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Progress Report for the period April 1, 1998 to September 30, 1998 of the
UNLV High Pressure Science and Engineering Center,
part of the **High Pressure Materials Science Research Partnership**
with the **DOE National Laboratories** prepared for the
Stockpile Stewardship Program at the DOE Nevada Operations Office

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DISCLAIMER

OVERVIEW OF THE PROGRAM

In Spring 1998, UNLV established the High Pressure Science and Engineering Center (HPSEC) as a multidisciplinary, materials research partnership among UNLV, the Nevada Test Site (NTS), and several DOE National Laboratories relevant to DOE's Stockpile Stewardship Program (SSP). This partnership emphasizes:

helping to engineer JASPER and future higher velocity accelerators at NTS,
participating in dynamic high pressure experiments at NTS and the DP Labs,
making laboratory measurements essential for interpreting results obtained at JASPER and other NTS shock wave facilities, and
developing new approaches for and doing leading-edge computational studies critical to SSP and related DOE/DP activities.

Although this official starting date of the first budget period for HPSEC is April 1, 1998, funding was approved only in late June; and operations began July 1. The effective period of this report, thus, is three months. During this period, each of four major programs got underway on campus. HPSEC investigators initiated many contacts with DP personnel to make detailed research plans by exchanging visits between lab and campus sites. By the end of the period, new HPSEC laboratories were being assembled, and work was well underway. The manuscript of the first publication from the collaboration was being finalized; it was submitted as a letter to Nature in mid-October. In late September 1998, the HPSEC Advisory Committee, composed of researchers from Bechtel-Nevada, LANL, LLNL, SNLA, and Shock Dynamics Institute at Washington State University, reviewed these plans and accomplishments. We were pleased with their strong endorsement of our accomplishments and activities.

WORK STATEMENT

HPSEC emphasizes scientific and engineering studies at high static and dynamic pressures directed toward validating and improving models of *d*- and *f*-band metals, energetic materials and their detonation products, foams, and low-Z elements of programmatic interest over a largely unexplored range of pressures and temperatures. We will measure equilibrium thermochemical properties, mechanical properties, reaction kinetics, and reaction products at static pressures using *in situ* x-ray diffraction; absorption, emission, light-scattering spectroscopy from infrared to x-ray wavelengths; and other chemical and physical analytical methods. We also plan to study the chemistries, microstructures, and mechanical properties of new and aged high explosives and composite foams; to synthesize novel engineering and energetic materials; and to improve theoretical and computational models of these phenomena. We also will help to design facilities and diagnostics for extending the range of dynamic studies beyond the capabilities of conventional launchers.

HPSEC also fosters interdisciplinary collaborations among chemists, engineers, geoscientists, and physicists from UNLV, NTS, and the DP labs. We plan to involve each HPSEC experimentalist and engineer in a project at NTS and to have each theorist collaborate with NTS and DP lab personnel in modeling closely related problems. Until HPSEC personnel gain appropriate clearances, they will work in laboratories at UNLV and develop collaborations elsewhere where they can do state-of-the-art high pressure, preparative and analytical measurements, and modeling studies. Whenever appropriate, we will develop collaborations rather than duplicating facilities available elsewhere to make best use of DOE resources. We expect to establish within three-to-five years UNLV as a world-class center for high-pressure research.

During these three months, efforts centered on:

1. Making contacts with personnel at NTS, the DP labs, and related DOE-supported facilities to establish near- and long-term research and development goals for HPSEC;
2. Building the UNLV infrastructure for preparing and analyzing samples for dynamic experiments to be done at NTS and for doing static high-pressure studies needed to support the dynamic experiments;
3. Developing research capabilities to study both mechanical *and* chemical properties of the *same* sample of fresh and aged programmatic and prototypical foams used to support, insulate, and protect nuclear devices;
4. Performing accelerator and diagnostics design studies aimed at extending the experimental frontiers of dynamic high-pressure research at NTS;
5. Developing new computational approaches and fundamental theoretical insights to help experimentalists at HPSEC, NTS, and the DP labs to understand of electronic structures of matter ranging from elemental metals to exotic materials whose existence has been predicted by not confirmed.

Progress on each of these activities during this brief period is described in the following section.

PROGRESS REPORT

Making contacts: From July through September, faculty associated with HPSEC visited one or more of the DP labs, hosted lab personnel at UNLV for discussions, and/or corresponded about project directions by phone, mail, and e-mail to learn about specific stockpile stewardship issues and to formulate detailed research plans. For many of these faculty, this was the first or second visit to DP facilities, following an orientation visit to LANL and SNLA in April. Return visits to LANL and SNLA were especially helpful in expanding contacts and focussing plans for the foams project. Several meeting with personnel from H Division at LLNL were useful for defining near- and long-range goals for static high-pressure studies to support shock equation-of-state (EOS) and other dynamic experiments planned for NTS. Three leaders of theoretical projects at LLNL were invited to campus for seminars and planning discussions during the Fall Semester. Lab and HPSEC personnel also attended several planning sessions for new high-pressure synchrotron projects that will be valuable for measuring EOS and other important mechanical and physical properties of programmatic materials in the near future. We very much appreciate the hospitality and advice provided by Drs. Jim Asay, Hyunchae Cynn, Ray Finucane, Joseph Fiore, Richard Fortner, Neil Holmes, James Lula, Christian Mailhiot, Andy McMahon, John Moriarity, Stephen Sheffield, Tamara Ulibarri, Choong-Shik Yoo, and David Young and apologize to anyone we may have omitted by oversight.

Building the UNLV infrastructure for high-pressure research: Professor Nicol is establishing a new laboratory for preparing and analyzing samples for static and shock experiments and for doing related diamond-anvil-cell static high-pressure spectroscopy and structural studies. During this period, he began to acquire appropriate spectrometers, optics, high-pressure cells and tools; these components began to arrive in September. He also began to recruit for suitable postdoctoral candidates.

The June 1998 award restricted spending funds for construction of synchrotron beam lines so we examined alternative approaches for structural work at high static pressures. We visited the Carnegie Institution of Washington and met with scientists from other laboratories to learn about state-of-the-art laboratory diffraction instrumentation for high-pressure research and trade-offs with regard to 2nd- and 3rd-generation synchrotron sources. We concluded that, even if we develop a laboratory facility at UNLV, we must have access to 3rd-generation hard x-ray synchrotron sources to meet our long-range goals and that a permanent presence at APS, the only such source in the US, is crucial to our mission. We reviewed this position with the HPSEC Advisory Committee in September and are pleased that they strongly endorsed this option. We will continue to pursue funding for this presence from DOE and private sources. Selection of a laboratory-based diffractometer was deferred while we devoted our attention to funding part of the proposed APS line.

We also made plans to join with Drs. Cynn and Yoo for a five-day run at the ESRF, the European 3rd-generation source, in November. There, we will study a number of samples of carbon dioxide prepared by different routes at various pressures and temperatures to identify the crystal structure of $CO^{++}CO_3^{--}$, the ionic dimer discovered by Yoo, Cynn, and Nicol by burning graphite at 9 GPa. These conditions are achieved behind the detonation front of programmatic high explosives, and this discovery challenges codes use to model detonation chemistry. Although Raman spectra provide evidence for the composition of this dimer, its structure and that of a similar nitrogen dioxide dimer are not known. That work is the reported in the manuscript of a letter submitted to Nature by in October. From the ESRF run, we will also learn about capabilities that may be developed at the proposed high-pressure materials science beam line at the APS.

Mechanical and chemical properties of foams: During this period, Professors O'Toole and Sapochak visited LANL and SNLA to learn about the precise nature of the foams of programmatic interest and to define more clearly model systems for studying damage and aging effects. After discussions with Dr. Asay and Ulibarri (SNLA), Sheffield (LANL) and Lula (Kansas City Plant), they developed an agenda focussing first on polyurethanes that are of interest to all of the DP labs and later on specific composite foams. Mr. Greg Schmett, an undergraduate student, is now preparing to synthesize the model foams under Prof. Sapochak's direction. They also received foam samples from LANL and SNLA for preliminary experiments. Orders were prepared for attachments to UNLV's Universal Testing Machine (mechanical tester) for handling low-density materials; the order will be placed when FY 99 funds are released.

Professor Lindle reassigned Dr. Wayne Stolte, a UNLV post-doc to support the project effective July 1. Dr. Stolte interacts with scientists at LBNL to obtain access to equipment and beam time for preliminary analytical experiments on the foam samples obtained from the labs. He uses an x-ray-absorption (XAS) apparatus for photon energies above 2 KeV under construction at LBNL to which UNLV has regular access. Drs. Mel Klein and Rupert Perera from LBNL have agreed to perform XAS experiments at lower energies on foam samples using their beam line and to match UNLV's contribution to the salary of a second postdoctoral scholar to collaborate on studying foams and similar samples. Included in this arrangement is additional beam time at ALS. Complementary support for studying foams and other complex materials using x-ray spectroscopy and microscopy is being pursued through NSF EPSCoR.

Accelerator and Diagnostics Design Studies: Over the summer, Professor Pepper's group got their compressible flow code up and running. A postdoctoral scholar, Dr. Yitung Chen; two graduate students Tim Debues and Dave Carrington; and two undergraduate students, Vernon Lau and Jason Malvey, worked full or part-time on this project. This code incorporates adaptive modeling (refined and unrefined) for inviscid as well as viscous compressive flows. The simulations include flows in a tube with axial symmetry and comparisons with 1-D gas dynamic calculations. The group also obtained an algorithm which they will use for simulating chemical effects for flows above mach 5 from Professor David Pratt of the University of Washington.

Theory and Computation: In this initial phase, we have identified potential difficulties in doing path-integral quantum Monte Carlo simulations of hydrogen at high pressure and the means to overcome them. We presented our plan to the Advisory Committee and discussed it with the committee members. An announcement of postdoctoral positions was distributed by e-mail, and one candidate was identified for hiring. We are searching for a second candidate. The literature search on the progress and the status of the experimental as well as theoretical work on the subject to date has been completed.