innovations from the operators have enhanced the electrochemical marking process to make a higher quality mark with greater ease.

Mechanical Operations

Assembling pits is a unique process that starts with placing the parts into a precise configuration and securing them in place. These complex operations are performed in a downdraft room, which is designed to accommodate processing the plutonium parts outside the normal glovebox confinement. The personnel performing this work are experienced and take all safety precautions as directed by radiological control technicians. Operators bring this unit back to the downdraft room several times during the assembly process for hardware modifications, so coordinating multiple personnel and skills is required to accomplish an assembly. Pratice of assembly enables smooth performance of an assembly when radiological conditions exist.

Surface Preparation: Using surface-preparation technologies developed at Rocky Flats, ESA-AET performed cold demonstrations to prove that the

equipment's function was not damaged during shipment and storage. When Los Alamos began these operations very limited documentation was available to reassemble the equipment and ensure its function.

Tube Crimping: To guarantee that the radioactive material is contained within the pit, we crimp the tubes used to access the interior of the pit; crimping provides a temporary seal that is eventually welded. Again, the equipment used to perform this function was developed at Rocky Flats, but little documentation of its configuration was available. So, we thoroughly investigated and documented the parameters affecting the crimp's performance and acquired additional hardware to improve operational reliability.

Gas Analysis: Many processes required the use of high-purity, inert gas to ensure that the highly reactive plutonium would not be affected. One process required the development of a control system upgrade with a dedicated argon line and a new sampling system to provide quantitative evidence of process control. While proving-in the process, it became evident that the testing technique required more precise documentation on the sampling technique, as well as container-processing and subsequent baseline analysis. We have improved performance in those areas and now routinely obtain great consistency in our analyses. Work has begun to install a real-time, gas-analysis system on the equipment to reduce turnaround times on analyses and to provide real-time feed-back to operators so that potential problems are addressed as they occur.

Vacuum Operations

During the assembly process, several critical vacuum operations are performed to ensure the prod- uct's quality during and after the part has been assembled. The first series of tests is performed by using a special fixture to ensure that welds are acceptable and that they meet the requirements for the vacuum and pressure required for final

Pollution Prevention Initiative

Waste minimization is at the forefront of the manufacturing efforts in NMT-5, where each NMT-5 team takes steps to better control processing with the hope that the incremental improvements will add up to better business practices. The Assembly Team has focused its waste-minimization efforts on solvent usage by working with other groups, such as NMT-6, C-AAC, and C-ACT, to develop and implement testing strategies that extend solvent life.

These efforts have had dramatic results. NMT-5 and -6 received a 2000 Green Zia award from New Mexico for the systematic reduction of mixed waste streams from their processing activities. The Assembly Team, in cooperation with C-AAC and C-ACT, received two pollution prevention awards for minimizing the amount of mixed waste that is produced.

Reducing TCE

One award was for reducing TCE usage as a cleaning agent by developing a test that facilitated reusing the solvent. Using a fieldable pH test developed with C-ACT provides a quantitative value of the amount of acid stabilizer used within the process and provides the opportunity to avoid disposing of the TCE after each use. Efforts are now under way to replace the single usage of TCE solvent rinsing. These efforts began several years ago with the design of a compact washing unit, on which a patent is pending, and the washing unit will be installed during FY04. In addition to the pH testing and the washing unit, an FTIR technique, again developed with C-ACT personnel, will be deployed for additional analysis of the TCE used and a greater understanding of solvent degradation.

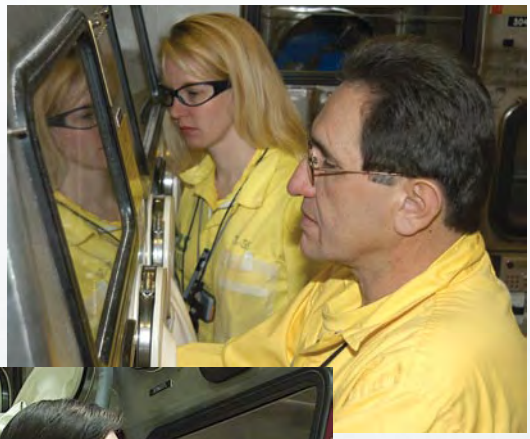
Bromobenzene

Another award involved bromobenzene, the medium used for density determination via the Archimedes' Principle. Historically, this well-characterized fluid has been used at Los Alamos for this purpose; however, in an effort to maintain quality control, the Assembly Team and C-AAC identified, developed, and implemented a test for the hydrogen bromide and bromine concentrations formed during processing. This test, like the one for pH in TCE, has allowed the extension of solvent life and thereby reduced waste generation.

Distillation and filtration techniques are under consideration to enable reuse of the spent fluids. These techniques were originally conceptualized for the TCE waste stream. However, the success with waste minimization has led to the expansion of the approach to all fluids in NMT-5 manufacturing processes. Investigation into long-term replacement of all fluids listed in the Resource Conservation and Recovery Act is also under way.

Our approach to solvent usage in NMT-5 has dramatically reduced the production of mixed waste, and good teamwork and planned resulted in exceptional waste minimization. The tasks involved in accomplishing the principles of pollution prevention require skills that are unique to each person. We hope to continue fostering the ideals of pol- lution prevention within the organization through the promotion of innovative approaches.

assembly. This ensures that the part can move downstream for further processing.



After each processing step, vacuum testing is used to verify that the assembly has maintained its integrity. The parts are heated to help remove residual contaminants and then tested to ensure that continued evolution of volatiles meets the prescribed levels. A residual gas analyzer is used to confirm initial contaminant removal and gives a quantitative indication when off-gassing has stopped. A leak-tight and clean part ensures that the subsequent operations meet the prescribed specification.

During fabrication, several changes occur to the pit hardware that allow various operations to be performed. The part is pressure-tested to ensure mechanical integrity of the complete system. The part is evacuated on a pumping station filled with an inert gas to ensure that the quality of the pit materials is not compromised. The gas is subsequently analyzed to ensure that the gas fill meets specification.

The final step is to ensure that the unit is completely sealed—an operation that is performed in a leak-testing chamber. This final check ensures that no leaks are present in the pit and that it will remain in a stable configuration.

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The Catacombs: Archiving Nuclear Test Debris

Postshot nuclear test debris collected in support of the Nuclear Weapons Test Program is stored at Los Alamos National Laboratory in a room known as the Catacombs. This collection of debris represents more than 50 years of US nuclear test history. Although the Catacombs may not be viewed as a national treasure, it is the repository with the most complete collection of postshot test debris samples.

From the days of the Trinity test to the end of testing in 1992, radiochemical (radchem) analysis of postshot debris has provided a direct measure of plutonium and/or uranium fission yield and integrated neutron fluence; it is the method by which other diagnostic techniques are calibrated.
The original purpose for archiving test debris was to provide weapons designers with material that could be reanalyzed at a later date to answer questions related to device performance. Analytical methods used in the past may not have provided optimal data. It was anticipated that future chemistry and measurement techniques would require reanalysis of test debris. Today, these archived samples provide an opportunity for weapons stockpile stewards to reexamine performance issues to benchmark modern weapons codes.

A sample analyzed by mass spectrometry was, for example, a combination of several individual samples because the importance of phenomena such as physical fraction of the debris was not recognized at that time. We now know the significance of some of these physical processes and their impact on the interpretation of radchem results. These samples are available, the integrity of the samples is excellent, and modern radchem analytical and mass spectrometry methods may help refine original assessments. Reanalysis of these samples may provide researchers with important answers to stockpile reliability and confidence issues in the absence of testing.

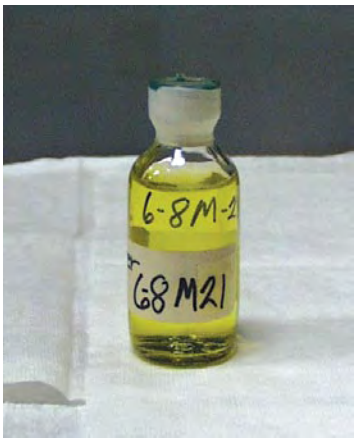
Archived debris exists in three different forms: filter paper, core samples, and acid solutions. We have between 300 and 400 filter papers obtained by aerial collections of post-shot debris from atmospheric tests and more than 10,000 core samples containing nuclear test debris incorporated into fused rock formed as a result of underground testing. Many of the filter papers and fused rock samples originally collected were dissolved in strong mineral acids; the resulting solutions were processed to obtain radchem diagnostic information. More than 3,000 acid solutions containing dissolved debris are archived in the Catacombs.

We have evaluated each of the archived samples on a set of criteria to verify that they are still useful for radchem diagnostics. These criteria included sample container integrity, physical state, and quantity.
We have evaluated the physical condition of the containers used to store the samples. The major problem encountered in the Catacombs was that many of the original storage containers holding the individual debris samples are nearing the end of their useful service life due to corrosion by acid fumes, aging plastic, etc. Among the problems encountered during the assessment of the archived samples were evaporation of the solutions, salting out (precipitation) of material from solution, salt deposits on the exterior of the lids, deterioration of bottle lids, deterioration of silastic seals, and embrittlement of plastic containers. Over 99% of the archived samples have met our criteria and are still useful for radchem diagnostics.

We are now undertaking the major effort of repackaging and stabilizing each of the archived radchem samples so that they will remain viable for radchem diagnostic analyses for an additional 50–100 years without any future stabilization efforts. We are replacing the old lids, which are phenolic, with polyvinyl liners. The acid fumes over the

years have caused deterioration of polyvinyl liners, which in turn have caused cracking and blistering of the phenolic lid. The replacement lids are also phenolic but contain a Teflon™ liner and a polyethylene film/foam backing that provides a tight seal for excellent chemical resistance. The lids are then wrapped in Teflon™ tape and sealed with heat-shrink tubing.

The majority of the postshot debris archived at Los Alamos is still suitable for radchem diagnostics. The debris is stored to ensure its integrity for at least 50–100 years. Pertinent information about each debris sample is placed in a database to facilitate use and management of the materials. The debris is an enduring and valuable resource for the Nuclear Weapons Program.



The pertinent information for the archived test debris is currently in hardcopy form in note- books housed in the vault in Building RC-1. We are developing a database to consolidate the information and make it more readily available for scientists who are evaluating previously obtained radchem results. This database will also facilitate future measurement requests. The database is being populated with the original information, uniquely identifying each sample, and each sample is being assigned a barcode that is readable by an optical scanner. The database cross references the samples to the chemists' laboratory notebooks and contains many unique comments about sample collection or analyses. In the future, the database will be expanded to incorporate search and sort routines. ✹

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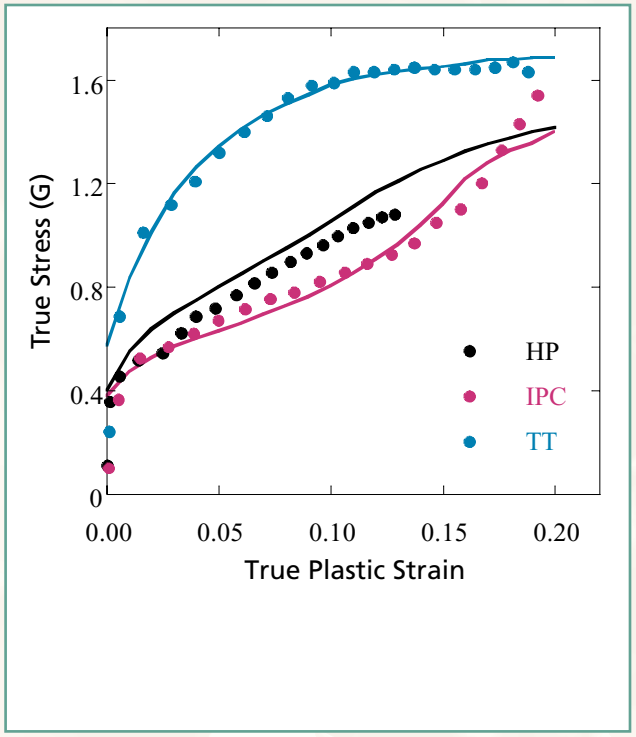
Beryllium at High Strain Rate

Beryllium is a low-density, high-stiffness, high-thermal conductivity metal that possesses unique neutronic properties. It is an integral part of many nuclear applications, including fission and fusion reactors as well as weapons. The ability to predict its strain response over strain rates that range from quasistatic to in excess of $5000s^{-1}$ is integral to the use and accuracy of models that simulate weapons performance.



To make such predictions, it is necessary that we understand the influence and interplay of metallurgical factors that include twinning and texture. To validate existing codes and advance the state of the art, a multigroup team (MST-8, MST-6, and LANSCE-12) has been studying beryllium that has been deformed at high strain rates by using a Hopkinson bar. Samples are characterized by using conventional metallography and neutron diffraction; the constitutive response is then modeled by using a viscoplastic self-consistent (VPSC) model, which is one of the first to explicitly and quantitatively incorporate a measured bulk texture, a feature integral to the prediction of the anisotropies indicated below.

It is well known that high or low temperature, as well as strain rate, changes mechanical response. However, it is less well understood that rather subtle changes in the crystalline texture (relative alignment of grains) of a polycrystalline metal can produce directional anisotropies in mechanical properties that are significant to overall properties and which are particularly apparent in high strain rate regimes. Changes in texture sufficient to alter properties are frequently invoked by changes in a fabrication process. Thus, as we shall show below, in addition to heat treatment, temperature, and strain rate, the initial and developing texture of a material must also be taken into account if quantitative predictions of mechanical response are to be made.

To illustrate the effects of texture, the graph shows the room-temperature load response measured at $5000s^{-1}$ for three beryllium samples nominally in the same heat treat condition. The differences among them is their starting texture. The hot-pressed (HP) sample has an essentially random texture, whereas the in-plane compression (IPC) and through thickness (TT) samples were both removed from a rolled plate but were loaded perpendicular and parallel to the plate normal, respectively. The mechanical response of the three samples is quantitatively and qualitatively different.

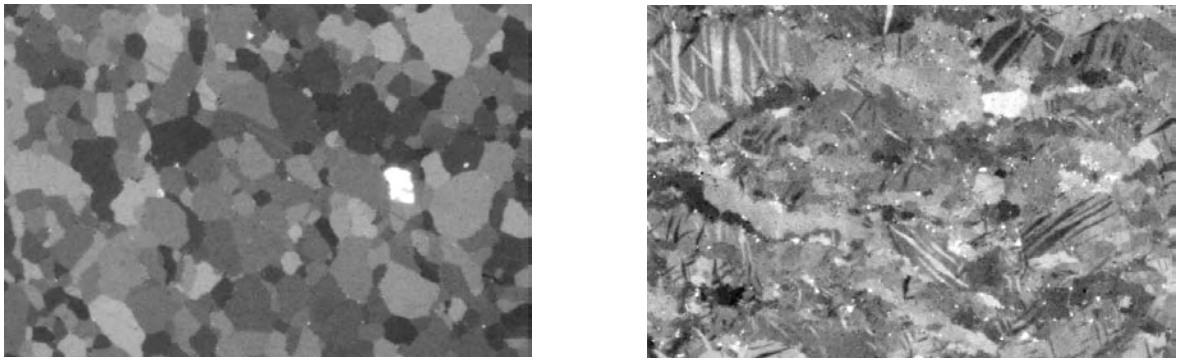
To explain the disparities in the graph, one must consider the manner in which inelastic deforma-

tion takes place in a polycrystalline metal. First, it is necessary to recognize that metals having different crystal structures exhibit different behavior. For example, a face-centered cubic metal like copper has sufficiently high crystallographic symmetry that it can always deform by slip. Conversely, the ability of a hexagonal close-packed material like beryllium to deform inelastically depends on the orientation of grains in the microstructure with respect to an applied load. More specifically, beryllium and some other materials may undergo twinning, in which a substantial portion of grains in a particular orientation (with respect to an applied load) undergoes a gross realignment due to a shear event. The resulting twins can be seen metallographically in the optical micrographs and quantified by using neutron diffraction.

Since the ability to twin is limited to grains in preferred orientations with respect to an applied load, characterizing their presence as well as the original crystallographic configuration in a bulk specimen is integral to predicting mechanical response. We used the new neutron high-pressure preferred orientation (HIPPO) diffractometer, a unique capability at LANSCE. This instrument takes advantage of the penetration of neutrons into bulk materials to generate pole figures, which represent the orientation distribution of grains. By measuring before and after deformation, quantitative validation comparisons can be made between experiments and models.

A predictive VPSC model was developed by researchers in MST-8 that describes the initial (and evolving) texture in the context of twinning and allowable slip systems. By optimizing and validating the model in comparison with measured texture data, the model can accurately simulate the macroscopic stress/strain curves. Moreover, the model provides insights concerning the activity of the various deformation mechanisms, a quantity that cannot be easily measured. Notably, the code accurately predicts the increased flow strength of the in-plane (IP) sample.

In metallurgical terminology, the reason for the disparity in the mechanical response becomes clear if one considers the crystallographic texture of the material relative to the applied load. The microstructure of the HP sample is randomly oriented, and easy basal or prismatic slip can be activated in most grains. Also, in the limited number of grains that are not oriented for slip, twinning may also occur. In the IP sample, the preferred orientation (basal poles normal to load axis) predisposes the material to twinning (thus it is comparatively soft). In contrast, for the TT specimen, the texture (basal poles parallel to load axis) does not exhibit the same predisposition. Thus the inelastic deformation must be accommodated by hard pyramidal slip, accounting for the increased strength (and the conventional hardening behavior).



Optical micrographs showing beryllium microstructure pre-deformation (left) and after compression (right) to -8.2% at 5000s^{-1}. The compressed beryllium exhibits twinning.

An accurate, physics-based description for beryllium has proved vital in describing its constitutive response over the range of thermo-mechanical conditions of interest. A major advantage of the resulting model is the ability to confidently predict the response of beryllium to thermo-mechanical conditions that have not been probed experimentally. This study showed that the initial texture has a significant effect on the morphology and magnitude of the stress-strain response.

Our focus has been to gain a basic understanding of the crystallographic mechanisms of deformation, their interaction, and the role of crystallographic preferred orientation (texture) on the mechanical response of beryllium. However, in complementary activity, we are making a systematic analysis of hexagonal close-packed metals, such as magnesium and titanium, because of their relevance in the industrial arena. Ultimately, the goal of each activity is to develop predictive computational codes that can be incorporated in industrial forming simulations or large-scale weapons calculations.

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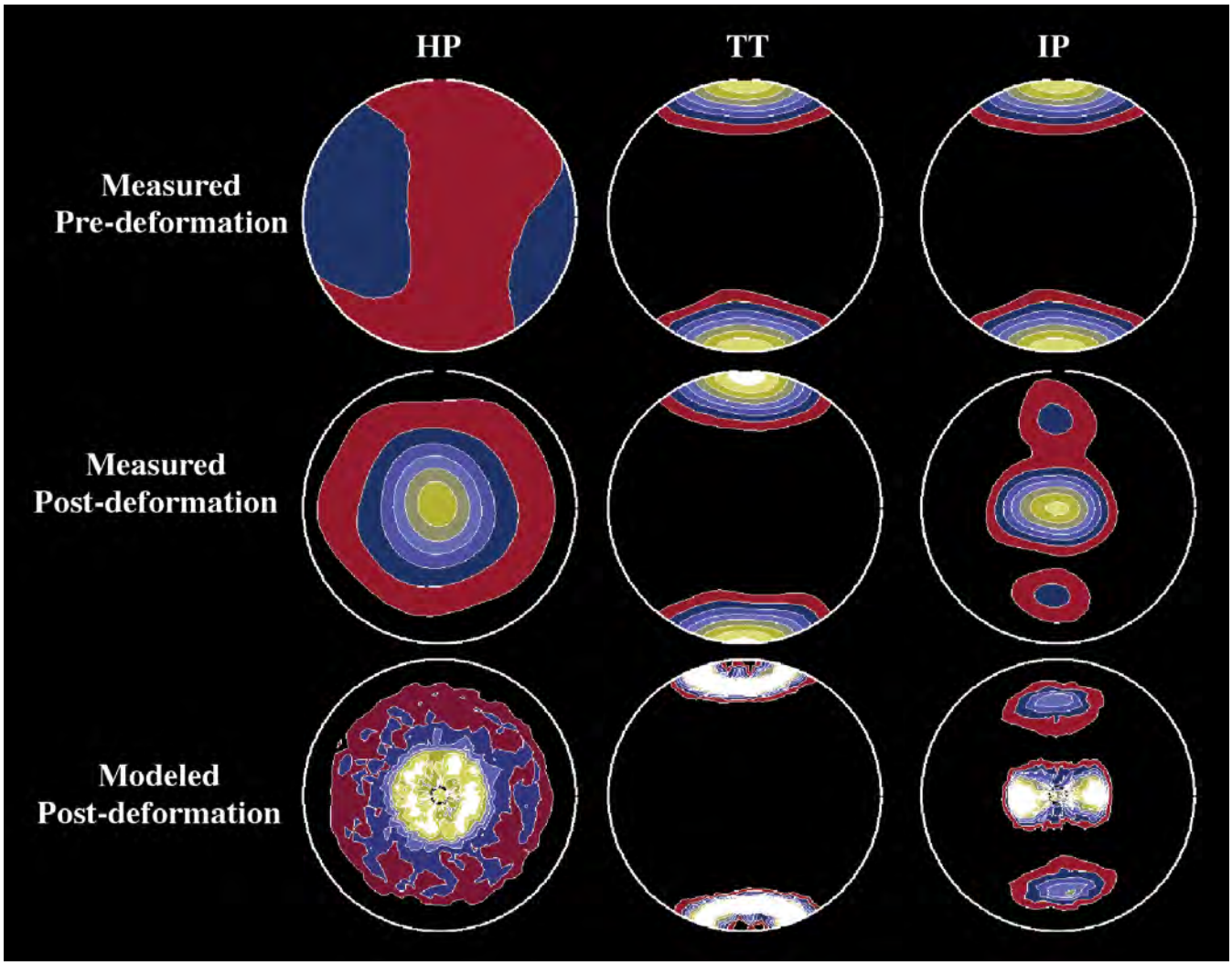
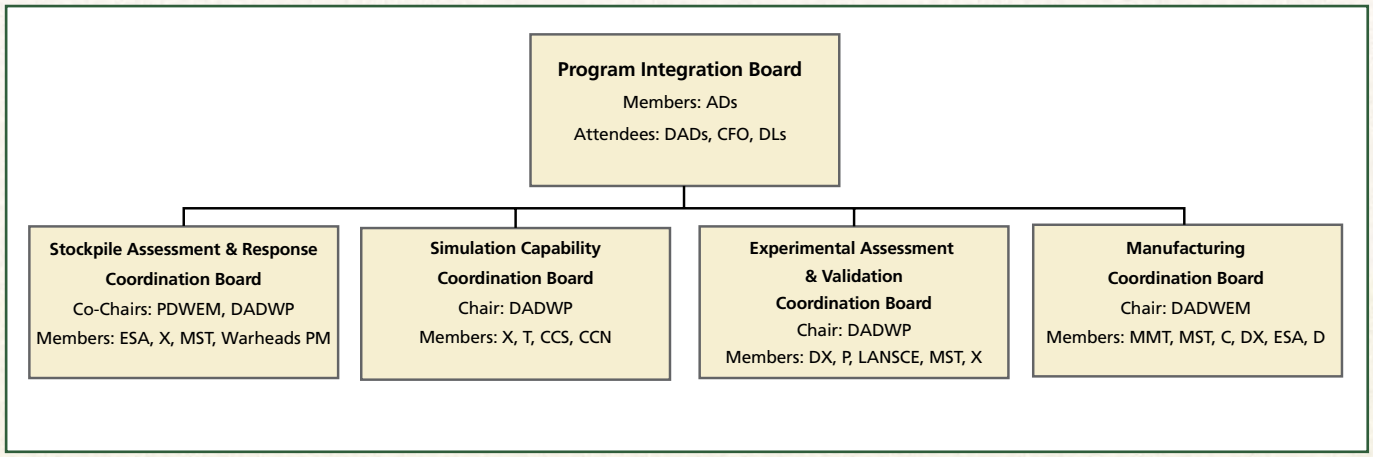


Basal pole figures showing the texture evolution pre- and post-deformation as well as the model's success in describing the final texture. Straining direction of the HP and IP samples is into the page of the paper; that of the TT sample is up and down the page.

Stockpile Assessment and Response Coordination Board

The Stockpile Assessment and Response Coordination Board (SAR CB) supports the Program Integration Board (PIB) and is an important element within the Laboratory's Nuclear Weapons Integrated Program. Its primary mission is to identify, validate, prioritize, and approve programmatic requirements and tasks to support stockpile activities that maintain the certification of existing warheads and that certify new design warheads (if tasked).

- To interface with and provide prioritized internal and external requirements to the EAV CB, the S CB, and the M CB, as necessary, to resolve issues that transcend the boundaries of the assigned program elements within the coordination boards.
- To define and prioritize the Readiness in Technical Base and Facilities (RTBF) component that supports SAR CB program elements.



All four Coordination Boards are expected to provide integrated requirements and plans, review the *Five-Year Program Element Plans*, monitor program element progress, and manage program element change control. Each Coordination Board supports the PIB by implementing *Weapons Program Guidance* through detailed program element requirements, implementing *PIB Fiscal Guidance* by issuing *Coordination Board Fiscal Guidance*, providing input into the PIB on requirements and fiscal issues and resolving integration issues at the coordination board level.

Major supporting SAR CB missions include the following:

- To interface with the Associate Director for Strategic Research as necessary to resolve issues involving nuclear weapons program research and development activities within that directorate.
- To provide management oversight and tasking to the following program elements defined in the NNSA budgeting structure:
  - Campaign 1 – Primary Certification
  - Campaign 4 – Secondary Certification and Margins
  - Campaign 5 – Enhanced Surety
  - Campaign 6 – Weapons Systems Engineering Certification
  - Campaign 7 – Nuclear Survivability

- Campaign 8 – Enhanced Surveillance
- Campaign 12 – Pit Certification (engineering and physics)
- Directed Stockpile Work (DSW) D3 – Dismantlement and Disposal
- DSW D6 – Stockpile Research and Development

- To approve closure plans for significant finding investigations (SFIs).

The SAR CB is organized around five program elements: Stockpile Surveillance, Stockpile Assessment, Stockpile Response, Base Stockpile Program, and Nuclear Weapons Complex Support.

The members of the SAR CB communicate regularly with their points of contact at the NNSA, US Strategic Command, and the POGs to convey status and changes within the program, to enhance quality oversight and integration, and to facilitate effective management within the Laboratory. The SAR CB meets weekly to discuss issues and respond to tasks from the PIB.

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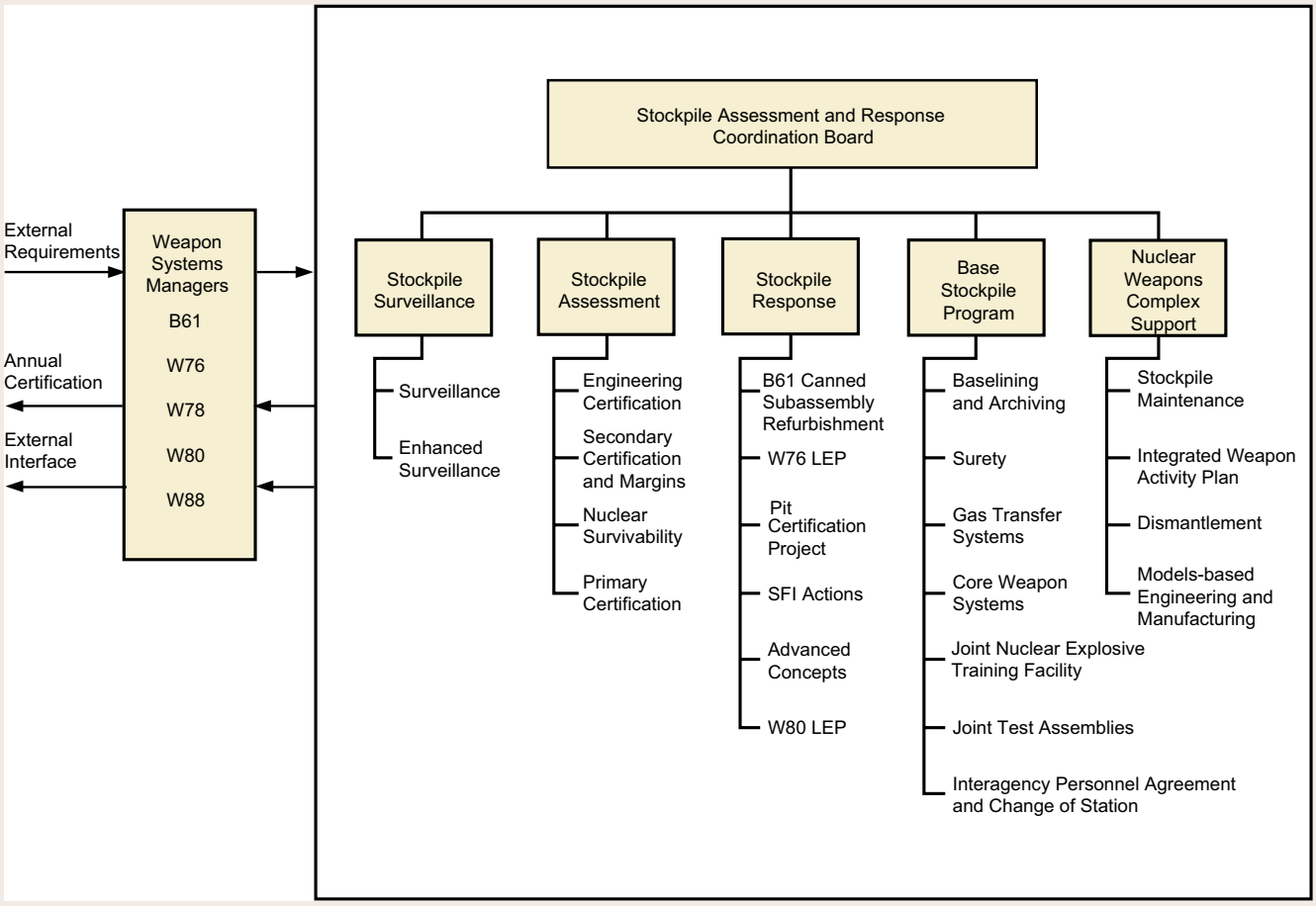

Security: Modeling Entry and Exit Inspections

By using Analytical System Software for Evaluating Safeguards and Security (ASSESS) and either Monte Carlo simulation or Joint Combat and Tactical Simulation (JCATS) modeling tools, S-1 conducts vulnerability analyses, compiles force-on-force exercise validation data for vulnerability modeling, and develops the Site Safeguards and Security Plan.

To enhance the utility of ASSESS and JCATS, we presented a graded approach to controlling access to mission-critical facilities in Modeling the Effectiveness of Entry/Exit Inspections (LA-UR-03-2000). A generic model can be used to quantify (1) the probability of detecting the transport of illicit, prohibited, or unauthorized materials or documents past an inspection point (detection models); (2) the amount of illicit, prohibited, or unauthorized materials or information transported before detection occurs (loss quantification); and (3) the effects of traffic on entry/exit inspections (traffic models). We obtain values for the model's parameters from automated login/logout data, per- formance test data, and reasonable assumptions; we have found that the model applies equally well to both entry and exit inspections and can be used for inspections of personnel, equipment, or a combination of personnel and equipment.

We have identified the parameters that affect each detection model, the relationships between models, and the equations and formulas used to calculate detection probabilities. In vulnerability analysis, it is also important to quantify the amount of material or information that could be lost prior to detection and the effects of traffic intensity on the probability of detection, and we also have techniques to calculate those quantities.

Ultimately, these formulas and techniques establish three main strengths. They will (1) put evaluation of entry/exit inspections on a firm objective footing, (2) allow a trained professional to discover the strengths and weaknesses of entry/exit inspections, and (3) aid organizations in modeling the effectiveness of entry and exit inspections.

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***Point of View** continued from page 1*

incorporates conventional high explosive and enhanced nuclear detonation safety features.

Development began in 1973, and the W76 was fielded in 1979 with an original design life of 20 years. However, the Navy projects the life of Ohio-class submarines to extend until 2042 and requires that the warheads on the Trident missiles be available during this period.

The NWC approved the W76 refurbishment in 1998, and Phase 6.2/2A was initiated to review weapon components and subsystems and to evaluate their ability to meet all performance requirements for an extended service life. This effort was completed in only 15 months.

The NWC granted conditional approval to begin Phase 6.3 activities in March 2000 and final, unconditional approval in December 2000.
A comprehensive refurbishment of the W76, including the primary and secondary, is planned to support the extended lifetime of the weapon system. Planned Phase 6.3 activities for the refurbishment will include small-scale energetic tests, full-scale hydrodynamic tests, joint ground tests, joint flight tests, physics modeling and calculations, and material studies.

Production engineering (Phase 6.4) is scheduled to begin in the third quarter of FY05. Delivery of the first production unit (Phase 6.5) is planned for the fourth quarter of FY07.

Top Priorities

The LEPs for the W76 and the B61 are top priorities for the weapons program at Los Alamos. Our B61 and W76 teams are aggressively attacking these challenging projects and look forward to an exciting and rewarding time during the upcoming years. These refurbishments will exercise nearly all the capabilities of Los Alamos and the entire nuclear weapons complex and will ensure the robustness of the US strategic nuclear deterrent well into the future.

First Step to Safety

To plan work, we must define our tasks, analyze the hazards and threats, and develop controls to prevent or mitigate the consequences of those hazards. These first three steps of the Integrated Safety Management (ISM) process form the basis of every hazard control plan (HCP). But sometimes, even with an HCP, something goes wrong— a worker can be injured or the environment or property damaged.

We have learned from those instances when we have failed to fully analyze or control hazards.
The ISM process always begins with defining the work—critical because if the work is inadequately defined, the subsequent hazard analysis will fail.

One of the more subtle mistakes we can make is our failure to recognize that all of our activities in the workplace should be examined. Not all work requires documentation—the existence of an HCP, however germane, would do little to control commonplace hazards—but all work does require ISM, even administrative assignments. The moment we enter a chemistry lab, a radiological area, or a construction site, our work becomes potentially hazardous because of that environment. We may take a tour, perform a walk-around, or read a gauge— that is work, and in the presence of hazards, it becomes potentially hazardous work.

Another way we can fail on the first step is to define work too generically. We may mask hazards by covering too many activities; by not identifying where and when the work takes place; or by ignoring tasks, materials, and equipment. It is important to define work specifically. Some employees fear that this approach will create interminable paperwork. The key is to write only what is required and informative and not overdocument the process, but we must include the important information because
a complete definition of the work facilitates our recognition of the hazards.

Finally, we must be aware of the impact of changes. Modifications to the way we do the work, the scope of the job, the materials or equipment that we use, or the location may introduce new hazards, but these are all integral to defining work.

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Organizational Acronyms and Abbreviations

ADs	Associate Directors
C	Chemistry Division
C-AAC	Actinide Analytical Chemistry Group
C-ACT	Applied Chemical Technology Group
CCN	Computing, Communications and Networking Division
CCS	Computer and Computational Sciences Division
CFO	Laboratory Chief Financial Officer
D	Decision Applications Division
DAD	Deputy Associate Director
DADWEM	Deputy Associate Director for Weapons Engineering and Manufacturing
DADWP	Deputy Associate Director for Weapons Physics
DLs	Division Leaders
DoD	US Department of Defense
DOE	US Department of Energy
DX	Dynamic Experimentation Division
DX-2	Materials Dynamics Group
EAV CB	Experimental Assessment and Validation Coordination Board
ESA	Engineering Sciences and Applications Division
ESA-AET	Applied Engineering Technologies Group
ESA-WMM	Weapons Materials and Manufacturing Group
LANSCE	Los Alamos Neutron Science Center
M CB	Manufacturing Coordination Board
MST	Materials Science and Technology
MST-6	Materials Technology: Metallurgy Group
MST-8	Structure/Property Relations Group
NMT-5	Weapons Component Technology Group
NMT-6	Manufacturing Quality Systems Group
NNSA	National Nuclear Security Administration
P	Physics Division
PIB	Program Integration Board
PM	Project Management Division
POGs	Project Officers Groups
S CB	Simulation Capability Coordination Board
S-1	Security Plans and Programs Group
SAR CB	Stockpile Assessment and Response Coordination Board
T	Theoretical Division
X	Applied Physics Division

A BACKWARD GLANCE

Bikini Atoll: Operation Crossroads

Late in 1943, Navy Captain William S. (Deak) Parsons, the wartime Ordnance Division Leader at the Laboratory, suggested developing a nuclear tor- pedo, the first proposal for a tactical nuclear weapon. J. Robert Oppenheimer killed the idea, citing his own research showing that shock damage from a nuclear torpedo would not be very effective in the shallow waters of a harbor—the most likely combat scenario.

Two years later, the idea of a tactical nuclear weapon was presented to Oppenheimer again, this time by Glenn Fowler, who was working with Norman Ramsey in the Delivery Group. Noting the fierce and savage combat conditions in the Pacific Theater, Fowler proposed developing a tactical nuclear weapon that could be used against Japanese-held caves, which represented a particularly vicious and deadly form of combat for Allied Forces. Fowler noted that if nuclear bombs were reserved for combat delivery only by airplane, their targets would be limited to cities, since aerial bombardment was notoriously inaccurate. World War II ended before any action could be taken on Fowler's idea.

Immediately after the war, Parsons again brought up the idea of developing a tactical nuclear weapon. Changing his argument from the development of a specific weapon to the broader concept of tactical use, Parsons asked mathematician John von Neumann to analyze the possible effects of a nuclear burst on naval vessels. Von Neumann quickly warmed to the idea and calculated that a ship could be sunk from an explosion occurring at a depth roughly equal to its distance from the target. Von Neumann suggested that serious attention be given to developing an underwater delivery system and using atomic bombs against single ships. In addition to making a technical argument, von Neumann also noted that "during the war, building a battleship was cheaper than building an atomic bomb, but now the situation is reversed." It was now cost effective to target individual vessels.

Building on von Neumann's analysis, the nascent Navy Atomic Bomb Group [Parsons, Frederick Ashworth (the Nagasaki weaponeer), and Horatio Rivero] began planning a series of atomic bomb tests against naval vessels that ultimately became known as Operation Crossroads. They proposed four tests with a target array of ships: detonation of a device suspended by a blimp, a deep-water detonation, a shallow-water burst, and a high-altitude delivery by a B-29 bomber. The blimp test was quickly eliminated, while planning proceeded on the remaining three proposals.

In the first nuclear tests held in the Marshall Islands, the Able test was a high-altitude drop that occurred over the Bikini Lagoon on June 30, 1946, followed by the Baker shallow-water test on July 24. Impressed by the extensive damage caused by Baker (eight ships were sunk, and eight others were severely damaged) and mindful of the very small stockpile of nuclear weapons, scientists abandoned the deep-water test.

Although Parsons' and Fowler's

concept of a tactical nuclear device was not proven during World War II, the Crossroads tests did demonstrate that tactical use of an atomic bomb was possible.

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Baker test, July 24, 1946