LA-UR 09-07771

A Summary Report on the 21st Century Needs and Challenges of Compression Science Workshop

Bishop's Lodge, Santa Fe, NM

September 22-25, 2009

Organizers:
Dave Funk, Rusty Gray, Tim Germann, and Rick Martineau

Image by NASA/JPL-CalTech

Table of Contents

Executive Summary

The influence that compression science has had on national security science and its manifestation through discovery and application cannot be overstated. In addition to supporting the certification of our nuclear stockpile in the absence of underground testing and a broad spectrum of engineering and defense applications, compression science has altered our view of the material world around us. The discovery of unexpected physical and chemical phenomena and new materials through the application of compression science techniques has led to a new and refined understanding of the nature of chemical bonding in extreme environments. However, it is clear that many important aspects regarding the response of materials to compressive loading are still not understood, let alone modeled in a predictive mode. As a result, we have not derived the many benefits that a predictive understanding would bring. As one product of the workshop we held, we identified five challenges that capture the scientific needs that are required to achieve full understanding and that ultimately support our ultimate goal of moving from *"observation to control."*

These five challenges are as follows:

- Acquire time and spatially resolved *in situ* measurements at all length scales (i.e., atomistic, micro -, meso-).
- Discover new physics and chemistry in extreme environments.
- Incorporate material complexity into multi-scale simulations to achieve predictive capability.
- Unify static and dynamic compression understanding across relevant length and time scales.
- Leverage scientific knowledge derived from theory and experiment to the design and control of real materials (i.e., chemistry, microstructure, defects, etc.)

Making progress on these challenges will require a suite of new experimental tools and diagnostics as well as a suite of conceptual frameworks and theoretical constructs. The suite of experimental tools must include the development of diagnostic capabilities, such as next generation light sources, for peering into and achieving time-resolved measurements in compressed materials at the lowest relative length scales while simultaneously characterizing them at higher length scales. The theoretical suite must include new frameworks of computation that will allow the incorporation of the stochastic nature of matter, as well as the ability to accurately describe the essential physics without the invocation of phenomenological models, while linking the atomistic to the continuum response.

Progress on these challenges will not only allow us to develop a full understanding of compression science, it will create an environment in which we can train the next generation of scientists and provide them with the tools needed to make progress and move from studying "Ideal" to "Real" materials.

1. Introduction

For applications in the future, the design, synthesis, and manufacture of new materials with increased performance and functionality require an increase in our fundamental understanding of matter over the broadest range of thermomechanical conditions. Furthermore, access to extreme states of matter results in a rich array of physical and chemical changes that requires a broad range of science—from quantum physics to the collective continuum response—to interpret. In fact, current research reiterates this need: "Compression induces changes in bonding properties, giving rise to altogether new compounds and causing otherwise inert atoms or molecules to combine. When coupled with changes in temperature, altogether new forms of matter may be produced. For example, it has recently become possible to use laboratory techniques to compress materials to the point where the interatomic spacings are reduced by up to a factor of two and densities increased by over an order of magnitude. At these densities, the changes in the electronic structure begin to influence our very notions of chemical interaction and atomic bonding."[1]

Thus, fully exploiting the possibilities of chemical bonding, as derived from the application of pressure and tuned with temperature, will require new tools to generate these extreme environments, but will also require an ability to diagnose and "calculate" them. The field of compression science has generated rich insight and made us aware of the fact that we do not fully understand the nature of the processes that we induce with pressure. Presently, pressures reached during static compression can exceed the 300 GPa (3 Mbar) range and can temporarily exceed temperatures greater than that of the surface of our sun (> 6,000 K), while those pressures reached during dynamic compression can exceed the TeraPascal (TPa or 10 Mbar) range. In addition, the dynamic processes of shock compression are so fast that the loading is usually adiabatic, the typical durations range from femtosecond to microsecond time scales, and temperatures reach greater than 10^4 K, depending on the rate of loading and the magnitude of the peak compression. Developing new capabilities for reaching further extremes and diagnosing these equilibrium states of matter with unprecedented spatial resolution will inform and advance our understanding, assisting in our goal of moving from "observation science" to "control science."

To quantify these needs and future directions, leaders in the static, dynamic, and theory of compression sciences participated in a workshop entitled, "21st Century Needs and Challenges in Compression Science," held September 22-25, 2009, in Santa Fe, New Mexico. A series of plenary talks were given (see Appendix I), followed by a day of breakout discussions in the areas of static compression science needs, dynamic compression science needs, and theoretical needs of compression science to define the decadal technical challenges and necessary developments to meet these challenges

[1] "Basic Research Needs for Materials Under Extreme Environments," a report of the Basic Energy Sciences Workshop on Materials Under Extreme Environments, June 11-13, 2007, Jeff Wadsworth, Chair, George Crabtree and Russel Hemley, co-Chairs.

At its highest level, the needs of compression science could be captured by the following five challenges:

- Acquire time and spatially resolved in situ measurements at all length scales (i. e., atomistic, meso-, micro-).
- Discover new physics and chemistry in extreme environments.
- Incorporate material complexity into multi-scale simulations to achieve predictive capability.
- Unify static and dynamic compression understanding across relevant length and time scales.
- Leverage scientific knowledge derived from theory and experiment to the design and control of real materials (i.e., chemistry, microstructure, defects, etc.).

The ability to address these challenges will require a new set of characterization tools, temporally and spatially enhanced diagnostics, and the development of new predictive models to characterize the behavior of matter under these extreme conditions. The information gathered in static compression science experiments, when combined with information acquired dynamically, offers the opportunity of understanding the fundamental mechanisms that drive the processes occurring in the matter observed throughout the universe, ultimately leading to an ability of controlling matter to meet our energy and national security needs.

2. Breakout Summaries

2.1 Static Compression Science

Static compression science is a burgeoning field that is undergoing unprecedented growth in addressing a broad range of materials problems that span the physical, engineering, and biological sciences. Methods that rely on static compression experiments have many advantages, including the availability of multiple simultaneous diagnostics. These diagnostics have the potential for full materials characterization with an accuracy, precision, and sensitivity that approaches measurements on materials at near ambient conditions. The field is turning its attention to addressing major grand challenges in materials science, including the DOE Grand Challenges of moving from observation to control science and harnessing materials far from equilibrium. There is a strong synergy between conventional static compression, dynamic compression method, and theory; indeed, many problems cannot be addressed without the combination of all three of these approaches. With the prospects for the creation of new facilities, including major radiation sources, many breakthroughs are on the horizon.

2.2 Scientific Discovery Challenges: Static Compression Science

2.2.1 Structure and bonding at high compression

Based on recent work, we currently have a limited understanding of structure and bonding in condensed matter at very high compressions. Making measurements with an accuracy and resolution equal to those attainable at ambient conditions over a broader range of P-T conditions, particularly at higher pressures, will allow the development of truly predictive theory: a new paradigm for understanding condensed matter. We will extend this knowledge across the periodic table over the full range of pressure and temperature, and extend chemistry from valence to core electrons, effectively to explore and develop "kilovolt" chemistry.

Our knowledge of materials is largely based on understanding obtained from systems at near-ambient conditions. Because of this, there are numerous examples of intriguing and poorly understood phenomena, nearly all of which were not predicted theoretically or were simply unexpected. Among the many examples are the recent observations of the novel $(O_2)_4$ cluster-based structure of dense oxygen; the unprecedented polymorphism of Na which exhibits some 11 different phases and melting below room temperature at megabar pressures; and the remarkable pressure-induced transformation of both Li and Na from metal to insulator. The origin of the behavior in all three previous examples at the level of truly predictive, general theory is lacking. Current static compression data observations are based on phenomena observed to pressures of 200–300 GPa. What happens at higher pressures, e.g., at 1 TPa and beyond? There are numerous possible other applications/fields for static higher-pressure compression, including materials science, and planetary science, astrophysics.

2.2.2 New physics in cold dense matter

Theory suggests the existence of new physics in materials at very high pressures (e.g., 0.5–1 TPa) and low temperatures. There are currently no experimental data in this regime; indeed, it is likely that experiments will reveal altogether new phenomena not predicted by theory. Achieving higher pressures together with variable temperatures and other extreme fields in combination with new diagnostics will lead to a deeper understanding of the nature of matter. The new physics that will be revealed, for example, will drive new theory into the mechanisms of magnetic and electronic order.

An excellent example is the predicted metallic superfluid; it is a proposed magnetic technique that would be a signature of the predicted new state of matter: a superfluid superconductor. The first challenge is reaching the combined pressures, temperatures, and fields needed and containing hydrogen to explore this. The diagnostics would involve imaging the vortex matter that would be created, as predicted by theory. Beyond fundamental physics, there are numerous potential implications for energy, planetary science, and astrophysics.

2.2.3 Fundamental thermodynamics

We currently have a limited understanding of the basic thermodynamic properties of many materials, including relatively simple elemental substances, in the currently accessible megabar pressure range. These properties include phase diagrams of many systems, where in some cases extremely large discrepancies in melting temperatures exist between static studies, shock compression, and theory. Since each of these approaches has its own limitations, and more important, may explore different phenomena or states of materials (e.g., stable versus metastable, relaxed versus unrelaxed), the existing putative discrepancies may provide evidence for new behavior in materials. Excellent examples include the melting curves of bcc transition metals, such as Ta. By bridging the current gaps that exist between these methods, we will find solutions to apparent discrepancies in phase stability, structures, transitions mechanisms, and dynamics, and thereby develop an understanding of the general phase behavior of materials at extreme P-T conditions. For this, accurate in situ probes of structures, dynamics, and equations of state are needed up to multimegabar pressures (e.g., 0.5 TPa) and temperatures from millikelvins to ~1 eV.

Another example of fundamental thermodynamics at extreme P-T conditions is the nature of equilibrium defects and grain boundaries under these extreme conditions in pure systems as well as interfacial phenomenon in alloys, composites, and complex materials. So far, there has been very little work on studying interfaces directly under any degree of compression. An interface at high pressure is a buried interface, so the most prevalent tools of surface science are useless. Interfaces currently may be studied using a monolayer of a material with a unique signature or using a surface-sensitive spectroscopic method such as sum-frequency generation. New interface sensitive *structural* probes are needed. The scientific challenges include understanding how interfaces and interfacial interactions between similar or dissimilar materials are affected by high pressure, how interfacial structure (e.g., interfaces with high surface free energy versus interfaces with lower surface free energies) changes with pressure, and how interfacial reactivity (e.g., the reactivity at the surface of a heterogeneous catalyst) responds to pressure. The applications include (1) lubrication resulting from the behavior of thin layers of lubricants between surfaces; (2) adhesion,

adhesion failure, and material aging, e.g., the interactions of adhesives with the surfaces of materials; (3) catalysis and electrocatalysis where the structures and, therefore, reactivities of the catalytic entities can be continuously varied by the application of high pressure; (4) control of the strength of materials by controlling the grain boundary structure; and (5) geoscience and planetary science in which this information is crucial for understanding the large-scale structure and physical properties of planets, including their evolution and dynamics of their deep interiors.

2.2.4 Time-dependent transformations

Equilibrium phase diagrams and stability relations are only a first step. In general, equilibrium properties do not adequately describe material behavior in dynamic processes. Compression-rate dependence of phase nucleation, growth, melt, and microstructure are vital to understanding and modeling dynamic events. By pioneering a broad range of time-resolved diagnostic probes (e.g., with x-rays, neutrons, or lasers), we need to selectively interrogate materials during pressure-induced transitions with the precision characteristic of static compression techniques. Such measurements will provide rate-dependent kinetic phase diagrams and establish an experimental basis for implementing predictive capability.

Development of a fundamental understanding of the influence of kinetics and compression-rate dependencies of phase transition will have a profound impact on high-pressure science and technology. Measurement and study of kinetic phase diagrams are crucial to understanding, modeling, and simulating dynamic processes. As a material is dynamically driven across a phase line, the nucleation and growth kinetics are the critical parameters determining the development of the new phase. Indeed, at exceedingly high-compression rates, the material may transform to altogether new (e.g., amorphous) phases rather than the thermodynamic equilibrium phase. Experimental data regarding kinetics at high pressures is very limited and credible predictive theoretical approaches do not exist. Pressure-drives with precise control and tunability across a broad range of pressures, temperatures, and compressions rates will provide crucial data for establishing insights into this challenging area of research.

This work will address the largely unexplored area of phase transition kinetics and dynamics and will be valuable in developing models of meteoritic impacts (geophysics) and other impact phenomena (DOE/NNSA and DoD). Control of phase transformation kinetics directly impacts the microstructure and associated constitutive properties of materials for technological applications. In addition, at high-compression rates, the possibility exists that the synthesis of materials with unique identification of novel metastable materials along reaction paths could have important technological and geoscience implications.

2.2.5 High-pressure strength, plasticity, and rheology

Material response under compression is a function of chemistry, phase content, microstructure, defects, impurities, as well as pressure and loading rate. By developing novel x-ray diffraction and nano-imaging techniques and pressure devices with the ability to apply controlled and characterized uniaxial or shear strain in well characterized environments, we will quantify the complete stress state in materials exposed to high pressure and the deformation mechanisms and flow stress as a function of strain rate and across grain boundaries.

The limited static (or quasi-static) high-pressure strength measurements performed to date rely on assumptions (e.g., magic angle analysis, peak broadening), and do not take advantage of new developments (e.g., emerging nanobeam probes and imaging methods). Required are new imaging techniques as a function of time, which will require in turn advances in anvil cell designs. These designs will permit pre-defined and controlled loading paths, direct nanoimaging of the stress state with nanometer resolution at nanosecond time scales, 3D tomographic mapping of strain of grains in composite materials, and full definition of the stress state as a function of material, pressure, and loading rate. Determination of stress tensors across material microstructures as a function of hydrostatic and deviatoric stresses provides critical input to theory, modeling, and simulation. The results would potential provide the basis for new physically based models for high P-T strength, including strain rate dependence. This information is of crucial importance for weapons physics, but there are also profound implications for geoscience, astrophysics, and planetary physics.

2.2.6 Synthetic chemistry frontier

Pressure can be used as a novel reactive variable in chemical synthesis. By interrogating intra- and intermolecular bond characteristics using novel x-ray and optical spectroscopies, by utilizing time-resolved probes following compression, and by using theory to develop recovery strategies and elucidating thermodynamic path dependencies, we will predict and control chemical reaction of novel materials and thereby develop a better understanding of the deeper intramolecular and intermolecular interactions under extreme conditions.

As one the largest ranges of any external variable, pressure can be used as a tool or "catalyst" for affecting new chemical reactions and bonding constructs not observed under atmospheric conditions, opening up intriguing possibilities for the discovery of new matter and novel methods of synthesis. Pressure increases local reactant concentrations, producing molecular (steric) configurations that have been shown to influence transition states or intermediates, and resultant product species along the reaction coordinate. The combination of controllable and well-defined high-pressure/temperature conditions offered by modern high-pressure cells devices, combined with advanced tools for probing these molecular states along the reaction coordinate, such as optical and vibrational spectroscopies, x-ray spectroscopies, and x-ray and neutron scattering methods offers exciting possibilities for controlling chemical reactions and discovering or designing new materials under these conditions.

The challenges to probing chemical reactions under high-pressure/high-temperature conditions include small sample volumes, the potentially low thresholds for material damage subjected to ionizing radiation, a lack of methods for temporally-controlled pressurization combined with transient probes of bond-breaking/making steps, and dearth of in-situ techniques typically used in the chemical synthesis laboratory within high-pressure devices in the absence of recovery and post-mortem analysis. Structural relationships for a wider variety of chemical functionalities under a range of high-pressure/temperature conditions and pathways are needed. This fundamental knowledge, combined with theoretical calculations of high-pressure reactant surfaces, could eventually lead to rational design of synthetic targets, much like the current status of the field of

organic chemistry. Here again, we must move from *observation* to *control*, an approach that so far is essentially lacking in high-pressure chemical synthesis at pressures above 1 GPa.

2.2.7 Optimized new materials

As indicated above, high compression has the possibility of creating new, quenchable materials with enhanced properties and functionality. By using the altered bonded states under such conditions, we will create new, useful materials that are recoverable to, and stable at, ambient conditions. Combined with developments in theory to predict material properties, suitable catalysts, and recovery pathways, we will develop new materials with enhanced superconducting, magnetic, thermoelectric, hydrogen storage, solar, and physical properties.

The highest temperature superconducting temperatures are found under pressure. For example, the Hg-Ba-Ca cuprate has the T_c of 164 K measured in 30 GPa; however, the high Tc does not persist when recovered to ambient pressure. Can these active mechanisms be understood and harnessed under ambient or moderately cool environments? Other possibilities, such as "green" hydrogen storage based on H_2O ices, and the prediction and creation of various ultra-hard materials, some with properties superior to diamond are expected to be possible in the future. It is known that double and triple bonds, for example, are particularly active under high-pressure conditions. Polymerization reactions, driven by electronic interactions, occur as "reactants" and are brought into closer contact with applied pressure. Small molecules, such as N_2, and its isoelectronic relative CO, have been predicted and shown to polymerize under moderate pressures. A polymeric form of CO has been recovered to ambient conditions and shown to be highly energetic, decomposing exothermically to gaseous CO, and offering the exciting possibility of new classes of explosive materials, prepared in the absence of catalysts and solvents. Still other examples include the recent creation of bulk metallic glasses under pressure and the prospect of making other types of glasses based on the observation of pressure-induced "polyamorphism." For these, the challenge is the recovery of these materials in large quantities for useful applications. There are obviously significant implications for materials science, energy science, and national security science.

2.2.8 Radiation-induced high-pressure chemistry

Ionizing radiation (e.g., x-rays, visible light, neutrons, and protons) can be used as a novel source of electronic rearrangement in chemical synthesis as well as an unwelcome mechanism of damage. By predicting bond ionization for the synthesis of desired products with a given functionality, and by investigating molecular bond breaking via time-resolved x-ray and optical spectroscopies, we will be able to design chemical reactions to target novel materials as well as calibrate and even control damage.

Understanding the behavior of materials under extreme conditions of high pressure and high radiation flux is vital for understanding and improving the performance and reliability of nuclear weapons and nuclear reactor components. In addition, as so many studies of materials are conducted using lasers, neutrons, and x-ray beams as part of current and next generation sources, it is vital to quantitatively calibrate and assess the damage caused by ionizing radiation. We have discovered that the rate of damage from x-ray beams has a strong and reproducible dependence upon the pressure (at least in the case of TATB,

slowing with pressure), which suggests that materials can be studied, despite radiation damage, by subjecting them to sufficient pressures or using time-resolved probes.

Techniques used to study radiation-induced chemistry to date include white beam energy-dispersive x-ray diffraction, x-ray Raman spectroscopy, and monochromatic angular dispersive x-ray diffraction. Samples are interrogated both before and after radiation bombardment to assess mechanisms and rates of damage. The challenge will be to develop additional probes and to use diagnostic in real time to determine atomic and electron level mechanisms with varying sources (light, neutrons, varying energy, varying x-ray flux). The benefits of this work would be twofold: (1) developing quantitative benchmarks for radiation-induced damage in materials *and* (2) using various kinds of radiation in combination with pressure, temperature, and other fields for the rational design of new materials with new properties and functionalities.

2.2.9 Earth science, planetary science and astrophysics

Static compression science is creating an ever-expanding picture window of increasing clarity and resolution on the interiors of our planet. Despite this advancing vision, many regions of the Earth remain poorly understood in terms of material properties. An excellent example is the Earth's core. This region of the planet is mainly composed of iron, but in a state that is far different from the element found near the surface of the planet. Iron has interesting, if not unusual polymorphism, elasticity, and strength; there are dramatic changes in chemical and magnetic properties, and iron is even a superconductor under pressure. We need to understand not only the high-density solid phases, but also the fluid states to pressures above 350 GPa. This information is crucial for modeling the Earth's magnetic field and determining the temperature distribution and heat flow from the interior.

Another rich area of study is the core-mantle boundary region, where oxide and silicate phases exist that are never seen on the Earth's surface and have completely different physical and chemical properties from near-surface rocks and minerals. Moreover, advances in observational planetary science and astronomy have led to materials questions about bodies throughout the cosmos. By reaching higher pressures and temperatures, and by making accurate determinations of the physical and chemical properties of planetary materials at such conditions, we will determine the structure, composition, dynamics, and evolution of the full range of planetary bodies and other astrophysical objects. This will have profound implications for our current understanding of the evolution of solar systems and the possibility of life elsewhere in the universe. Planets, stars, and other astrophysical bodies are natural high-pressure chambers, so interpreting the wealth of new geophysical and astronomical data in terms of their component materials will also add new understanding of information that is important for fundamental physics, chemistry, and materials science

2.2.10 Life in extreme environments

We do not currently know the limits of life in extreme environments. By developing new methods for making in situ measurements of structure-function of biological systems, from whole communities of organisms to component molecules, we will be able to define the habitable zone in the cosmos, the limits of life on Earth, the possible origin of life, new

methods for directed evolution, and thereby develop the new field of high-pressure genomics/proteomics.

2.2 Technical Grand Challenges in 'Static' Compression Science

2.2.1 Reaching 1 TPa and beyond

The recent dramatic improvements in high-pressure generation and extreme condition diagnostic capabilities are clearly leading to important scientific advances, but this is only the tip of the iceberg. Achieving pressures exceeding 1TPa, far beyond the current capability of ~400 GPa, will enable studies in entirely new regimes of physics. Novel high-pressure apparatus design and materials are needed to extend current pressures limits. New anvil materials, for example, could be based on CVD single crystal, nanocrystalline diamond, and new types of composites. Using a nano-focused x-ray beam to measure anvil nanostrains together with large synthetic diamond with enhanced physical properties, for example, we will optimize pressure cell design. Such breakthroughs will enable open extreme compression laboratory environments to myriad of diagnostic tools available in static compression studies and herald new understanding of matter under extreme conditions.

2.2.2 Developing multi-probe 'intelligent' devices

The next generation high-pressure designs that will extend pressures limits to 1 TPa and beyond will require tailored anvils that enable the measurement of a broad range of physical properties with high spatial resolution. Extension of tailored designer anvils can measure new physical properties, including electrical conductivity, thermal conductivity, and NMR. Nano-scale manipulation and sub-micron patterning and modification on anvils will result in a dramatic extension of measurements that will be enabled in extreme environments. The results could also lead to novel nanosensors with applications beyond extreme environments.

2.2.3 Stress-strain states and P-T calibration

Accurate characterization of the stress-strain state of materials is central to all aspects of high-pressure science; it also underlies the challenge of calibrating pressure as one reaches ever more extreme conditions. With the development of multi-diagnostic probes, "ab initio" calibrations of pressure can be developed (i.e., by measuring bulk modulus and density on the same loading state). However, we can now go much further and produce detailed maps of the micro-strains in samples from which the 3D stress distributions can be determined. The development of micro-focusing capabilities is crucial. Nano-focused x-ray beam will allow measurements of nanostrains in not only the anvils and gaskets but also the samples and pressure (stress) calibrants. Such high-spatial resolution probes can make detailed mapping of material properties. New theory and modeling of composite materials is needed to provide robust and reliable stress-strain inversions. Accurate calibration of temperature at very high pressure is also needed; this calibration needs to be carried out by combining static and dynamic compression and theory. Addressing these technical challenges is required in order to open extreme compression environments to the myriad of diagnostic tools available in static compression studies.

2.2.4 Advancing x-ray methods

Inelastic x-ray spectroscopies such as x-ray Raman Spectroscopy (XRS), x-ray absorption spectroscopy (XAS), x-ray emission spectroscopy (XES), extended x-ray absorption fine structure (EXAFS), nuclear forward scattering (NFS), and nuclear resonant inelastic x-ray scattering (NRIXS) will be harnessed to interrogate deep core-level bonding changes and phonon density of states (DOS) determinations under extreme conditions. Using techniques rooted in the phonon modulation of Mossbauer nuclear energies, the phonon density of states can be determined. In the XAS, XES, and EXAFS techniques, valence electronic states are probed by photoelectron absorption and emission. Temperature can be determined by appropriate fits of the phonon DOS, which can allow potential novel methods to ascertain sample temperature under extreme conditions. For experiments performed to date, Be gaskets are used to allow x-rays into and out of sample region. There is also likely to be sample decomposition with bombardment. XES is usually achievable for primarily heavier atoms. XRS reveals bonding changes (e.g., hybridization alteration) under extreme conditions. XAS and XES provide a measure of changes in valence and deeper electronic changes (cf., "kilovolt" chemistry). Though these are now established techniques, the measurements are, in general, photon limited.

NRIXS and NFS measurements are only possible with high flux sources due to their inherent low signals for conventional high-pressure-sized samples (nanoliters, cubic microns) and the requirement for highly filtered x-ray light using double monochromators to achieve meV energy resolution. Thus, long detection times are required due to low signal to noise; moreover, measurements at the highest pressures are impossible with current technology because the signal overwhelms the background. Only Mossbauer-sensitive nuclei can be used (NRIXS and NFS). Most measurements cannot be performed over the wide range of pressures needed (e.g., multi-megabar pressures) or with sufficient spatial resolution to address the above science challenges. Hence, higher brightness x-ray sources are required.

2.2.5 Real time x-ray imaging with nm resolution

The above dual advances in x-ray spectroscopies and time-resolved methods need to be combined ultimately for in situ time-resolved imaging. Such imaging methods are essential for understanding the time evolution of defects in materials, starting at the subpicosecond scale. Another example is the technological challenges for studying interfaces at high pressure, which stems from issues of sensitivity, i.e., detecting a small number of interfacial species, and selectivity and suppressing the background of the associated bulk media. For planar interfaces buried within opaque media, such as bimetallic interfaces in metal, grazing x-ray scattering could be useful. But for buried opaque complex interfaces, such as the grain boundaries inside a polycrystalline metal, good techniques do not yet exist. One suggested possibility, based on the paradigm of nonlinear optics, might be the use of nonlinear x-ray optics using intense short-duration coherent x-ray pulses, for example, imaging grain boundary structures using 2-photon x-ray microscopy.

2.2.6 Neutron scattering to multi-megabar pressures

Neutrons are complementary to x-rays, as they probe nuclei (not electron distributions), magnetic structure, are sensitive to hydrogen, and have high penetrating power. However, neutron scattering studies are currently limited to ~30 GPa by the need to use large sample volumes to overcome the inherent weakness of neutron sources. By using micro-focused

neutron beams, higher-intensity neutron sources, and larger sample volumes available using novel pressure cell technologies, neutron scattering measurements can be performed to above 100 GPa. The goal is accurate measurements to at least 300 GPa to address the scientific challenges described above. These measurements include both elastic scattering (e.g., diffraction) as well as the more difficult inelastic scattering (e.g., spectroscopy) measurements. Meeting these challenges requires advances in both high-pressure apparatus (e.g., larger sample volumes) and significant increases in neutron flux—not incrementally—but both by orders of magnitude. Such advances will enable the numerous strengths of neutron techniques to be extended to extreme compressions.

2.2.7 Challenge of liquids and amorphous materials

The inherent weakness of scattering from liquids and amorphous materials has long limited their study. Yet a wide range of novel extreme-conditions phenomena exists in such materials, including both polyamorphism and liquid-liquid phase transitions. We currently have a limited understanding of the nature of amorphous materials under high static and dynamic pressures. How are the atoms or molecules distributed spatially, and what is the range of local density variations? What new probes can bring insights into liquid-liquid transitions and melting phenomena at high-pressure conditions? How can melting be defined or determined (for metals, small molecules, etc.)? Likewise, second-order transitions between amorphous phases, such as glass transitions in polymers, are difficult to discern with current techniques. Methods such as neutron and x-ray scattering (SANS, SAXS, pair distribution function) currently give information about the distribution of atomic pairs in amorphous or liquid domains, but the scattering cross-sections are low, signals are often difficult to distinguish from diamond Compton scatter or other backgrounds, and analysis is difficult. Acoustic measurements used to derive bulk volumetric information are frequency dependent and do not offer atomic-level insights into compressive responses.

This area of study will require developing novel detector technologies to enable inelastic Compton scattering to be removed, extending neutron scattering techniques to higher pressures, and using nano-imaging techniques. For example, new methods are needed with enhanced signals (or enhanced detection) for interrogation of amorphous samples at high pressures in small sample volumes, coupled with high accuracy knowledge of local temperature and stress states. Potential improvements can be gained from back-drilling the diamond anvils along the incident x-ray axis, use of slits, or increased flux. Likewise, neutron scattering measurements with smaller focused beams in large volumes at even higher pressures, as discussed above, will open up a large number of potential measurements on amorphous phases. The measurements must be coupled with modeling efforts aimed at capturing and interpreting the stochastic nature of these forms of matter. Finally, extending these new tools to the time domain and combining them with transient measurements of transport properties, viscoelastic properties, and kinetics of liquid-liquid and liquid-solid phase transformations will be necessary for interpreting the dynamic aspects of phase diagrams, improving equations of state for amorphous or multiphase materials (including melt), and evaluating bonding in new forms of matter.

2.2.8 Filling the strain rate gap: Static to shock

Interesting and largely unexplored physics lies between the static and dynamic time-scales at high pressure. Mode transitions, as well as phase transformation kinetics, are known to

be strong functions of loading rate. By developing high-pressure cells with precisely controlled and calibrated loading rates capable of compression rates to 10^5, cycles at kHz, and single-shot rapid decompression, and by developing detectors and probes consistent with these new experimental capabilities (sub-micron spatially, sub nano-second temporally), we will elucidate the rate-dependent properties for the first time.

Systematic studies of phase transitions can be achieved using tunable precise pressure-drives in conjunction with time-resolved diagnostic probes (e.g., x-ray, neutron, and laser). The time-resolved probe can be synchronized and timed to selectively interrogate the sample as it is driven across the phase transition. The dynamic diamond anvil cell (dDAC) is one example of a tunable pressure-drive suitable for these types of studies. Pulse-selection hardware and high-speed detectors at high-performance sources are necessary technical components to perform these proposed studies.

2.2.9 Transport properties

There are few measurements of thermal and transport properties at high pressures/temperatures. Examples of desired measurements include thermal conductivity, diffusivity, and viscosity in small volumes at high-pressure/temperature conditions. The present state-of-the-art concerns the use of designer anvils for resistivity measurements, NMR and rolling-ball viscosity measurements at low pressures, and laser-based foil heating methods to estimate thermal conductivities. These challenges could be met with advances in pulse-probe NMR methods, development of non-magnetic diamond cells capable of high pressures, exploitation of confocal, ultrafast optical methods for both heating and detecting temperature changes spatially in high-pressure sample volumes, and design of new embedded-probe anvils for measuring heat flow.

2.2.10 Thermochemical measurements at multimegabar pressures

In addition to constituitive, transport, and dynamical measurements, there remain great challenges in measuring fundamental thermochemical data needed to address the science challenges discussed above. New techniques are needed, for example, to determine free energies, enthalpies, entropies, and heat capacities of pure, complex, and nanophase materials starting at even modest pressures. A combination of time-resolved optical methods combined with highly sensitive nanolithographic techniques need to be developed for measurements to be performed in concert with the in situ studies described above.

3. Dynamic Compression Science

Dynamic compression science has historically been a field in which measurements have been made (primarily) at the bulk or continuum level. Details of the effects of phase transformations, defect generation, chemical composition, shock-induced chemistry, and the effect of grain boundaries and grain orientation on dynamic material response have only been inferred through wave profile analysis and/or post-experiment examination. That said, the level of detail gathered in the first decades of compression science was adequate for the simulation and modeling capabilities available at the time, and the weapons community was able to design modern weapon systems through a combination of "simple" simulation and experiment. This is no longer the case.

Today, we are on the verge of transforming dynamic compression science from science focused on developing understanding at the continuum level to a scientific discipline focused on developing understanding at the atomistic and mesoscopic scales, ultimately leading to the linking of scales and the ability to predict and control performance under dynamic loading conditions. Our current modeling and simulation capabilities have unprecedented temporal and spatial resolution: a result of modern platform development and better understanding of material response (though we have not yet reached simulation linking all scales), but we have not reached our goal of fully predicting and controlling material response. Reaching this goal will require a suite of new diagnostic tools and capabilities that can help answer the scientific challenges, described below, and provide validation data for next generation simulation capabilities. We will not succeed if we do not meet these challenging opportunities.

3.1 Scientific Discovery Challenges: Dynamic Compression Science

3.1.1 Kinetics and mechanisms of melting, freezing, and solid-solid phase transformations

A long-standing problem in compression science is the identification of the location (in Pressure-Volume-Temperature [P-V-T] space) and characterization of phase transformations, including melting, freezing, solid-solid transformations, and their associated kinetic rates. Of concern is the fact the static and dynamic measurements do not always yield the same location in phase space. This could be a result of differences associated with the transformation path dependence in P-V-T space, and/or the effect of strain rate (which can include both loading and release paths) on the transformation dynamics, or simply that the sample must be superheated during shock experiments to observe the transformation on the timescale of the experiment. Moreover, we have very few techniques for characterizing phase transformations, particularly dynamically. In principle, pyrometric techniques should yield characteristic signals associated with the temperature arrest that is indicative of a phase transformation, and transient X-ray techniques should provide structure information that ultimately could be quantified to yield fractional phases as a function of time. Neither technique has reached a maturity level that unambiguously meets our needs, and the data will be unimportant if our theoretical constructs regarding transformation are inadequate or at best phenomenological. Thus, in addition to advanced

diagnostic tools, we require the development of theories that accurately represent the physics of transformations and capture the path and rate dependence effects.

3.1.2 Warm dense matter (WDM): metallization, release around critical points

The metallization of matter when subjected to extremes of temperature and pressure has been considered and pursued since the development of band structure theory and the recognition that extreme pressure could cause a closure of such bands. That said, metals can also behave counter-intuitively. For example, lithium and sodium can become insulators under the extremes of pressure. Perhaps more importantly, the class of matter known as warm dense matter (WDM) lies in "no-man's land." It is not hot enough for direct application of Thomas-Fermi, yet too hot to accurately calculate the properties using classic cold-curve techniques. More important, we have very few methods for creating and characterizing such matter, both on initial compression and subsequent release. As an example, if one could reliably measure the conductivity under these unique conditions, while simultaneously measuring the temperature, pressure, and volume, the data set obtained would challenge and expand our current thinking regarding the equation of state (EOS) of matter in this regime. Furthermore, if we could create comparable conditions in a static setting, we could make a connection to between static and dynamic regimes that will improve our overall understanding. Thus, there is a significant need to develop capabilities for creating and diagnosing this state of matter, both to develop a fundamental understanding of such things as the nature of matter at the core of planets, but also to gain an understanding that can impact applications such as fusion, first-wall material studies for the International Thermonuclear Experimental Reactor (ITER), and enhance our understanding of nuclear weapon performance, including boost.

3.1.3 Evolution of microstructure under dynamic loading including defect distributions

Most metallic materials are polycrystalline in nature, such that they are an aggregate composite of metallic single crystals. As the polycrystal is deformed, the single crystals interact with each other so that the internal stress within the polycrystal is highly non-uniform. Simulations predict a factor of two or so difference between the minimum and maximum stress within the aggregate. If these materials are deformed a great deal, the temperature will certainly increase, and they begin to develop damaged regions and failure zones. The location of these damaged and failed regions is highly dependent upon microstructural characteristics (e.g., grain size distribution, impurity content, grain boundary strength) and the nature of the loading (e.g., time rate of loading, total strain, maximum stress). Figure 1 shows an image of tantalum deformed by plate impact loading. This image displays a snapshot of a material that has failed by the process of pore nucleation, growth, and coalescence (a ductile process). Note that the failed regions are spread out and indicate that the physical processes involved are stochastic in nature.

Predicting when and where material failure will occur with current theoretical and computational tools is still one of the biggest challenges facing the material modeling community. Failure is the final step in a complex physical process of microstructural evolution. The ability to understand and predict when and where failure will occur for any type of aggregate material (e.g., polycrystalline metals, high explosives, concrete, fibrous composites, etc.) requires that we not only understand the statistics of material initial

conditions such as grain size and morphology (for the case of polycrystalline metals), inclusion content and location, grain boundary shape, misorientation across grain boundaries, etc., but also how these quantities combine and evolve under service environments leading to failure. Deformation events that add to the initial heterogeneity are such things as inhomogeneous temperature change, dislocation cell formation, slip band formation, twinning, and phase transformation. Further microstructural evolution leads to discrete damage/failure processes, such as pore (ductile materials) or crack (brittle materials) nucleation, growth and coalescence, shear band formation and growth. These events also occur in three dimensions, of course, so we need to push our experimental and theoretical/computational capabilities to deliver this type of information in 3D. A two-dimensional characterization will never allow us to achieve success.

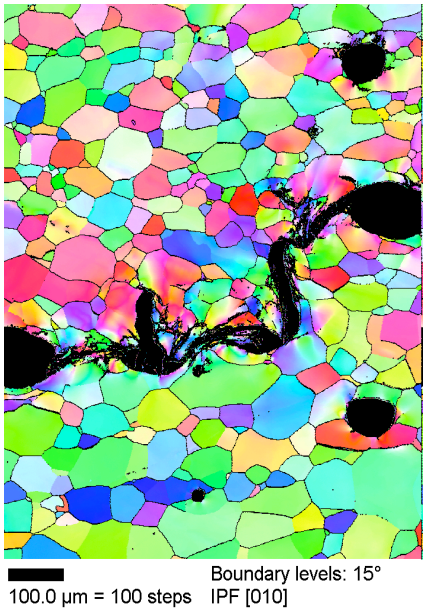

Fig. 1. Orientation Image Map of a deformed tantalum plate impact sample.

Thus, we have the need for a new experimental capability to track, in situ, the 3D microstructural (including defect distributions) and temperature field and their evolution. The information is needed to characterize and develop associated theories that incorporate the details of defect distributions leading to pore nucleation, pore growth and coalescence, dislocation cells, slip bands and twins, as well as shear bands.

3.1.4 Experiment/theory convergence: Developing the ability to reproduce simulations of 'real systems' for better understanding of experimental observations.

One of our greatest challenges is to be able to conduct experiments and perform associated simulations that are so precise in their initial conditions (such as the defect distribution and/or polycrystalline orientations and sizes) that we are modeling the "real" and not the "ideal" system. One approach would be develop experiments that directly evaluate the results of molecular dynamics (MD) simulations, such as an LINAC Coherent Light Source (LCLS) experiment with exactly the same number of atoms as an MD simulation, and validating at the appropriate length scale. Moreover, experiments might be designed to probe a particular physical regime to isolate and provide a means for better comparison with the simulations. Too often, we end up compromising on both the experiment and the simulation, with results that need interpretation or speculation to make the connection between the experiment and the simulation. Thus, the development of a series of experiments that are standards and/or the choice of simulations that we can properly diagnose in an experiment is critical to develop real understanding and to move from "observation to control."

3.1.5 Resolving the details of detonation and shock-induced chemistry

It has been the firm belief of many in the Energetic Materials (EM) community that the key to predicting explosives behavior for both performance and safety lies in the intimate understanding of the molecular-level processes. Energetics are complex systems that involve inter- and intramolecular bonding, numerous morphologies, different polymorphs, crystal defects, impurities, and component inhomogenities. EM can be made stable under ambient conditions, can be stimulated to energetic decomposition, will crystallize into a knowable structure with a given density, and can be fabricated into incredibly elegant shapes and strong mechanical structures. The crystal structure and intermolecular bonding strongly affect the density of the material and, thus, the energy delivered per unit volume of explosive. The molecular structure and the intermolecular bond energies will also affect the rate at which energy put into a molecule might escape to the bulk material, which in turn strongly affects the sensitivity and safety of the compound. Unfortunately, these molecular-level processes are not known even for systems that lack many of the complicating factors listed above. Without this detailed data, we cannot develop molecular-level predictive capabilities. Present theories can only lump most of the chemistry into overall reaction rates or energy release rates. The overall goal is to develop a complete time-dependent description of detonation and the evolution of the product's equation of state for military purposes as well as to facilitate the introduction of new energetic materials for military, counter-terrorism, surety, and industrial applications. These new energetic materials include explosives, rocket and gun propellants, and pyrotechnic devices. Various driving forces (which can be different for the wide variety of applications) include increased performance, increased safety margins, decreased cost, and decreased environmental impact. It is important to have optimal screening measures so that confident decisions can be made more rapidly on whether to proceed or not with a particular formulation. We need to develop the ability to screen, measure, and predict the performance of new or proposed materials for optimal use and/or unique applications.

3.1.6 Discovering new phases and forms of matter at ultra-high compression using tunable pathways and controlling reaction chemistry through pressure and temperature

As stated in the introduction, one of the key contributions of compression science has been through discovery, as generated by novel extremes of pressure and temperature. For example, the nature of the phase boundary in sodium and lithium was completely understood when the experiment elucidated its concave downward nature (in P-T space) and, in general, that the nature of bonding can significantly change with compression (imagine core electron participation in the extremes). Furthermore, chemical reactions that are forbidden on the ground state potential surface (e.g., Woodward-Hoffman forbidden) may be accessible under the extremes of pressure and temperature. Thus, the exploration of potential energy surfaces as a function of pressure may offer new routes for the synthesis and/or manufacture of materials that would otherwise be unachievable. The classic example of this is the conversion of graphite to diamond using pressure/temperature, but other examples such as the formation of polymeric nitrogen have demonstrated the utility of these concepts. Thus, using *ab initio* calculations as guides, and through the development of a robust experimental program (including the ability to tune pressure and temperature through the proper choice of wave profile, e.g., ramp, shock, etc.), we will be in a position to predict and/or discover new materials that may have functional behavior that meet our needs under extreme service conditions (e.g., armor, high neutron fluxes of reactors, etc.).

3.1.7 Discovering and understanding of the partitioning between dissipative and non-dissipative mechanisms

The concept of a shock is well defined. However, the underlying processes within the shock wave and the partitioning between dissipative and non-dissipative mechanisms are not well characterized nor well predicted. Predicting and measuring the Hugoniot Elastic Limit (HEL) and strength under loading is a must. We currently have little means for measuring and calculating transport properties, and therefore, our description of the loading process is incomplete and we cannot connect with theory. We must develop diagnostics at the appropriate scale (e.g., diffraction for atomic-level information) that allow the elucidation of mechanisms important in all rate processes, including transition from shockless loading to shock compression, and provide physical details that resolve phenomenological models of deformation such as the Swegle-Grady fourth power law. In addition to better experimental characterization, we have a need for the ability to predict transport properties, damage evolution, and localization phenomena.

3.1.8 Determine the role of shear in deformation processes

Shear can play a major role in initiating and controlling the physical and chemical processes that take place under dynamic loading, but needs to be quantified and better understood. We currently have little experiment and diagnostic capabilities for resolving shear so as to ascertain its role in dynamic material processes, including chemical reactions. For example, we would like to know the mechanisms that cause inelastic deformation, damage evolution, and failure and the extent to which shear contributes to these processes. Experiments designed to examine shear contributions would provide data that, in turn, would guide the development of a predictive capability by providing a mechanistic understanding of structural, chemical, inelastic deformation, fracture, and second-order phase transitions that can be driven by shear.

3.1.9 Develop understanding of the role of interfacial boundaries

There is a lack of understanding of the interaction of waves with boundaries (including spallation) and the stability of materials (or lack thereof) that result in the dynamic mixing of materials within local environments. Thus, we must conduct controlled experiments with high-resolution dynamic imaging to measure the velocity field evolution and dynamic mixing as a function of time, which would imply the need for measuring flow within opaque materials. Furthermore, this information is of little value without basic theories for prediction of the local geometries as well as thermodynamic states in the mixed phase regions. The mixed phase regions include heterogeneous interfaces of grain structure and their evolution. In addition, we need to understand the morphology, size of particulates, and their relation to global variables such as density evolution. Finally, we need the ability to determine material properties from observations of interfacial evolution under general loading conditions, which will allow us to predict and optimize material behavior to meet our functional requirements.

3.1.10 Develop an understanding of the transition in material plasticity and damage evolution across the ‘thermally activated’ to ‘shock’ to ’drag control’ regimes

There is a lack of understanding of the operative mechanisms of defect generation and storage across the transitions from thermally activated plasticity under uniaxial stress to

uniaxial strain shock loading. Furthermore, as we increase strain rate, the transition to drag control occurs as relativistic effects become operative. To date, only surface diagnostic tools have been applied to studying these fascinating transitional regimes in plasticity with little insight. Accordingly, theory has not achieved physically based models to address these transitions owing to a lack of mechanistic understanding of the changes in defect generation, motion, and thereafter storage processes as a function of the applied strain rate.

3.2 Technical Grand Challenges in 'Dynamic' Compression Science

3.2.1 Characterization of melting, freezing, and solid-solid phase transformations

We need to develop a comprehensive definition of melt. We know that loss of shear modulus, loss of long-range structure, and loss of autocorrelation are indicators, and we need diagnostics that connect to this definition. (We also recognize that there is a distinction from amorphous solids.) Tools should include the following:

- Phonon dispersion measurement—LCLS diffraction correlation instrument?
- Measurement of shear modulus
- Fully utilize advanced light sources
- Coherent imaging and diffraction
- Tomography (grain scale microstructure)
- Time resolution (kinetics)
- Diffuse scattering (statistical representation of defects)
- Small angle scattering (nucleation and growth kinetics)

3.2.2 Real-time diagnostics for dynamic mapping of the thermo-mechanical field

We have a need to develop predictive capability that describes the generation and evolution of defects that control continuum material properties. We must develop and field multiple diagnostics for such experiments to achieve thermodynamic field measurements, in particular temperature measurements and specification of the full stress tensor. These diagnostics must include in situ temperature and stress diagnostics applicable to different compression regimes and time scales. This will allow the specification of time-resolved thermo-mechanical variables at different spatial locations. Thus, we need the following:

- Accurate temperature and strain/stress field measurements
    - Local environment temperature probes
    - Multi-axial stress probes, e.g., single molecule spectroscopy
    - Multi-axial strain probes, diffraction
- Pre- and post-experiment characterization

- Tomography
- Diffraction Contrast Tomography

3.2.3 Ability to make experimental measurements to link length scales ranging from atomic to continuum dimensions

Continuum response depends on material behavior at lower length scales**.** A suite of in situ time-resolved measurements at different length scales is required to validate theoretical models as they transition from one length scale to the next. To reach this goal (need), we must develop new experimental capabilities that provide these linkages. The linkage of measurements at different length scales will lead to the first realistic models required for predictive capability.

3.2.4 Ability to make in situ spectroscopic measurements including those of electronic structure

Spectroscopic probes provide a characterization tool for measuring both the average and localized environmental effects of compression, depending on the probe and its practical implementation. Data regarding the effect of compression on molecular structure and/or chemical changes can be obtained through vibrational spectroscopies (e.g., Raman and IR absorption), while electronic spectroscopies provide a measure of the changes in conductivity (as manifested through changes in Fresnel coefficients) and changes in the potential surface. Nuclear spectroscopies (e.g., XANES/EXAFS) can also provide information regarding bonding and nearest neighbors. Thus, modern facilities must have capabilities for implementing the following spectroscopies in order to make stronger connection with theoretical models:

- Reflectivity
- Raman
- X-ray spectroscopy
- XANES and EXAFS
- XEL

3.2.5 Complex loading path control

As discussed previously, the application of compression can provide routes to other forms of matter that would normally be symmetry disallowed or inaccessible on the noncompressed potential surface. Thus, the proper combination of ramp and shock can provide the mechanism for tuning the path and creating an environment conducive to generating new forms of matter or for "allowing" normally disallowed chemical reactions. In addition, the ability to quantify the partitioning of energy between dissipative and non-dissipative mechanisms requires techniques that allow for changing the relative contributions of these processes. Thus, ultimately achieving dynamical control of these processes will require the ability to carefully tune the loading profile, from isentropic to shock loading and anywhere in between, in order to vary the thermal content as well as access portions of the potential energy surface that can only be accessed under compression.

3.2.6 Develop first-order continuum analyses that produce better subscale models and capture defect evolution

Many of the current descriptions of dynamic loading are phenomenological in nature and cannot be connected in a "real" sense to the material world. As an example, to design optimal experiments for direct comparison, we have a need for realistic descriptions of inelastic deformation that incorporates material phenomena at lower length scales (microstructure, defects, texture, etc.). Often, experimentalists and theorists define experiments that are "ideal" in the sense that they are capable of being performed, even though the experiment or theory may not be modeled or tested. Thus, we need stronger experimental and theoretical collaboration to define optimal conditions and diagnostics from which to draw more accurate comparisons and, as a result, a better analysis and interpretation of experiments.

3.2.7 Learn how to conduct and diagnose experiments relevant to 3D applications

Real-world applications are inherently three-dimensional and will often involve phenomena that may not occur in one-dimensional experiments. Thus, we have a need to develop experimental methods and diagnostics that achieve and quantify controlled 3D loading conditions in such a manner as to allow interpretation. This work inherently includes the development of material models that are pertinent to 3D loading and devoid of knobs, if at all possible.

3.2.8 Design experiments that overlap different loading regimes and experimental platforms

We currently have at our disposal a large number of platforms for conducting dynamic experiments, with the Z machine and National Ignition Facility (NIF) as examples. However, we have not developed methods that guide the best use of these different experimental platforms and loading regimes. To achieve maximum effectiveness, we must learn how to coordinate and integrate experiments on different platforms and different time regimes. When coupled with a variety of volume- and time-scale probes (flexibility to span scales on facility), these types of experiments will aid in developing the understanding of the load path and strain rate dependence of material properties needed to achieve realistic and complete models.

3.2.9 Increase experimental throughput

We are often limited in dynamic compression science by the rate at which we can conduct experiments. We must work toward the development of new experimental methods that allow easier and faster measurements of dynamic properties while simultaneously developing new experimental paradigms for combining multiple diagnostics that yield increased efficiencies, decreased cost, and faster turnaround. These new experimental methods will allow for a more complete set of observations, which in turn, will increase development of realistic models, thereby advancing the field.

3.2.10 Develop improved materials and standards for uniform comparisons

Lastly, we have a need for the development of a set of standard materials that will allow us to connect measurements on a variety of platforms and using a diverse set of diagnostics. For example, loading a 50-micron thick tantalum sample on NIF may require the development and

production of an extremely fined-grained material to ensure that the data is not dominated by grain boundaries. To make a direct comparison of this data with that obtained on guns may not be an easy task. To start, we should make gun measurements with the fine-grained material, but our results may still be confused with loading rates that may influence the shock wave rise time. They may be further confounded by time-dependent changes in the wave profile. One example is the change in amplitude of the elastic precursor simply as a function of sample thickness. Thus, connecting these disparate temporal and spatial regimes will require careful thought and analysis. Furthermore, if we could develop better impedance matching materials that are transparent, we could begin to imagine (nearly) looking in at the processes that are taking place in bulk. These observations will be required if we truly expect to achieve control.

3.3 Theory Needs and Challenges in Compression Science

An accurate material description involves the characterization of many variables that can only be captured in a statistical sense, e.g., chemical composition, defect density and distribution, texture, grain size, etc. Our premise is that these intrinsic properties and their linking across scales determine a material's properties (or functionality) and its performance. To develop control, we need to establish the correspondence between a 3D description of a material and its properties, from which we may develop a set of principles that provide an intelligent system for tailoring materials functionality. To make progress in linking behavior of materials to their processed characteristics, we must develop and maintain the intimate coupling of experiment with theory and simulation.

In other words, to develop "process-aware" models linking materials behavior with its 3D characteristics, we require tools that seek to couple and link the spectrum of materials length scales—from the electronic through the continuum and to the application or integrated system level. In fact, a long history of successful models punctuates the lineage of materials science in this quest. Some models, such as optical device theory, rely on fundamental physics; others, such as time-temperature heat-treating curves, arise from phenomenology; and most, such as phase diagrams, combine theory and empirical observation. Within the past three decades, the subspecialty of computational materials science has strived to provide additional modeling tools to the materials scientist, ranging from (i) fundamental (*ab initio* electronic structure and molecular dynamics) calculations at the atomic (usually single crystal) scale, to (ii) dislocation dynamics and phase field modeling at mesoscopic length scales, at which microstructural aspects such as texture and interfacial effects become important, to (iii) single crystal and polycrystal plasticity models that describe "bulk" materials behavior that can be encapsulated in (iv) Equation of State (EoS) and dynamic material strength models suitable for engineering-level simulations. Our computational materials science goals are to enable an integral and predictive capability, not postdictive, and to provide a link between materials, design, manufacturing, and functionality that will ultimately enable "control" of material functionality.

This panel attempted to envision this future research path and elucidate the advances in multi-scale modeling techniques and also the experimental capabilities needed to measure the required validation data that will be required to meet this goal. The heterogeneity of real materials and the non-equilibrium processes underlying dynamic compression phenomena are two key aspects absent from current models based upon a description of average homogeneous, equilibrium behavior. A proper treatment of such aspects will enable

predictions of a probabilistic bulk performance rather than just the ideal macroscopic behavior. The ultimate goal is to develop the scientific understanding that will enable a tailored "control" of the chemical and spatial structure of materials to be tolerant to extreme environments, replacing the conventional trial-and-error approach.

3.4 Scientific Discovery Challenges for Compression Science Theory and Modeling

3.4.1 Track dynamic microstructure evolution in situ

The response of materials to dynamic compression involves a wide range of length scales, ranging from individual point, line (i.e., dislocation), or surface defects at the nanometer length scale, to the nucleation and growth of voids, twins, or product phases at tens to hundreds of nm, collective dislocation microstructure at micron length scales, and finally the 10–100 μm grain scale. Current computational materials science techniques have been developed for each of these length (and corresponding time) scales, but a corresponding set of direct in situ experimental probes has not yet been developed. This leads to two choices for design and parameterization of the higher length-scale models: either postdictive fitting of the end state of highly integrated experiments (e.g., Taylor cylinder impacts or recovered incipient spall samples) or an "upscaling" of dynamic material properties from one method to the next. The latter remains an extremely challenging task and introduces a typically un-quantified (but potentially quantifiable) error from one step to the next (*ab initio* electronic structure, to semi-empirical potentials for MD simulations, to mesoscale and finally continuum-scale models). Thus, there is an enormous benefit to direct in situ measurements of the dynamic microstructure evolution at the mesoscale, which lies in the gap between the microscale where theory is most reliable and the macroscale where experimental measurements are most readily made. Two of the most promising candidates in this regard are the following:

- X-ray scattering, which is sensitive to microscopic defects such as voids and dislocations. An outstanding challenge is the "inverse problem" of inferring such defect content from experiment.

- Microprobes on synchrotron light sources have reached a level of maturity where the 3D microstructure of a volume containing tens of grains can be mapped within an hour of beamtime. The grand challenge is to do such measurements in situ during static compression and ultimately during dynamic compression.

3.4.2 Discover new and unexpected high-pressure and temperature solid phases

The high-(P,T) equilibrium phase diagrams of elemental materials are in many cases still poorly mapped out, and the situation is even worse for alloys and compounds. The discovery of the hcp ε phase of iron by dynamic shock experiments, only subsequently confirmed by static experiments and theory, is a landmark achievement that greatly enhanced the stature of that community. The accuracy and predictive capability of *ab initio* and molecular dynamics has reached a state where that community should strive to seek such a discovery, by exploring the vast regions of phase space which lie between the principal Hugoniot, isentrope, and isotherms that dynamic and static experiments have already accessed. The question of the structure of iron at Earth's core and related planetary

science issues are being actively explored by these approaches, but otherwise this is a largely untapped area prime for discovery.

3.4.3 Design novel experiments to isolate key physics

To date, the vast majority of simulations has by necessity simplified the material description but, as a result, has neglected the material complexity that often dominates behavior under extreme conditions. The physics that are relevant for understanding the state of matter at extreme conditions include composition, phase, crystal structure and stability, elastic moduli, and local stress of the perfect crystal. In addition, real materials are composed of a collection of crystalline grains with various orientations, shapes, and internal defects that play a dominant role in determining the material behavior. Such material complexity includes internal vacancies, impurities, alloy elements, dislocations, inclusions, second phase particles, and grain boundary or other interfaces. As simulation and experimental scales are approaching each other, it is crucial that such complexity be incorporated in simulations.

To bridge this gap between the often idealized theory and simulations and the experiments using often insufficiently characterized engineering materials, there is a need for novel experiments involving samples with controlled (or at least adequately characterized) grain and defect structures. Simulations can thus be performed on identical samples (statistically if not exactly), and experiments can be performed with internal measurements of strain rate, temperature, and stress state that directly correlate to simulation observables.

3.4.4 Move beyond planar impact: Non-uniaxial strain experiments

Uniaxial and hydrostatic loading conditions have been most studied primarily because they are the most easily achieved in experiments, and modeled, but represent only a very limited subset of stress and strain tensor states that are accessed in complex integrated experiments. Experiments involving oblique impact, sweeping waves, bulge tests, etc., have been performed and modeled, but further work is needed to understand the dynamic material response to these more complex loading conditions and to enhance our confidence in dynamic material models and codes under the entire range of stress and strain states at which they are utilized.

3.4.5 Design novel simulations to isolate key physical mechanisms and observables

The behavior of material following a change in external conditions is determined by the defects inside the materials. By designing simulations that directly model these key unit processes, simulations will make a better connection to the experimental observables. Today's high-performance computing platforms enable the direct modeling, at an atomistic level, of materials starting from an experimentally characterized dislocation microstructure. A direct numerical simulation of the shock compression of material at the atomistic level reveals the deformation by dislocation mechanisms, which may be directly observed with experiment via diffuse X-ray scattering.

3.4.6 Develop ability to predict the kinetics of phase transitions (solid-solid, solid-liquid, and liquid-solid)

Materials exist in many states, and the kinetics of transformation between such states is poorly understood. To date, heuristic models have been fit to macroscopic experimental measurements, such as Velocity Interferometer System from Any Reflector (VISAR) wave profile records, but provide no insight into the transition mechanisms. Direct numerical simulation of transformations provides insight into the nucleation and growth of the product phase and can inform physically based models. For instance, the Kolmogorov continuum model requires nucleation rates, lag times, interface velocities, and other fundamental parameters that can be directly determined from simulations at lower length scales, including molecular dynamics and phase field simulations. However, these lower length scale models have never been validated at extreme conditions by experiment. In situ small-angle scattering experiments reveal the distribution of nuclei at a given point in time; such distributions at multiple times can provide information on the kinetics.

3.4.7 Understand relationship between microstructure and constitutive properties (e.g., strength) during dynamic processes

The dynamic behavior of a material depends upon its constitution, which includes phase, microstructure, and loading path and rate. The development of a predictive material model for that response requires the knowledge of the microstructure evolution along the loading path at the given loading rate. In particular, strength is primarily determined by dislocation unit mechanisms. The dislocation content changes during deformation, and the rate of change is largely unknown. Phenomenological strain hardening models account for this effect in a macroscopic way but do not represent the underlying microscopic physics. Mesoscale dislocation dynamics models can account for this microscopic physics; however these models need to be extended to include deformation, polycrystals, crystal rotation, and experimental information on dislocation mobilities under extreme conditions. Atomistic molecular dynamics simulations can also provide information on the mobility of dislocations at extreme conditions, including conditions in the presence of other defects such as vacancies, impurities, other dislocations, inclusions, or grain boundaries. This microscopic evolution of the dislocation microstructure must be captured in a continuum rate model. The validation of this microstructure evolution is essential and can only come from emerging in situ, real time, X-ray, neutron, and/or proton probes with high spatial and temporal resolution.

Nothing is known about the microscopic state of the material following a phase transition, for instance the dislocation density or grain (and subgrain) structure. The history dependence of a material element, following its evolution through phase transitions, can strongly affect its resulting strength and other dynamic properties in an as-yet poorly known manner, which needs further investigation.

3.4.8 Understand material failure

Material failure under shock compression may result from the localization of deformation and during release the nucleation, growth, and coalescence of microscopic voids or fractures may lead to ductile or brittle failure, respectively. Heuristic models omit such physics, for instance, by assuming that material failure occurs at a specified maximum compression (or

tensile stress) η_{min} (or P_{min}). Nucleation and growth models have been developed for a number of other physical situations but have not been widely applied to material failure to date. Direct numerical simulations of material failure under shock compression can reveal the evolving porous state of the material under load and the underlying physical processes. For example, mesoscale crystal plasticity models with an explicit representation of nucleation sites, informed by atomistic simulations of the nucleation and growth processes, can be developed. Dynamic in situ radiographic imaging, and eventually 3D tomography, can provide details of the void growth process needed to validate the models, overcoming the limitations of existing post-recovery analysis of incipiently spalled samples.

3.4.9 Resolve melting discrepancy in transition metals

Despite several recent attempts involving new theoretical calculations and static high-pressure experiments, the compression science community has failed to resolve a glaring discrepancy between the high-pressure melt curves in several body centered cubic (bcc) transition metals, most notably Mo and Ta. Whereas static high-pressure diamond anvil cell (DAC) experiments using laser heating reveal a very gradual rise in melting temperature (a few hundred degrees K) at high pressures, dynamic shock experiments and quantum molecular dynamics (QMD) simulations both predict a much steeper melt curve, rising thousands of degrees with remarkably good agreement between the dynamic experiments and theory. The fact that several groups in both the United States and Europe have demonstrated the reproducibility of many of these calculations and experiments makes this discrepancy even more intriguing and suggests an overlooked explanation that may potentially raise questions about a wider range of experiments or calculations. For instance, on the one hand, the assumption of a hydrostatic stress state and thermal equilibrium in DAC experiments, and neglect of electron temperature in virtually all QMD and MD calculations, even as temperatures approach 1 eV, could introduce significant errors. On the other hand, static and dynamic experiments are in excellent agreement with each other (and with theory) for non-transition metals, including Al, Fe, Mg, and Ni, which could suggest that an intermediate semi-ordered phase akin to a liquid crystal may be a precursor to melting for bcc transition metals, confounding the interpretation of what melting actually is.

3.4.10 Understand the behavior of the full anisotropic stress state at extreme pressures and temperatures, e.g., Poisson's ratio approaching melt

Related to the previous challenge, material properties such as Poisson's ratio and strength approaching melt are still poorly understood. The existence of new phases, or drastic changes in behavior of existing phases near melting, could affect the interpretation of experiments and provide insight into various theories of melting, from Born's proposed elastic instability to more modern theories of dislocation-mediated melting.

3.5 Technical Grand Challenges for Compression Science Theory and Modeling

3.5.1 Multiscale modeling free of ad hoc parameters: linking subscale processes to higher length/time scales

The field of multi-scale modeling today contains several theoretical and computational tools, which together span the time and length scale ranges of interest to static and dynamic

compression science. Each modeling tool, in general, contains both physically based and non-physical quantities (parameters) that allow the representation of material response. The non-physical quantities exist due to our lack of understanding about either the physical processes that occur in real materials or how to represent known physics into a theory or computational tool adequately. Our lack of experimental information about dynamic responses and structural evolution of materials at length scales of importance to the physical processes prevents us from developing the theoretical and computational tools to adequately achieve predictive models at the relevant length scales for our problems of interest.

The information deficit can be addressed through high-fidelity diagnostics applied to critical experiments. Eliminating non-physical parameters from today's models is the goal at all length scales.

3.5.2 Better theoretical tools in the mesoscale (1–10 mm) regime

The mechanics and physics community has over many years collectively produced theoretical tools that have started at the continuum level and worked down in length scale or at the atomic scale and worked up in length scale. Although these continuing efforts are critical, we do not have adequate theoretical tools that describe the complex ways in which dislocations interact and form substructures or how they interact with microstructural features such as inclusions, grain boundaries, point defects, precipitates, dislocation sources, etc. Present polycrystal plasticity models have demonstrated our deficiency in describing the development and evolution of subgrain heterogeneities and structure.

These theories must also represent real material length scales in their formulation in order to eliminate many of these deficiencies and provide microstructural size dependence, which is known to exist in all materials. At present, crude theories attempt to represent real material length scales, but these theories are very complex, less than physically based, and computationally expensive. We must drive our understanding to the point at which we can represent these length scale dependent behaviors with physically based models that are as simple as practically possible and include sufficient information to link across the length scales, which that particular model divides.

3.5.3 Transferable density functionals, pseudopotentials, and classical MD potentials valid at extreme conditions

Present day interatomic potentials are limited to the regimes of response within which they were calibrated. This limitation prevents translation to a wider set of physical regimes, which thus limits predictive capability. We must develop new computational frameworks that enable a wider range of known interatomic interactions to allow representation of the detailed complexities of real materials, which inherently contain defects and are exposed to extreme environmental conditions of loading. Particularly for dynamic compression experiments that access extreme pressure *and* temperature states, there is a need for further research into two techniques that promise to correct potentially fatal weaknesses in current density functional theory (DFT) and MD calculations: temperature-dependent density functionals and classical potentials for MD simulations that are electron temperature-dependent.

3.5.4 Equation of state treatment of materials beyond simply pressure and volume

- Avoid reliance on simple separation into hydrostatic and deviatoric stresses
- Two-temperature (electron and ion) EoS's

Present day theories are built upon the simplification of decoupling the effects on materials of the hydrostatic (pressure) and deviatoric (shear) partitions of stress. In reality, the equation of state for any crystal structure (except a cubic at reference configuration) compresses through application of hydrostatic pressure by changing both volume and shape. Theories used today do not account for the effect of the shear response during hydrostatic compression. Theories accounting for this coupling at present lack sufficient experimental information to enable their complete development and use. The lack of coupling between pressure and shear prevents an adequate treatment of pressure dependent plasticity and calculation of thermodynamics. Additional data from both experiments and simulations can be used to calibrate more complete EoS formulations.

Current EoS frameworks assume the Born-Oppenheimer approximation that electron contribution to the thermodynamics state variables is negligible. This forces the assumption of local thermodynamic equilibrium (LTE) at all conditions. It is currently believed that LTE does not exist under strong shock conditions and in warm dense matter. Extending formulations to two temperatures (electron and ion) is a first step toward providing a better treatment for non-LTE conditions.

3.5.5 Codes that preserve the integrity of material models

Current numerical frameworks do not handle steep gradients in loading and material state adequately. This diffuses fields, preventing the adequate treatment of surfaces (either material variables or interfaces). Many of these steep gradients are below the resolution of the computational grid. Numerical schemes are required to more adequately represent steep gradients and/or track material state without diffusion.

3.5.6 Quantitative dynamic x-ray probes (diffraction, XANES, EXAFS, etc.)

- In situ determination of phase
- Measure volume fraction of growing product phase

To acquire necessary experimental information at length scales that are not presently achievable, new diagnostic probes will be required. In general, diffraction techniques are used to distinguish material phase information in a volume averaged fashion. Diffuse scattering is impacted by the existence and evolution of disorder in which the materials can be both thermal and structural. Of particular interest is the spatial distribution of dislocations and the evolution of dislocation density with deformation, which is crucial in understanding the evolution of strength. Small-angle x-ray scattering is sensitive to the presence of density heterogeneity in the materials, and these materials include precipitates, voids, second phase particles, and phase nuclei. Both diffraction and small angle scattering can be used to determine the growing volume fraction of phase.

The XANES and EXAFS techniques probe the electronic state of the atom and are sensitive to the local environment surrounding the atom, including nearest neighbor spacing, stress, and temperature. These techniques or new techniques must be developed to enable the measurement of the nucleation of these phase changes events at very small time and length scales. In addition, new visualization and data processing tools will be necessary to deal with the large data sets produced from the three-dimensional measurements.

3.5.7 Develop local temperature and stress tensor gauges

Present temperature probes are limited to the surface of the sample or are invasive and have the potential to influence the results by their existence (e.g., thermocouples). Surface probes are based upon the emissivity of the sample, and theories describing emissivity as a function of temperature are inadequate for the basing measurement upon emissivity. Temperature is a fundamental quantity in determining the thermodynamic state of the material and in the influence that the thermal state has on the constitutive response of the material. We must develop the tools to enable the measurement of in situ temperature in a deforming body at length and time scales that are consistent with present modeling tools (e.g., 1 micron and 1 ns). Advancements of photonic crystals that could be embedded into a materials and images produced with a radiation source could hold potential for attaining a real three-dimensional temperature field.

As we have discussed earlier, we must begin to account for the complex three-dimensional stress state in both the treatment of EoS and strength theories. To do this, we must develop techniques to make in situ measurements of the full stress tensor field in materials as a function of position. This will allow us to more completely evaluate the local constitutive behavior of materials. Measurement of only the deformation field will still require us to estimate through modeling the kinetic response of the material. Manganin gauges are presently used and are limited to finite volumes and are used for traction only—no shear. The panel did not offer good suggestions for technologies that might show promise in making these measurements in situ and at a small length scale.

3.5.8 Local structural identification in static experiments, e.g., DAC, for amorphous materials and liquids

Static high-compression experimental techniques do well for crystalline solid materials – particularly diffraction techniques. The same diagnostic capabilities do not exist for other classes of materials such as amorphous solids and liquids, yet their behavior is not well characterized. We must develop the diagnostic techniques to enable the measurement of local scale strain, stress, structure for materials that lack crystallinity or are at least only partly crystalline.

3.5.9 3D orientation image mapping to dislocation length scales under dynamic conditions

The response of metallic materials to externally imposed loading is not simply a function of the types of elemental materials existing in the materials. Their response is also a function of the spatial position each of those elemental materials has in the bulk material. Imperfections and defects (e.g., grain boundaries, dislocations, impurity inclusions) also play a major role in determining the deformation behavior of metallic materials. The spatial arrangement of atoms and defects in the material comprise what is commonly termed as the material

microstructure. The microstructure also evolves substantially with deformation (distortion, dislocation movement/evolution/arrangement, heterogeneity evolution) and when conditions are extreme, this evolution leads to material damage and failure. These are unsolved problems from a theoretical perspective. We simply are not yet able to model these complex processes in a predictive manner. We need to be able to measure the evolution of the microstructure during dynamic loading conditions to enable us to make in situ observations of how microstructural heterogeneities evolve and lead to damage and failure. Orientation Image Mapping (OIM) is a well-known 2D technique, which is presently used to characterize the crystallographic orientation of polycrystalline metallic materials. Coupled with laborious mechanical serial sectioning, it can presently be used as a way to characterize the 3D microstructure of a material for a sample recovered from a mechanical deformation history. This 2D technique teaches us a great deal about the behavior of a material but only in 2D and after the fact. To get to the next level of understanding, we need have a tool which will tell us information like OIM is able to now but in 3D and during dynamic loading responses.

3.5.10 Extracting useful information from high-resolution 3D data (e.g., from 3D tomography or large-scale simulations)

As our ability to produce very large experimental or computational data sets becomes greater, so too is the need to be able to extract useful physics information from those large data sets. As we begin to think about how material microstructures evolve to produce an observed behavior or as we begin to be able to use new physics understanding to enable us to produce material microstructures that take advantage of inherent heterogeneities to our advantage, it will be increasingly important to make the linking between different physics events. For example, we may wish to derive an evolving 3D velocity, strain, or strain rate field, by performing image correlations for 100 time-sequenced 3D microstructural images to the level of resolution of the images. This will require characterizing each image (OIM type information) but also linking each image to the next image or next few images to be able to propose an evolving field. The same can be said for the analysis of large-scale MD calculations. Much information is produced during those simulations and the correlations of each atom with its nearest neighbors will define a lattice strain field but also may help to define a new solid phase depending upon the local structure. The analyses performed will generally have a basis in a particular physics question, which we may wish to address. Many of the processes we have discussed here have been around the concept of evolving statistics. We will also need higher order statistical models to be able to tractably capture the statistics of material behavior into something which we can use to help us link the evolution of heterogeneities to observed or designed properties. We can also use these statistical models to help define initial condition microstructures for MD, phase field, and polycrystal models that represent real materials of interest, which will always begin at an initial state of heterogeneity (defect structure).

4.0 Conclusions

The workshop offered an opportunity for open discussion of the problems and challenges in the field of compression science. These problems and challenges present opportunities for advancing our field and moving the field from that of discovery and observation to that of prediction and control. This transition requires that we diagnose and develop an understanding of materials, not in an ideal sense of theory alone, but also in a real-world sense of experiment and measurement. To make progress on these high-level goals requires the community to meet a set of challenges that include the following:

- Acquire time and spatially resolved in situ measurements at all length scales (i.e., atomistic, micro, meso).
- Discover new physics and chemistry in extreme environments.
- Incorporate material complexity into multi-scale simulations to achieve predictive capability.
- Unify static and dynamic compression understanding across relevant length and time scales.
- Leverage scientific knowledge derived from theory and experiment to the design and control of real materials (i.e., chemistry, microstructure, defects, etc.)

Furthermore, we have identified detailed challenges and opportunities within the framework of static, dynamic, and theoretical compression science that work toward attaining our end goal of control. Resolving all of these challenges is necessary for true predictive understanding, while partial resolution will lead to new paradigms regarding our thought processes on the material world around us. Compression science offers opportunities for discovery, yet challenges our ability to fully comprehend the controlling chemistry and physics. As scientists, we recognize the complexity and acknowledge the underlying beauty in the field of compression science, and we look forward to the surprises to come and the expected success of our predictive capability.

Appendix I Workshop Agenda

21st Century Needs and Challenges in Compression Science Workshop

Bishop's Lodge, Santa Fe NM
Tuesday, September 22, 2009

7:00 PM Dinner Tesuque A,B

If you are available, we are expecting a speaker on Tuesday, September 22, 2009

(unfortunately, not confirmed): 8:00 PM

Wednesday, September 23, 2009
Tesuque A, B

8:00 – 8:30 AM Continental Breakfast
Tesuque Pavilion

8:30 AM Welcome, Introduction and Workshop Kickoff……David Funk and Rusty Gray
Los Alamos National Laboratory

9:00 AM The Future of Static Compression Science……Malcolm McMahon
University of Edinburgh

10:00 AM Discussion

10:30 AM The Future of Dynamic Compression Science ……Yogi Gupta
Washington State University

11:30 AM Discussion

12:00 PM Lunch – Workshop Co-chair will lead discussion on the morning Plenary Talks
Tesuque Pavilion

Tesuque A, B

1:00 PM Experimental Needs for Material Phase, Strength, and Damage …….Neil Bourne
Atomic Weapons Establishment

James Asay
Sandia National Laboratories

2:00 PM Discussion

2:30 PM Break

3:00 PM Theory Needs for Material Phase, Strength, and Damage……. James Belak
Lawrence Livermore National Laboratory
Curt Bronkhorst
Los Alamos National Laboratory

4:00 PM Discussion

4:30-5:30 PM Summary Discussion

6:00 PM Reception / Informal Discussion
Tesuque Pavilion C

7:00 PM Dinner – Workshop Co-chair will lead discussion from breakout discussions (using key questions to stimulate discussion)
Tesuque Pavilion C

Thursday, September 24, 2009 - - Breakout Sessions
Las Fuentes Alcove Room—Future of Static Compression Science
Las Fuentes Fiesta Room—Future of Dynamic Compression Science
Tesuque Pavilion C—Theoretical Needs of Compression Science

8:00 – 8:30 AM Continental Breakfast
Tesuque Pavilion

8:30 AM Retire to side rooms for independent discussion and presentation of each participant's materials (ten minutes per participant)

12:00 PM Lunch – Panel Chairs will report back on the progress from the morning sessions; and that progress will be used by all in the afternoon breakout sessions
Tesuque Pavilion

2:00-4:00 PM Panels develop summary presentations (5 slides)

Tesuque Pavilion A

4:00 PM Panel Chairs present summaries (20 minutes each)

5:00-6:00 PM Summary Discussion

6:30 PM Informal Discussion / Reception
Tesuque A, B

7:30 PM Dinner – Panel Chair/Co-chair will lead discussion to refine workshop information presented in the afternoon session
Tesuque A, B

Friday, September 25, 2009 - - Report Writing

8:00 – 8:30 AM Continental Breakfast
Tesuque Pavilion Portal

Tesuque Pavilion C

8:30 AM Panel Chairs and Plenary Speakers draft reports (5-7 pages from each)

12:00 PM Workshop Adjourns

Appendix II Participants

21st Century Needs and Challenges in Compression Science Workshop

James Asay	Sandia National Laboratory E-mail: jrasay@sandia.gov
Cris Barnes	Los Alamos National Laboratory E-mail: cbarnes@lanl.gov
Richard Becker	Lawrence Livermore National Laboratory E-mail: becker@llnl.gov
James Belak	Lawrence Livermore National Laboratory E-mail: belak1@llnl.gov
Reinhard Boehler	Carnegie Institution of Washington E-mail: rboehler@ciw.edu
Neil Bourne	Atomic Weapons Establishment E-mail: neil.bourne@mac.com
Curt Bronkhorst	Los Alamos National Laboratory E-mail: cabronk@lanl.gov
Michael Desjarlais	Sandia National Laboratories E-Mail: mpdesja@sandia.gov
Micheline Devaurs	Los Alamos National Laboratory E-mail: devaurs_micheline@lanl.gov
Dana Dlott	University of Illinois Email: dlott@illinois.edu
Jon Eggert	Lawrence Livermore National Laboratory E-mail: eggert1@llnl.gov
William Evans	Lawrence Livermore National Laboratory E-mail: wjevans@llnl.gov
David Funk	Los Alamos National Laboratory E-mail: djf@lanl.gov
Timothy Germann	Los Alamos National Laboratory E-mail: tcg@lanl.gov

George “Rusty” Gray	Los Alamos National Laboratory E-mail: rusty@lanl.gov
Yogendra “Yogi” Gupta	Washington State University E-mail: ymgupta@wsu.edu
Russel Hemley	Carnegie Institution of Washington E-mail: larson@lanl.gov
John Klepis	Lawrence Livermore National Laboratory E-mail: klepeis1@llnl.gov
Marcus Knudson	Sandia National Laboratories E-mail: mdknuds@sandia.gov
Christian Mailhiot	Lawrence Livermore National Laboratory E-mail: mailhiot1@llnl.gov
H.K. Dave Mao	Carnegie Institution of Washington E-mail: Mao@gl.ciw.edu
Rick Martineau	Los Alamos National Laboratory E-mail: rickm@lanl.gov
Stephane Mazevet	Universite De Brtagne Occident E-mail : stephane.mazevet@cea.fr
Malcolm McMahon	University of Edinburgh E-mail: mim@ph.ed.ac.uk
John Moriarty	Lawrence Livermore National Laboratory E-mail: moriarty2@llnl.gov
Nigel Park	Atomic Weapons Establishment E-mail: nigel.park@awe.co.uk
Michael Pravica	University of Las Vegas E-mail: pravica@physics.unlv.edu
Paulo Rigg	Los Alamos National Laboratory E-mail: prigg@lanl.gov
Adam Schwartz	Lawrence Livermore National Laboratory E-mail: schwartz6@llnl.gov
D. Scott Stewart	University of Illinois E-mail: dss@illinois.edu
Sarah Stewart-Mukhopadhyay	Harvard University E-mail: sstewart@eps.harvard.edu

Justin Wark — Oxford University
E-mail: justin.wark@physics.ox.ac.uk

Phil Withers — University of Manchester
E-mail: philip.withers@manchester.ac.uk

Sasha Zivaljevic — Los Alamos National Laboratory
E-mail: sashaz@lanl.gov

Appendix III Cross-cutting issues identified during the workshop

Although materials under extreme environments of pressure, temperature, and strain rate are central to defense, energy, and other technologies, we know relatively little about how and why materials respond under these conditions. To understand the operative controlling mechanisms and learn to design and control the effects of extreme environments on materials, we must develop in situ experiments that see the dynamics in real time. Such experiments are coming within reach, as ever brighter sources of electrons, x-rays, and neutrons with ever higher spatial and temporal resolution allow sensitive measurements on ever smaller sections of materials.

A second reason for our limited knowledge of materials under extreme environments of static and dynamic compression is the enormous complexity of the effects such environments cause. Unraveling the emergent behavior of materials under extreme environments requires more than observing the response of the material in situ. We must understand and model this behavior to see how extreme environments damage, degrade, and ultimately disable materials. One of the most pervasive and difficult challenges blocking this understanding is the diverse range of time and length scales that govern compression behavior.

Discussion of the workshop attendees following the overview presentations led to the identification of a number of cross-cutting themes of relevance to static compression, dynamic compression, and theory as follows:

- How do we build confidence that classical MD provides representative and accurate physics in both atomic and polycrystalline simulations. Are the potentials accurate? That is, are the potentials accurate in both fully dense and defected materials? How do we develop a single simulation capability that can capture all of the relevant physical parameters (i.e., conductivity, phonon density of states, electronic structure, phase diagram, etc.)?

- How do we link static and dynamic results particularly in those situations in which large discrepancies exist? Are the issues kinetics/calibrations or misinterpretation of diagnostics, and how do we resolve this issue.

- Three-dimensional imaging of both single-crystal and polycrystalline materials is needed to drive our understanding of material response to compression.

- How do we elucidate linkage between microstructure, defects and other heterogeneities with constitutive properties under loading conditions; static or dynamic? Can we draw general inferences that will lead to predictive capability?

- When is local-thermodynamic equilibrium valid in dynamic systems (including static/laser coupling experiments)? How do we know when and if we have reached equilibrium?

- How do we build bridges between length and time scales that captures and hands off relevant physics? Can we look at multiple scales, both temporal and spatial, using multiple diagnostics in a single experiment and assess our multi-scale simulation capabilities?
- How do we create equilibrium conditions/states of pressure and temperature orders of magnitude greater than currently attainable in relevant sample sizes?
- How do we characterize and quantify the physical processes (viscosity, localization, instabilities/mixing, phase transitions, transport, defect generation and storage, damage) in an arbitrary loading event? [Geophysical to laser driven shock] How do we quantify the partitioning of energy between dissipative and non-dissipative processes?
- How do we characterize and potentially exploit chemical changes that occur either through static compression or material dependent changes induced by compression (polymer decomposition, detonation)?
- How do we formulate problems of study such that experiments look more like theory and theory looks more like experiments? What are the critical tests of theory that provide confidence in our predictive capability?
- How do we capture anisotropy in our constitutive and equation of state descriptions of real materials?
- How do we capture the stochastic nature of materials accurately with our simulation capabilities? Thereafter, how do we validate meso-scale simulations? What are the new numerical schemes that will capture subscale physics accurately; i.e., rare events?