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Sandia Dynamic Materials Program Strategic Plan

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Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

Executive Summary

Materials in nuclear and conventional weapons can reach multi-megabar pressures and 1000s of degree temperatures on timescales ranging from microseconds to nanoseconds. Understanding the response of complex materials under these conditions is important for designing and assessing changes to nuclear weapons. In the next few decades, a major concern will be evaluating the behavior of aging materials and remanufactured components. The science to enable the program to underwrite decisions quickly and confidently on use, remanufacturing, and replacement of these materials will be critical to NNSA's new Stockpile Responsiveness Program. Material response is also important for assessing the risks posed by adversaries or proliferants. Dynamic materials research, which refers to the use of high-speed experiments to produce extreme conditions in matter, is an important part of NNSA's Stockpile Stewardship Program.

Dynamic Materials refers to the use of high speed experiments to produce extreme conditions in matter

Impact of a 0.25"-diameter sphere at 4 km/s on a thick plate produces a debris cloud

Sandia National Laboratories has a significant effort in dynamic materials research. Our flagship materials capability today is the Z pulsed power facility, which drives mm-scale material samples to multi-Mbar pressures over time scales from 100 to 1000 nanoseconds. The large sample sizes and time scales ensure our capability to make precise measurements and assess the effects of microstructural features such as grain size or orientation, both of which are sensitive to manufacturing processes. A unique feature of our experiments on Z is that a wide range of hazardous materials can be tested, including the oldest existing plutonium samples taken directly from the stockpile.

In the next 20 years, stockpile modernization plans and security programs such as Nuclear Counterterrorism must address a number of dynamic material concerns. Capabilities available today cannot address several critical issues relevant to plutonium aging, remanufacture of components, additive manufacturing, and compression of heterogeneous materials. Addressing these issues will require new capabilities to reach weapon-relevant temperatures and pressures at relevant time scales for samples that are large enough to include representative microstructures with sufficient experimental capacity to address significant variability. We must implement these capabilities within the next 10 to 15 years to enable responsive, cost-effective, risk-informed decisions for the Nation's stockpile stewardship and defense programs.

Our dynamic materials strategy is addressing these gaps by building upon Sandia's strengths through targeted capability developments in order to improve our understanding of aging, microstructure, and phase transitions over the next 10 years. A centerpiece of our strategy is a new high-pressure, fast-turnaround pulsed power facility optimized for materials research that will address key plutonium issues, including aging and systematic evaluation of the effects of manufactured materials. In the near- to mid-term, we will focus on new diagnostics, improved experimental platforms, and advanced modeling to measure critical properties and reach weapon-relevant regimes to enable defensible decisions for stockpile stewardship and reasoned responses to proliferation concerns.

Strategic Objectives of Sandia's Dynamic Materials Program

> ***Vision***
> *In 10 years we will determine how kinetics, aging, and microstructure affect material response at pressures up to 15 Mbars.*
>
> ***Mission***
> *Provide predictive capabilities for national security on material behavior at high pressure and high temperature by integrating theory, simulation, and high-precision experiments on Z, STAR, DICE, and next-generation pulsed power facilities.*

1. **New pulsed power facility focused on dynamic materials.**
   There is a need for a large body of experiments, some hazardous, using macroscopic samples and loading paths that are currently unachievable, to address material aging, reuse, and remanufacture for stockpile programs scheduled for the late 2020s. We plan to develop and work to obtain approval for a new pulsed power facility with intrinsically-safe containment and flexible pulse shaping.

Near-term to Mid-term Objectives (3-5 years)

2. **Measurement of phase boundaries for hazardous and surrogate materials.**
   Identification of material phase on pulsed power experiments is critical to the national strategic goal of developing multi-phase equation of state and strength models. This capability is important for pulsed power because our experiments reach relevant regimes that are not accessible with other techniques. Our current velocity diagnostics provide only indirect evidence of phase changes under some conditions. We plan to implement a diffraction diagnostic to measure the crystal structure directly.

3. **Platforms to reach higher pressures and broader regions of phase space.**
   Nuclear weapons reach conditions of density, temperature, and pressure that are currently inaccessible with existing platforms, particularly for macroscopic scale samples, and material models are frequently highly inaccurate in extrapolated regimes. We plan to increase the pressures attainable on Z by developing an approach to take advantage of cylindrical convergence and to implement a shock ramp platform to probe phase boundaries. Improved analysis techniques will be needed to take advantage of these new platforms.

4. **Temperature measurements for hazardous and surrogate materials.**
   Temperature measurements are needed to understand properties of materials off the principal Hugoniot, where thermodynamic constraints do not apply. Experiments reaching these conditions are comparatively cold and do not produce enough emission for traditional approaches. In the near term, we will develop an infrared pyrometer and use it on shock ramp experiments for surrogates and Pu. In the longer term, we will pursue novel approaches such as reflectivity or Stokes techniques.

Mid-term to Long-term Objectives (5-10 years)

5. **Determination of the effect of microstructure on material response.**
Many components for the stockpile modernization programs will be remanufactured. New advanced manufacturing approaches that result in very different material microstructures have significant advantages for cost and agility. Understanding the effects of microstructure and manufacturing processes on materials is therefore critical. We will take advantage of our DICE, STAR, Z, and Thor capabilities to perform macroscopic sample tests in almost any pressure regime and loading history of interest to evaluate the continuum response systematically. We will team with Centers 1400 and 1800, as well as the other labs, to develop modeling techniques to use in conjunction with our experiments to build understanding.

6. **Time-dependent material response (kinetics) during dynamic compression**.
Many material responses, most notably strength and phase transitions, are sensitive to the time scale (kinetics) of a loading event. Shock and explosively driven systems may exhibit strain rates of $10^2 s^{-1}$ to $10^7 s^{-1}$. Material models based on experiments with much faster or slower loading rates can contain significant errors. Investigating the effects of kinetics during dynamic compression has been identified as a national priority. We will quantify the importance of kinetics and provide data for kinetics-aware material models by teaming with LANL and LLNL to evaluate experiments at various time scales across different platforms. We will also pursue pulse shaping on Z, Thor, and future pulsed power facilities to enable systematic control of time scales in order to isolate the phenomena.

7. **Physics for material strength.**
Resistance to deformation, or strength, can be important to material behavior for stockpile applications but the data are not sufficient to support accurate models. The data suggest significant sensitivity of strength to microstructure, phase, and loading path. National plans have identified multiphase strength models as a priority. We plan to build upon our ability to conduct experiments at a variety of pressures on large samples and use interlaboratory collaboration to address the role of microstructure, phase, and loading history on strength. Systematic variations at moderate pressures on Thor will help uncover the basic physics.

8. **Transport properties.**
The role of transport properties such as electrical and thermal conductivity, opacity, and viscosity are not well understood but are important for stockpile applications and for the design and analysis of high energy density (HED) experiments. Measurements and simulations of these properties on HED experiments are challenging because the techniques that have been developed for engineering applications are not applicable at HED pressures, temperatures, and time scales. We plan to improve our simulation tools, develop new diagnostics, and use the new tools to develop innovative experimental platforms.

9. **Magnetohydrodynamic and particle-based simulations to model Z conditions.**
Current modeling tools used to design and interpret Z experiments are missing key physics models and require unphysical simplifications. We anticipate that models that combine the features of particle-in-cell and magnetohydrodynamic (MHD) techniques will be needed to design new facilities and to optimize pulse shaping to realize the objectives discussed above.

10. **<u>Classical and quantum-mechanics-based atomistic simulation techniques</u>**
    Atomistic simulations are critical to develop high-fidelity physics models for the design and simulation of Z experiments and for calculating equations of state and electrical and thermal conductivities. Advances are needed to enable more realistic simulations and increase physics fidelity to support the material phase, kinetics, and transport objectives described above. We plan to expand our pioneering work in quantum Monte Carlo techniques and establish the capability of using *ab initio* calculations to build potentials for classical molecular dynamics approaches. We intend to be at the forefront of leveraging new computing techniques in the emerging initiative to develop exascale computing.

11. **<u>Impact on SNL's Stockpile and Counterterrorism programs</u>**
    Stockpile life extension programs (LEPs) present significant challenges to Sandia's system engineering and component teams. We have demonstrated that our experimental and computational capabilities can increase the scientific validity of engineering analyses in a responsive and cost effective manner. We will proactively seek deeper understanding of Directed Stockpile Work (DSW) issues and prioritize partnerships that benefit these programs. We will also seek synergies in the requirements of our traditional NNSA science program and the Nuclear Counterterrorism (NCT) program to amplify our impact on national security.

12. **<u>Academic Alliances</u>**
    Connections with universities are critical to maintain the quality of our work through peer interactions, provide intellectual excitement for the staff, and assure a pipeline of future researchers. We will nurture our existing collaborations by active engagement and support of the formal Z Fundamental Science Program. We will be alert for new opportunities through NNSA's Stockpile Stewardship Academic Alliances and by encouraging the work of universities with active research groups in planetary science, geophysics, shock physics, and plasma physics. Collaborations on Thor may offer uniquely interesting opportunities for joint projects in the very near future.

13. **<u>Collaborations with LLNL and LANL</u>**
    Collaborations with our sister laboratories are essential for understanding the material requirements of the nuclear explosive package and helping the NNSA deliver a nationally coordinated program that maximizes taxpayers' return on investment. Strengthening ties with our sister laboratories is an absolute priority; the known and anticipated requirements motivate this entire plan!

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I. Description of the Dynamic Materials Program

Our Dynamic Materials Program uses high-speed experimental facilities, primarily Z and gas guns, to provide critical high-strain-rate material response data at temperatures, pressures, and densities relevant to NNSA's Defense Programs and other national security applications. The NNSA Science Program is our principal sponsor, and Sandia's Nuclear Weapon PMU is a key stakeholder within the Laboratory. The mission of the NNSA Science Program is to

> *Provide the Nation with the scientific and technological means to assess the safety, security, and effectiveness of nuclear weapons; support resolution of SFIs; develop new technologies for future stockpile options, including LEPs; and provide a technical foundation enabling capabilities for nuclear security.*[1]

We support these missions by improving scientific understanding through the acquisition of high-accuracy data that defines material behavior under extreme conditions, thereby providing a reliable basis for models that will enable predictive simulations of material and component performance for nuclear weapons and other national security applications. For example, our notable successes to date have included Z ramp-compression measurements on Pu that led to major improvements in the models that support annual assessments and contribute to the completion of a comprehensive survey of high-pressure material properties that improves the nuclear safety in future stockpile options.

The DICE and STAR small-scale facilities ensure cost-effective, high-turn-around experiments at lower pressures. In addition to obtaining data, we develop diagnostics and techniques at these facilities for eventual implementation on Z. The DICE and STAR experiments support a range of programs, including Sandia's DSW activities, NCT, and intelligence efforts. Thor, a new intermediate-scale pulsed power driver currently housed at DICE, will enable high throughput experiments with adjustable loading rates to pressures of around 100 kbars in 2017 to a peak of about 1 Mbar in 2019.

The acquisition of high quality data in extreme regimes and the integration of theory and experiments are the hallmarks of our program. Tests are designed, analyzed, and optimized using a broad range of simulation codes and capabilities. Our program is particularly strong in atomistic modeling and MHD code development. Atomistic modeling supports development of tabular material models used in multi-physics codes and informs materials theories with detailed structure and process analysis.

[1] FY 2016-2025 Science Program Plan draft, January 2017, p. 4.

A. Critical Issues and Gaps in Predictive Capability for Material Response

1. Equation of State, Phase, and Transport Properties

The equation of state (EOS) describes material density as a function of pressure and temperature. It connects the thermodynamic and hydrodynamic evolution of materials in multi-physics simulations. High-fidelity equations of state are necessary to understand everything from HED experiments to nuclear weapon performance. The EOS, strength, constitutive properties, electrical conductivity, and optical characteristics all depend sensitively on the phase (*i.e.*, solid, liquid, or gas). Different phases or crystal structures display decidedly different properties. For example, metals in the body centered cubic (bcc) structural phase, in general, have higher strength than metals in the face centered cubic (fcc) phase. Transitions from one phase to another are often encountered in the dynamic material loading histories associated with weapon performance.

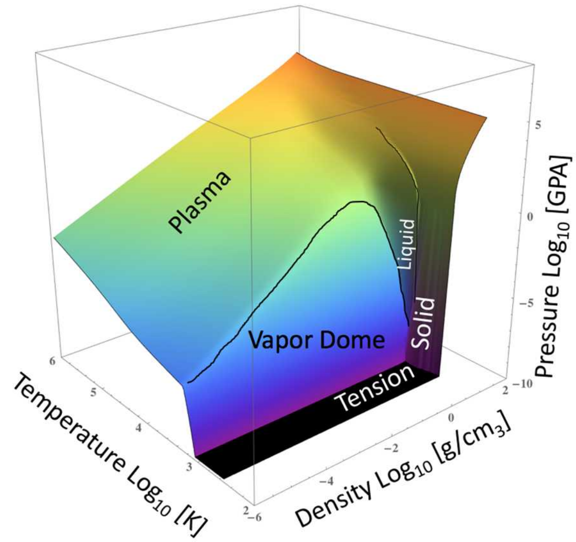

Figure 1. Equation of state for copper. An equation of state describes the pressure, density, and temperature and is used in multi-physics codes to model a material's response. The location of melt, vaporization, and rate of pressure increase with density in a solid is unique to each material.

Although Z data have contributed greatly to understanding material response at conditions of direct importance to the Stockpile Stewardship Program, critical regions in pressure, temperature, and density have remained inaccessible. A dearth of ramp compression data exists above 5 Mbars for most metals, particularly those relevant to the Stockpile Stewardship Program. In addition, many applications require knowledge of material properties at higher temperature states than can be accessed via ramp techniques and at lower temperatures than can be accessed via traditional single shock techniques. The available range of experimental data is constrained by the present limitations of diagnostics. The lack of definitive material phase identification for Z experiments and the difficulties with making reliable temperature measurements in many regimes are particularly problematic because these parameters are critical to formulation of material models for simulation codes.

2. Material Strength

Material strength controls the resistance to deformation. It is important to the behavior of a structural material during assembly, storage, and use. It is also a key consideration in accidents and other off-normal conditions that can affect the behavior of a system or component in dynamically driven applications. The assessment and modeling of strength embodies considerable complexity and depends on many factors, including the thermodynamic state, loading history, phase, age, kinetic effects, and microstructure. Current simulation codes explicitly account for almost none of these effects; however, national defense programs have identified the need for strength models that can address all of these factors. Pulsed power experiments, which can evaluate the effects of material microstructure and age using macroscale samples of representative materials, could provide the data to address the effects of these factors on strength. Improvements in pulse shaping, attainable peak pressure, and analysis are needed to realize the potential benefits.

3. Microstructure

Material response is sensitive to the detailed microstructure, which, in turn, is sensitive to manufacturing processes. Compressibility and strength may be affected by small (ppm) quantities of contaminants in an alloy as well as processes such as cold working and/or heat treatment. Even minor changes in traditional material production techniques are known to impact the microstructural properties. These relationships are not well understood or captured in continuum models.

Figure 2. Image from electron backscattering diagnostic of grains in an additively-manufactured stainless steel. The different colors represent different grain orientations.

Engineered materials, such as those produced by additive manufacturing (AM) processes, are being adopted for an increasing range of applications. This trend impacts reuse-remake-redesign decisions for LEPs and the introduction of advanced manufacturing to reduce costs and improve agility. AM materials respond differently than conventional materials;[2] the differences must be well understood if they are to be certified for nuclear weapons or other applications. Tools that can short circuit the development cycle by adding predictability to the process-structure-performance equation would have enormous value. Adequate experimental platforms, mesoscale sensitive diagnostics, and microstructure-sensitive analysis tools are needed, but do not currently exist.

4. Kinetics

Many materials undergo phase transitions at a wide range of pressures and time scales. There is evidence that many of these transitions occur over finite time periods, and the time and energy required for a phase transition affect the conditions of the material once it reaches the new phase. Refreezing of a material after melt is a critical transition that probably occurs on a finite time scale that may depend significantly on the loading rate.[3] Phase transition kinetics are currently modeled with empirical phenomenological models and are typically not addressed at all in large-scale continuum codes. Other physical properties, such as strength,[4] may depend strongly on kinetic effects. Our present measurement capabilities in this area are limited and significantly restrict our experimental data base for understanding the physics of kinetic effects. An important goal for the national dynamic materials program over the next 10 years is

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[2] J. L. Wise, D. P. Adams, E. E. Nishida *et al.*, "Comparative shock response of additively manufactured versus conventionally wrought 304L stainless steel," *Shock Compression of Condensed Matter – 2015*, AIP Conf. Proc. **1793**, 100015, AIP Publishing (Melville, NY, 2017).

[3] D. H. Dolan, K. D. Knudson, C. A. Hall, C. Deeney, "A metastable limit for compressed liquid water," *Nature Physics* **3** (5), 339-342 (2007).

[4] M. D. Knudson and Y. M. Gupta, "Transformation kinetics for the shock wave induced phase transition in cadmium sulfide crystals," *J. Appl. Phys,* **91**, p. 9561 (2002).

therefore to determine the effects of strain rate on the kinetics of phase changes as well as on the mechanical strength. At present, different experimental platforms at the NNSA laboratories produce different time scales. The capability does not exist to only vary the time scale without changing other critical parameters in order to address kinetics.

B. Role of pulsed power to characterize material response for weapon predictive capability

Since material issues are ubiquitous in the nuclear security enterprise, many platforms are used to address these issues. This section addresses the differentiating character of pulsed power, particularly on Z and Thor, to provide material response data.

Material models are assessed using laboratory facilities at all three NNSA laboratories using a variety of dynamic loading platforms such as high-power lasers, pulsed power, and gas guns. Each platform fulfils a unique role in developing, parameterizing, and assessing material models. Generally, gas guns focus on shock experiments with up to centimeter-scale targets at pressures up to several Mbars. High-power lasers, such as those at LLNL's National Ignition Facility (NIF), can address very high pressures (10s or even 100s of Mbar), but the sample sizes are limited to 10 to several hundred microns. The Z pulsed power facility is used for higher-pressure shock experiments (10 to 20 Mbars) than gas guns and on ramp and shock-ramp experiments up to 5 Mbars with millimeter-scale samples; such samples are large enough to address heterogeneous materials and still provide precise (less than 1 % uncertainty) measurements. The Thor intermediate-scale pulsed power driver, which is being constructed, will provide higher throughput for intermediate pressures up to 1 Mbar. Meeting the needs of the national dynamic materials program requires broadening the range of conditions studied, increasing the throughput to address the number and types of materials required, and providing more precise control of the material conditions.

Today, Z provides unique capabilities for dynamic materials properties experiments, including:

- flexible pulse shaping that enables ramp compression, shock-ramp compression, and very high pressure (10-20 Mbars) shock experiments,
- adequate sample sizes for extreme pressure experiments to investigate the effects of microstructure on material response and/or understand the response of bulk heterogeneous materials,
- stockpile and NCT-relevant pressures and/or time scales that cannot be attained on gas guns or the NIF, and
- experiments with hazardous materials including Pu and Be.

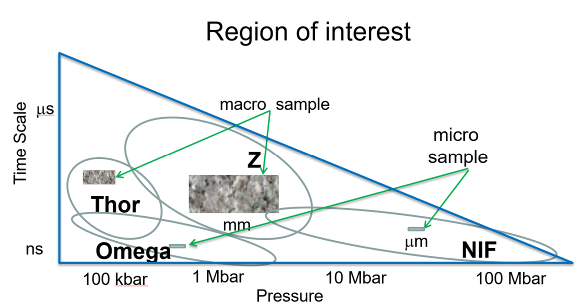

Figure 3. Materials for nuclear weapons and other national security applications are subjected to pressures of a few kbars to 100s of Mbars. Relevant time scales range from ms for some delivery and accident conditions, to μs for shock and implosion conditions, and to ns for very high pressure and thermonuclear processes. Grain sizes for solid

materials are typically 10s to 100s of μm. Z, and soon Thor, uniquely address mid-range pressures and time scales with samples that can include many 10s of grains to assess the continuum response to microstructural variations.

II. Strategic Objectives

We have developed a set of strategic objectives to capitalize on our differentiating strengths to meet national security imperatives over the next 10 years. A specific objective is to develop the business case to motivate an intrinsically-safe materials facility and then begin the construction.

Near-term to mid-term (3-5 years)

- Develop x-ray diffraction diagnostics to measure phase boundaries accurately, including for hazardous materials.
- Create platforms that reach higher pressures and access broader regions of phase space in temperature and density than can be reached in pure ramp or shock experiments.
- Measure temperatures in dynamic materials experiments for precise determination of the thermodynamic state.

Mid-term to long-term (5-10 years)

- Determine the effect of microstructure on material response, for example for aged and additively manufactured materials.
- Develop methods and determine the time-dependent material response (kinetics) during dynamic compression for deformation (strength) as well as solid-solid, solid-liquid, and liquid-solid phase transformations.
- Measure material strength at multi-Mbar pressure.
- Develop platforms for transport properties such as electrical and thermal conductivity.

Theory and simulation capability

- Improve MHD and particle-based simulation capabilities to model the unique conditions predictably that are encountered on Z and should be achievable on future pulsed power systems (*e.g.*, a new facility focused on dynamic materials experiments and Z-Next, a replacement for Z using new technologies).
- Apply as well as continue to develop leading-edge capabilities for calculating properties of matter in extreme conditions using methods based on atomistic quantum mechanics-based simulation techniques.
- Ensure the research is highly integrated among experiments, theory, and simulations. Our long experience in employing atomistic- and multi-physics simulations in combination with the data has led to significant new insights across research areas and in NNSA research programs.

Alliances

- Increase our role in Sandia's DSW and the NCT Programs by applying our expertise to problems of key importance to the Laboratory and the Nation.
- Create and maintain academic alliances for research and recruiting in order to make the Pulsed Power Sciences Center a magnet for talent in high energy density physics.
- Strengthen our collaborations with LLNL and LANL.

A. Obtain approval and funding for the design and construction of a new pulsed power facility focused on dynamic materials experiments

Z has been used to launch flyer plates to velocities far greater than can be reached with gas guns for shockless ramp compression experiments and recently for combining these approaches to shock-ramp samples. However, significant gaps still exist that cannot be addressed by Z or any other driver. Z does not have the power flow control to address the kinetics of phase change or the shot capacity to address the plethora of materials needed by the NCT program. Systematic experimentation to support microstructural-aware modeling will also be shot limited. Finally, existing containment systems are considered reliable only to a few percent, and any release could be disastrous for all programs on the facility.

A pulsed power driver of ~ 20 MA, coupled with advanced phase-sensitive diagnostics, would meet these needs. A proposed capability relies on switching each individual Marx component separately to enable very fine control over the temporal shape of the current pulse. This would allow control of the loading rate for experiments to investigate kinetic effects in phase. That proposed driver could be designed to handle hazardous materials by utilizing a valveless containment system that would be far less susceptible to failure than current systems. A new facility would significantly increase the number of experiments that could conduct experiments for NNSA's Dynamic Materials Properties (DMP) subprogram and all other programs and would provide an important opportunity for collaboration with the academic community.

To obtain the approval for this new capability, we will focus on generating community and Laboratory executive support to document the programmatic needs that would be met. We will also develop a set of design requirements to meet those needs, along with a conceptual design of the machine, which will allow us to estimate the cost. This information will be collected and submitted to NNSA to obtain CD-0, the first step necessary to obtain approval for a new construction project.

Time Line:

- 2016-2018:
  - Develop mission needs document and design requirements
  - Develop conceptual design and preliminary cost estimate
  - Seek support from SNL, LANL, LLNL, and NNSA executives
  - Obtain CD-0 approval
- 2018-2020:
  - Complete CD-1 evaluation of Analysis of Alternatives to meet the mission need
  - Obtain CD-1 approval
  - Begin machine design and component testing
- 2020-2023:
  - Build the machine

B. Short-term to Mid-term Objectives (3-5 years)

1. Develop capability to measure phase boundaries accurately for hazardous and surrogate materials

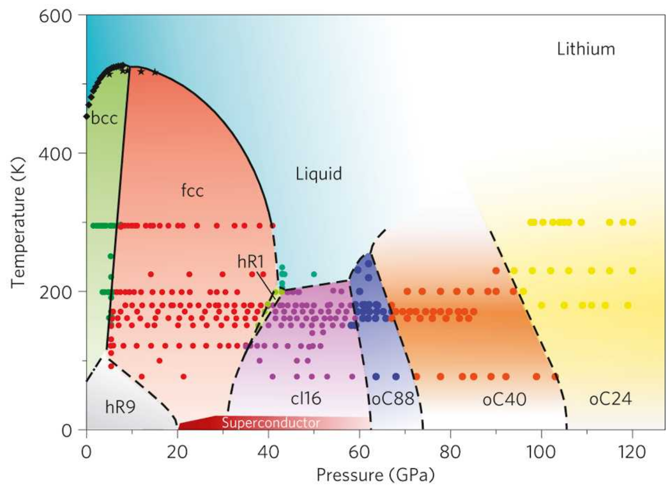

Figure 4. Phase diagram of lithium showing a number of solid phases with a large degree of complexity with increasing pressure. [C. L. Guillaume *et al.*, *Nature Physics* **7**, 211-214 (2011).

The tri-lab materials community has established a strategic goal of multi-phase EOS models to provide a high degree of accuracy in predictive simulations. Material properties such as strength and electrical and optical conductivity often depend sensitively on the phase of a material. An obvious prerequisite to developing "phase aware" EOS, strength, and transport property models is determining the phase diagram of a material over a broad pressure-temperature range.

An important goal for the Dynamic Material Properties group over the next 10 years is to develop new capabilities to identify phase transformations experimentally. Fiber-based techniques such as observing changes in reflectivity vs wavelength and ellipsometry may be useful but do not provide direct insight into the high-pressure phase. Thus, significant effort will also be expended to develop dynamic x-ray diffraction (XRD) techniques for Z and Thor. We will focus on developing methods and techniques that are compatible with our containment system for hazardous materials.

Time Line:

- 2017-2018:
  - Explore diffraction in Z-specific geometry on the Dynamic Compression Sector at the Advanced Photon Source
  - Develop suitable x-ray sources and survivable detectors on Z
  - Increase Z-Petawatt energy for x-ray sources
  - Explore diffraction sources for Thor
- 2018-2022:
  - Implement single frame diffraction on Z in 2018
  - Develop XRD detector systems compatible with containment on Z
- 2022:
  - Implement contained diffraction on Z

2. Develop and utilize advanced platforms and data analysis techniques to reach higher pressures and access a broad region of phase space

Nuclear weapons reach density, temperature, and pressure conditions that are not accessible with existing platforms, particularly for macroscopic-scale samples; material models are often highly inaccurate in extrapolated regimes.[5] Platforms capable of achieving order-of- magnitude higher pressures and of probing properties in broader regions of the phase diagram would therefore have high mission impact. Improved load-path flexibility to reach regimes between the Hugoniot and the principal isentrope is also needed to reach and identify phase boundaries.

Higher pressure can be reached by exploiting convergence. Our present cylindrical platform reaches up to 15 Mbars in most materials[6] but deviates from simulations around 5-6 Mbars. In the next 5 years, we will implement a combination of experiments, models, and code validation in an effort to create a reliable platform based on cylindrical convergence.

As shown in the figure, shock-ramp loading paths access a broad range of the phase diagram, including solid-solid phase transitions, melting, and solidification. Using analysis and diagnostics, including Bayesian forward techniques, we will mature the planar shock-ramp platform to infer the kinetics of phase transformations. However, current losses and variations in the load current, when using our present containment system limit their use on special nuclear material experiments.

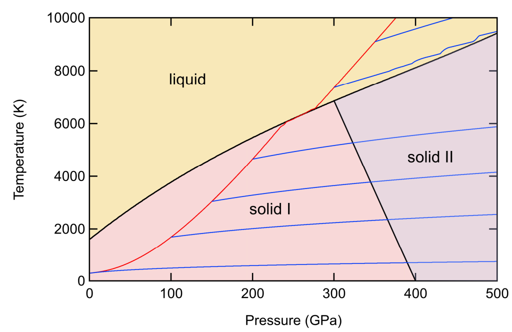

Figure 5. Shock-ramp compression enables experimentalists to map out complex phase boundaries.

A major new project is therefore to improve the containment system for Pu experiments that use the full capabilities of Z. For the Next Generation Containment (NGC) project, subject matter experts in power flow and high explosives are designing a system with reliable closure and significantly improved power flow. The two goals for the project (improving the power flow to the load and fast enough closure of the ultrafast explosive valve) compete in design space and, hence, there are challenges to overcome.

Time Line:

- 2018:
  - Infer EOS of a material from a cylindrical high-pressure experiment
- 2019:
  - Complete development and authorization of NGC system and use for high impact Pu experiments
- 2019:
  - Infer kinetics of solidification for a material via planar shock ramp
- 2020:
  - Complete rigorous uncertainty quantification analysis of ramp and shock-ramp experiments

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[5] S. Root *et al.*, *Phys. Rev. Lett.* **185**, 085501 (2010); T.R. Mattsson *et al.*, *Phys. Rev. B* **90**, 184105 (2014); C.T. Seagle *et al.*, *Appl. Phys. Lett.* **102**, 244104 (2013).

[6] R.W. Lemke *et al.*, *J. Appl. Phys.* **119**, 015904 (2016).

3. Develop the capability to measure temperature in hazardous and surrogate materials

There is considerable mission interest in understanding the properties of materials off the principal Hugoniot. Our recent efforts have therefore focused on quasi-ramp and shock-ramp compression experiments. The temperature data are particularly important to characterize the thermodynamic state under off-Hugoniot loading conditions.

Measuring the temperature in most of our experiments is very difficult because conditions in ramp or shock-ramp experiments range from 500 to 5000 K and do not produce enough emission for streaked optical pyrometry. For low temperatures, we must develop new techniques. In the near term, above 1000 K, we will develop an IR (infrared) pyrometry system for Z in collaboration with LANL. This IR approach would be especially useful for shock- ramp loading experiments. We will begin testing a new system soon with the goal of full operation in FY 2018.

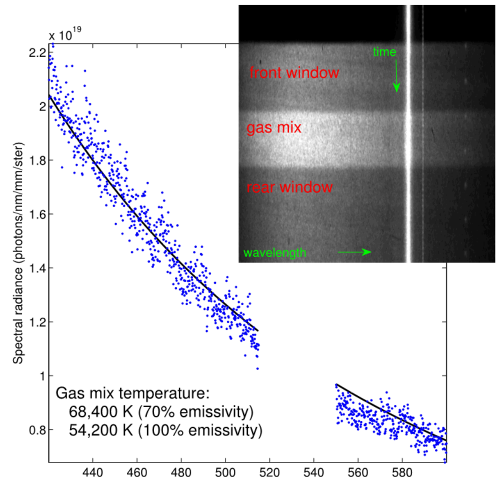

Figure 6. Temperature data using streaked visible spectroscopy. Wavelength is measured vs time, resulting in a 2D time-frequency map. For lower temperatures, infrared spectroscopy is required.

Our longer-term efforts will focus on novel techniques for very low temperatures (*e.g.*, temperature-dependent changes in the reflectivity of gold). To improve the techniques, we are testing these systems on gas guns and smaller pulsed power drivers. These new methods will provide a unique capability for present and future platforms on Z, Thor, and next- generation pulsed power facilities.

Time Line:

- 2017-2018:
  - Develop infrared pyrometer for temperatures between 1000 and 10000 K
- 2019-2022:
  - Implement infrared pyrometer on containment experiments on Z
  - Implement infrared pyrometer on range of facilities
- 2020-2025:
  - Develop reflectivity or Stokes technique for temperatures below 1000 K

C. Mid-term to Long-Term Objectives (5-10 years)

1. Determine effect of microstructure on material response

Engineered materials, porous materials, and new advanced manufacturing approaches such as additive manufacturing result in very different microstructures, with poorly understood dynamic material response (*e.g.*, residual stresses, elevated dislocation densities, complex textures, high porosity, and impurities). The manufacturing technique can affect the dynamic strength of the material.[7] Future weapon performance calculations will need models that are microstructure-aware and can be used in continuum-scale codes. This objective is challenging because appropriate data for analyzing relationships between microstructure and performance are sparse and modeling approaches are under development.

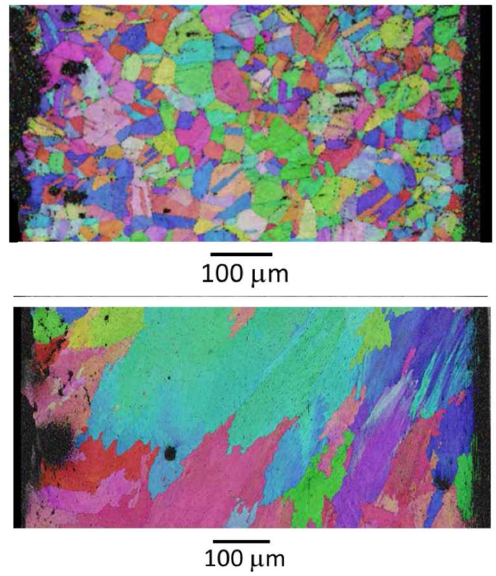

Figure 7. Microstructure of conventional 304L stainless (top) and Z-cut additively-manufactured 304L (bottom). Microstructural differences result in different dynamic strength.

We are uniquely positioned to contribute in this area because of our testing facilities and expertise in multi-scale modeling.

Using DICE, STAR, Z, and Thor, we can conduct macroscopic sample tests in almost any pressure regime and loading history of interest. Our team will work with customers (*e.g.*, component and system engineering) as well as researchers at our sister laboratories in materials science, modeling and simulation, and field tests to develop and implement a microstructure-aware approach to qualification of engineered materials.

Time Line:

- 2017-2018:
  - Build a multi-disciplinary team with 1400, 1800, and outside groups to develop validated, direct numerical simulation tools to inform models
- 2018-2019:
  - Investigate diagnostics to characterize material response at the mesoscale
  - Implement recovery of shock- and ramp-compressed samples
  - Pursue collaborations with LANL and LLNL for targeted Z experiments
- 2019-2020:
  - Demonstrate systematic characterization of a microstructural feature such as contaminant level or grain size on Thor for a relevant material
- 2020:
  - Document an integrated plan for 2020-2025 combining theory, computations, experiments, and partnerships

[7] J. L. Wise, D. P. Adams, E. E. Nishida *et al.*, *op. cit.*, 100015.

2. Develop methods to determine the underlying physics responsible for time-dependent material response during phase transformations and deformation

The conditions under which a material changes phase while undergoing dynamic compression can depend on a wide range of variables. For example, the pressure at which a phase transition occurs can depend on the rate of compression of the material and its mesoscale structure. In addition, the dependence on impurities or other variables may be different for dynamic compression compared to static measurements. Understanding these dependencies is essential for modeling dynamically compressed matter and relating dynamic to static properties.

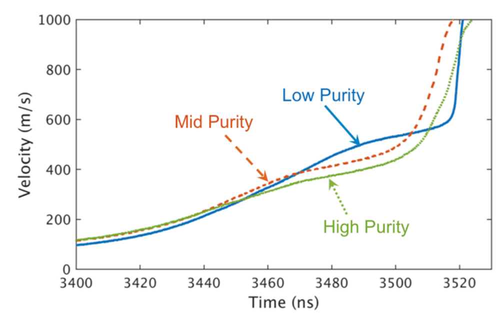

Figure 8. Timing of the Zr $\alpha \rightarrow \omega$ phase transition under ramp compression depends on sample purity.

A critical aspect for understanding the time-dependent material response is the capability to control the loading rate and make time-resolved measurements of the phase. We are developing diagnostics (ellipsometry and x-ray diffraction) to detect phase changes. Concurrently, we will develop simulation methods using atomistic classical and quantum simulations to understand the underlying physics responsible for the time-dependent materials response. A high degree of pulse shaping to vary the strain rate at interesting phase boundaries will be available in the near term at moderate pressures on Thor and eventually at higher pressures with a high-hazard driver. Graded density impactors also enable strain rate variation. We will utilize these new capabilities to study phase transitions at variable loading rates.

Time Line:

- 2017-2019:
  - Develop techniques to modify the strain rate on Thor experiments
  - Apply diagnostics for phase on Z and Thor experiments
- 2018-2020:
  - Explore and delineate material phase diagrams based on first-principles simulations (DFT and QMC)
- 2020-2022:
  - Quantify the role of kinetics and the physics of refreeze for key materials under ramp compression
- 2022-2025:
  - Use a new facility to obtain loading rate dependence on materials at high pressure, perform analyses, and participate in cross-platform collaborations.

3. Develop methods to determine the underlying physics for material strength, particularly effects of phase transitions, microstructure, and loading history

The resistance to deformation of a material (commonly referred to as material strength) can have important consequences for dynamic loading response. Models describing this property are developed to ensure accurate response predictions. Modeling is complex because strength depends on thermodynamic conditions, microstructure, phase, and loading history. A key goal is to understand the effects of material phase and mesoscale properties on strength. We support modeling efforts by conducting experiments to determine material strength as a function of these parameters. Our approach determines strength by measuring the material response during ramp loading followed by a release.

LANL and LLNL use alternative approaches, and comparing the results is an active endeavor in the national program.

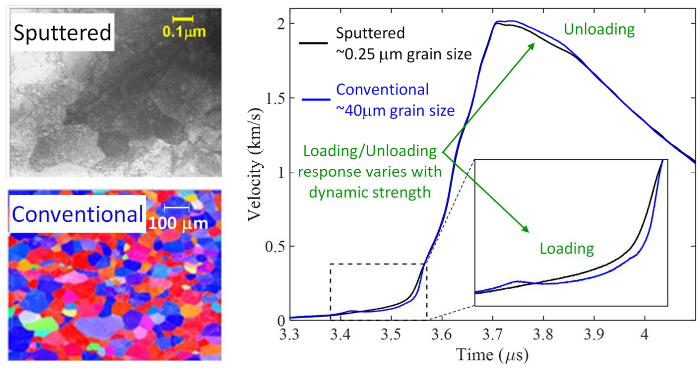

Figure 9. Z ramp-compression experiments on tantalum demonstrate a significant dependence of high-pressure strength on the material production technique and consequent microstructure.

The Dynamic Material Properties group seeks to include strength in our phase-aware EOS models. In particular, a key goal is to determine the strength of a material undergoing a solid-solid phase transition or melt and then refreezing. Kinetics can affect strength. We seek to develop loading techniques to examine strain rates from 10^4-10^8/s, which requires pulse-shaping capabilities offered by next-generation electromagnetic drivers.

Time Line:

- 2017-2018:
    - Make cross platform tri-lab Ta strength comparison to identify gaps in modeling and theory (no variations in phase or microstructure)
    - Evaluate multi-phase modeling capability
- 2019-2022:
    - Develop capability to vary shear stress on Z and Thor (such as magnetically applied pressure shear, or MAPs)
    - Optimize Thor for systematic strength evaluation
    - Use new temperature and diffraction measurements to constrain strength experiments on Z and Thor
    - Address modeling of dislocation effects
- 2022-2027:
    - Perform systematic studies of strength and phase, microstructure, loading rate, and path history on Z and Thor and cross platform initiatives
    - Assess modeling capability to separate hydrostatic and deviatoric components

4. Integrate new experimental and theoretical techniques to determine transport properties of matter at multi-Mbar pressure

Multi-physics simulations of complex dynamic materials and HED experiments on Z, NIF, and Omega depend on accurate transport models (*i.e.*, for electrical and thermal conductivity, opacity, and viscosity control of material and energy). Increased capabilities in transport properties will improve the fidelity of a broad range of multi-physics simulations. The transient character of dynamic experiments makes the measurement of these properties particularly challenging. First-principles calculations are also challenging since we must calculate the response of excited electronic states as well as collective atomic motion like phonons and plasmons.

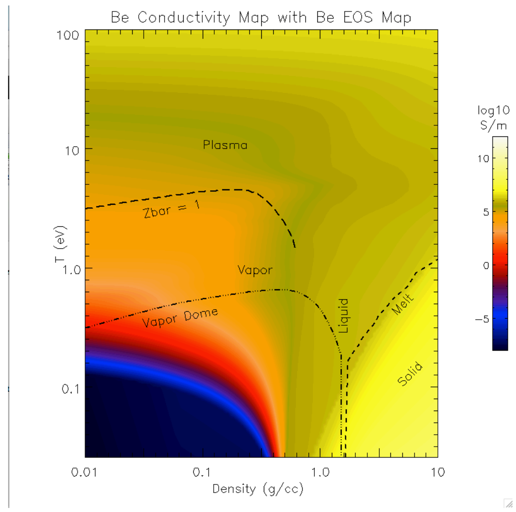

Figure 10. Electrical conductivity for beryllium in a color overlay of the equation of state. Changes in phase are correlated with changes in conductivity. The two properties are intrinsically linked and the behavior in simulations is closely coupled.

We will develop a new generation of theoretical and experimental techniques to address these challenges. We will continue to rely on, and improve, linear response-type calculations (Kubo-Greenwood) for electrical and thermal conductivity as well as to grow our capabilities in time-dependent density functional theory (TDDFT). We will also develop a platform to measure electrical conductivity directly under shock, ramp, and shock-ramp conditions and a platform to use ellipsometry-based techniques to measure the complex dielectric function of high-pressure states. Measurement of the complex dielectric function, in turn, includes information on the frequency dependence of electrical conductivity. Platforms targeting viscosity and thermal conductivity are even more challenging to develop. Although viscosity can be addressed by studying flow perturbations, and thermal conductivity can be assessed as energy balance in integrated experiments, we expect that first-principles simulations will play an important role in developing the models for these properties.

Time Line:

- 2017:
  - Perform x-ray Thompson scattering calculations from first principles (TDDFT)
  - Conduct experiments using ellipsometry on Z
- 2018:
  - Make direct 4-point measurements of electrical conductivity on Z
- 2020:
  - Perform direct calculation of electron-ion dynamics using TDDFT
- 2020-2025:
  - Develop platforms to measure viscosity and thermal conductivity

D. Theory and Modeling Objectives

1. Extend MHD and particle-based simulations to model unique conditions on Z

Z experiments are designed, analyzed, and optimized using multi-physics codes. Z's unique environment, which includes extremes in density and temperature, requires solving problems that span kinetic to fluid modeling. These problems are very complex and often require unphysical simplifications that modify the physical solution in some regions in order to obtain tractable simulations.

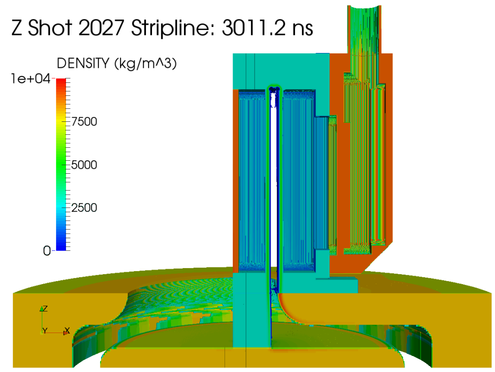

Figure 11. 3D simulation of high-pressure planar EOS experiment using ALEGRA MHD shows plasma generation at base of the load with a potential for causing losses.

We will develop new code capabilities to simulate key phenomena in high energy density physics that will work efficiently on the next-generation supercomputers. Physical effects important in pulsed power must be included. We anticipate the hybrid particle-in-cell/MHD capability will be needed to address power flow and plasma physics. This new capability will accelerate experimental progress on Z and allow for more accurate scaling studies of target physics and current delivery on future machines.

Our recent initial work extending solvers is encouraging and will serve as the foundation for future developments. Code development in this area requires teams spanning several organizations, including Pulsed Power Sciences, Center for Computing Research, and Radiation & Electrical Sciences as well as support from Laboratory Directed Research and Development and Sandia's Advanced Simulation and Computing program management.

Time Line:

- 2017:
  - Implement an initial Generalized Ohm's law, with an asymptotic preserving electromagnetic algorithm coupled to hydrodynamics on a regular mesh in ALEGRA
- 2018:
  - Develop capability to simulate the current distribution in a cylindrical geometry experiment to enable EOS inference to 10-15 Mbars
- 2020:
  - Implement Adaptive Mesh Refinement
- 2022-2025:
  - Develop a particle-in-cell/MHD coupled multi-scale capability on an exascale computer architecture

2. Pioneer classical and quantum mechanics-based atomistic simulation techniques to calculate key material properties at extreme conditions

Our dynamic material properties program has a distinguished record of collaborative efforts between experiments and corresponding *ab initio* calculations, principally those with density functional theory (DFT). In addition to the direct simulation of experimental conditions achieved on Z and other platforms, these calculations have been critical to developing high-fidelity physics models for the design and simulation of Z experiments. Use of DFT is now routine for calculating equations of state and electrical and thermal conductivities. We are applying DFT to calculate entropies, viscosities, diffusion rates, and path integral molecular dynamics (PIMD) for nuclear quantum effects.

Building on the success of our DFT efforts, we now have a complementary strong effort in quantum Monte Carlo (QMC) simulations. QMC methods, which do not rely on an approximate functional as does DFT, excel where very high accuracy is required. Since electrons are cold in this approach, it is particularly relevant for very accurate low temperature calculations. A primary application of this method will be to develop phase diagrams for a broad range of low-Z materials by 2020 and high-Z materials by 2025, through leveraging exascale computing capabilities.

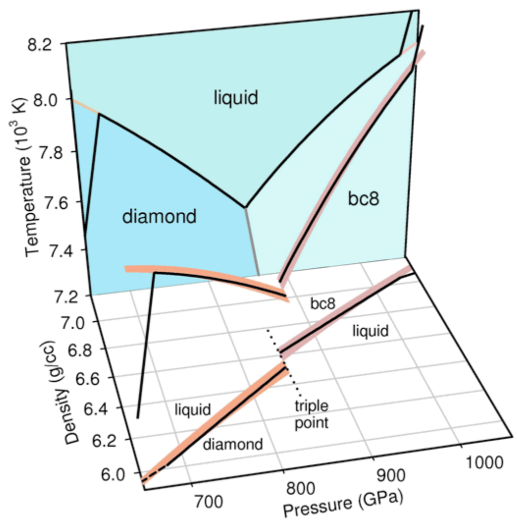

Figure 12. High pressure phase diagram of carbon determined from DFT simulations and Z experiments.

The *ab initio* methods used in DMP are limited to rather small systems, ranging from dozens to, at best, a couple of thousand atoms. For the direct simulation of loading and the dynamics of deformation and transformation under stress, the natural choice is a large-scale classical molecular dynamics (MD) approach. An area of ongoing and increasing research will be to expand our efforts with *ab initio* calculations to build high-fidelity model potentials for use in classical MD codes.

Time Line:

- 2017:
  - Use path-integral and nuclear quantum effect calculations routinely with PIMD
- 2020:
  - Establish a production capability for using *ab initio* calculations to build high-fidelity potentials for classical MD codes
- 2020:
  - Evaluate a broad range of low-Z material phase diagrams with QMC
- 2025:
  - Evaluate a broad range of high-Z material phase diagrams with QMC, leveraging exascale computing capabilities

E. Alliances

1. Increase our impact to SNL's Directed Stockpile Work and Nuclear Counterterrorism programs

Center 1600 provides key support for Sandia's mission in nuclear weapons and global security. Historically, most of our effort has been devoted to DSW related to nuclear weapon components. Recently, we expanded our role by supporting the Nuclear Threat Science (NTS) program. Leveraging our in-house experimental and computational capabilities, we provide highly valued data on materials and components under high strain rates and high pressures for DSW and NTS thrusts.

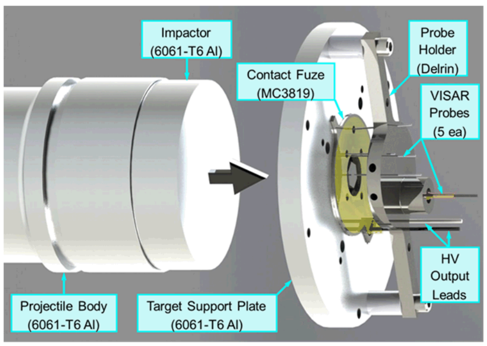

Figure 13. STAR and DICE gas-gun tests provide dynamic electrical and mechanical response data for fully functional contact fuzes under realistic stockpile-to-target-sequence conditions.

Our DSW activities address the design and performance of components such as impact fuzes, neutron generators, power supplies, energy absorbers, and radiation shields for major weapon systems. DMP personnel in Center 1600 will identify and engage with our nuclear weapon customers (*e.g.*, component and system engineering) and research groups (*e.g.*, materials science, modeling and simulation, and field test) to implement multi-faceted, science-based efforts related to changing component requirements and threat perceptions. A key objective will be to use our test facilities to rapidly and cost effectively produce extensive data sets to address a wide range of stockpile-to- target-sequence conditions to improve stockpile responsiveness. In a similar fashion, we will support NTS programs that involve materials or design configurations that have not previously been evaluated.

The DICE, STAR, and Z platforms provide unique material EOS data and nuclear weapon component testing capabilities. We are studying hazardous and non-hazardous materials and sharing our data with the LANL and LLNL to improve EOS models. Our future DSW and NTS activities will continue to investigate dynamic strength effects, examine compaction of electrically active, energetic, porous, and granular materials, and assess the resultant performance of weapon subassemblies and components. Furthermore, our research focus will be expanded to include AM materials, which are of interest to the DSW and NTS programs and relevant to our stockpile stewardship mission. For example, we will evaluate the differences in the dynamic strength of AM vs conventionally wrought metal alloys and examine the consequences of 3D printing on the performance and safety of explosives.

2. Create and maintain academic alliances for research and recruiting

The importance of university partnerships is evident in NNSA's Stewardship Science Academic Alliances (SSAA) program, is emphasized in Division 1000's strategic plan, and is well recognized within group 1640 and Center 1600. We plan to maintain our existing partnerships selectively and create new ones in order to underpin our world-class dynamic materials research. Universities with active research groups in the areas of planetary science, geophysics, shock physics, and plasma physics are natural partners for us. Academic partnerships bring concrete advantages in the area of recruitment, development of laboratory scientists, and increased creativity and productivity. Because of such collaborations, our scientists are able to participate fully in the international research community, engage with graduate students and their professors, and exchange research ideas. The importance of academic collaborations for retention of our first-class research staff cannot be overstated. We have two main avenues for partnering with academic groups: first, our formal Z Fundamental Science Program (ZFSP) for joint experiments on Z, and, second, direct collaborations with academic research groups with or without contracts and funding.

Our Center's research tools and resources are made available, through the ZFSP cycle, to academic scientists for state-of-the-art research. The third ZFSP call for proposals will be issued in June 2017 and will close on September 15, 2017. The program's objectives are to conduct fundamental research in HED science and to provide the research experience to maintain and grow the HED community, especially through the involvement of academic researchers. Proposals are solicited and evaluated by an independent review panel based upon their feasibility for a specific facility and their scientific merit.

Direct research collaborations with academia are organized in different ways. These ways include, for example, long-term relationships where we and an outside research group contribute complementary expertise, research contracts with outside scientists to work on a specific problem, support and mentoring of undergraduate or graduate students (either summer or year-round), or joint appointments between Sandia and a university. The formality differs depending upon the nature of the collaborations, as do our financial commitments. Going forward, we plan to engage purposefully in collaborations with groups that are highly recognized in their fields and have a high throughput of students. We will focus on developing future collaborations with universities engaged within the SSAA as well as with the University of New Mexico.

3. Collaborations with LLNL and LLNL

These collaborations are essential to understand the material science requirements for the nuclear explosive package. We have developed a deep understanding of these requirements by engagement with the community and careful reviews of national strategy documents (*e.g.*, *Dynamic Plutonium Experiments Plan*, *Stockpile Stewardship and Management Plan*). We reach out to LANL and LLNL by devoting Z experimental time to their requests. Specific experiments are identified in joint discussions and reviewed by the HED Council. Our most notable success is a set of experiments that address the Pu phase diagram via ramp and shock-ramp compression of specific stockpile alloys and the effects of Pu aging. Other collaborations with our sister laboratories focus on uranium, noble gases, comparisons of NIF and Z data, and NIF ablator materials. A current tri-lab effort is to determine how pressure, strain rate, and loading path affect the strength of tantalum, based upon cross-platform evaluations and cross-code comparisons.

We will continue to position our dynamic materials program to support high-priority national initiatives. Our experimental platforms are ideal for assessing the continuum-scale response to microstructural variations. For example, this capability dovetails well with NNSA's production science proposal and can help set the stage for MaRIE. Our Pu data from Z, in particular, help weapon designers optimize the impact of larger scale experiments without exceeding reactivity thresholds and by supporting the interpretation of integral data.

Strengthening ties with our sister laboratories is an absolute priority; their known and anticipated requirements motivate this plan!

III. Conclusions

Stockpile systems are composed of a large number of complex materials. Understanding, maintaining, modifying, and certifying the stockpile requires a detailed knowledge of these materials under the extreme conditions produced in nuclear weapons. The ability to assess aging, remanufacturing, and replacement of materials is critical to stockpile plans for the next decades. Understanding the underlying science behind these issues is necessary to address specific assessments quickly. This agility is needed to underpin a successful thrust to improve the responsiveness of stockpile activities. Our goal is to build on Sandia's strengths, namely the ability to produce high pressures and temperatures along variable load paths on large samples and to develop advanced capabilities that will provide the required knowledge. A new dynamic materials facility designed to produce relevant conditions that are difficult or impossible to create elsewhere and is optimized for high throughput and hazardous materials would have a major impact on the Nation's ability to address stockpile material science questions.

Achieving the objectives described in this strategic plan will allow us to conduct experiments that reach higher pressures and more relevant regimes using diagnostics, theory, and analytic tools to assess the material properties most important to weapons designers. We will take advantage of our existing strengths to study the effects of microstructure to address the national imperative to implement new production techniques for stockpile components. Our data will provide more precise materials models using defensible physics applicable to a much broader range of problems and allow deployment of advanced technologies for the stockpile. We will increase the agility with which aging and manufacturing issues can be addressed. Our dynamic materials program will support certification with confidence that the nuclear security enterprise can adapt to future requirements without underground testing.