Letter of Intent for

Dynamic Compression Collaborative Access Team (DC-CAT) at Advanced Photon Source

by

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Abstract

This Letter of Intent is to develop dynamic experimental beamlines (namely, DC-CAT) at the nation's brightest third-generation x-ray synchrotron source, APS. Washington State University will lead an effort to build and operate a new sector dedicated for dynamic high-pressure research, in partnership with DOE-NNSA National Laboratories (LANL, LLNL, and SNL) and the Carnegie Institution of Washington. The DC-CAT comprises (i) three independently operating beamlines (two double-undulator beamlines shared by a diamond monochromater and one high-energy bending magnet), (ii) various dynamic compression drivers including gas- and powder-guns, lasers, and a mini-pulser, (iii) enclosed and access controlled operation rooms on the experimental floor, and (iv) experimental laboratories and an office module. The main research objective is to perform atomistic/molecular-level investigations of dynamic materials response under extreme conditions of high stresses, temperatures, and strain rates. Recently, we have demonstrated the experimental feasibility of obtaining microscale response through x-ray diffraction data in shock compressed materials at the HPCAT/APS. We envision that the DC-CAT will foster successful and sustainable DOE-NNSA and BES partnerships benefiting a broad range of scientific research communities in both national laboratories and academia, and become a cornerstone for modern shock wave research in the 21st Century.

Scientific Objectives

Understanding the dynamic response of materials is not only at the heart of DOE-NNSA Defense Program needs but is also of fundamental importance to understanding the response of condensed matter (such as solids, liquids, glass, proteins, nano-particles, and many others) at extreme conditions, as emphasized at recent DOE workshops: one organized by the NNSA on the *Use of the DOE Basic Energy Sciences National User Facilities for NNSA Mission Needs in the area of Condensed Matter Physics and Materials Science*, February 9, 2007 and the other by BES on *Basic Research Needs for Materials under Extreme Environments*, June 11-13, 2007, in Bethesda, MD. Especially highlighted was the scientific significance of dynamic compression experiments, in the panel report on *Dynamic Response of Materials: Scientific Challenges and Opportunities* (Appendix A).

Dynamic loading (shock wave and shockless compression) experiments subject materials to extreme and unique conditions (very large compressions, high temperatures, and large deformations) on very short time scales (ps to μs) resulting in a rich array of physical and chemical changes. The extreme conditions encountered under dynamic loading provide an excellent opportunity to explore the delicate balance between mechanical (PΔV) and thermal (TΔS) energies to determine how this balance governs a wide variety of physical and chemical phenomena in the condensed state. The short times, inherent in dynamic loading experiments, result in the kinetics playing an important role in determining the governing mechanisms and in the attainment of metastable states, beyond thermodynamic constraints. Therefore, dynamic compression experiments offer an excellent approach to study how materials manifest the rising mechanical and entropic energies in melt curves, crystal structures, phase stability and metastability, microstructures and mechanical strength, and chemical bonding, over a broad range of the pressure (0-1000 GPa), temperature (0-1 eV), and time (1 μs – 100 ps) space.

Advances in computational modeling and simulations over the past decade or two have made it possible to examine condensed matter phenomena over a wide range of length and time scales. Predictions of novel structures and properties through computational modeling are quite common. Although many of the advances in multiscale modeling of complex condensed systems were driven by problems related to the dynamic compression of materials, multiscale measurements under dynamic loading remain an outstanding challenge-particularly at an atomistic level. Therefore, *in-situ* time-resolved x-ray diffraction of solids under dynamic compression constitutes a major scientific need in obtaining a comprehensive understanding of extreme material response. Such measurements will provide structure-stress-strain relationships of solids over a large stress-temperature-time range and, thus, add significantly to the fundamental knowledge base in condensed matter physics, chemistry, and materials science.

Challenges and Opportunities

Unlike the usual "pump and probe" approach, the transient and destructive (single event) nature of the shock wave pump makes probing of materials very challenging. Despite the developments in optical spectroscopy and x-ray diffraction measurements pioneered at Washington State University and elsewhere, microscopic probing of shock compression in condensed matter in a routine and regular manner remains a major scientific challenge. The single event nature of these experiments coupled with the short time scales requires that the probe beams (irrespective of the photon or particle energy) have exceptional brightness and extremely high quality.

In recent years, DOE has made many major investments to develop unique national facilities (APS, LCLS, SNS, NSLS-II, etc.), benefiting a broad range of user communities in the physical sciences, materials research and condensed matter physics, and bioscience. Surely, these facilities can benefit shock wave research, providing a wide-range of cutting-edge tools to probe more detailed atomistic information under shock wave loading. For example, the temporal structure of the third-generation synchrotron APS (~100 ps x-ray pulses separated by a few to 150 ns at 300 kHz) is ideally suitable for ns time-resolved shock-wave studies. Its highly collimated x-ray beam is sufficient to probe coherent diffraction of shocked lattice in a few ns, revealing the structural evolution of solids and species that last only for a transient period, as demonstrated in our proof-of-principle x-ray diffraction experiments on shocked materials at the 16IDD of the HPCAT/APS (Fig. 1). Therefore, it is timely to bring shock wave research into these national facilities. In this regard, the present proposal to develop DC-CAT at the APS will likely represent the first of such efforts, which will definitely stimulate further developments at many other facilities and greatly benefit, if not revolutionize, the dynamic experiments in the 21st Century.

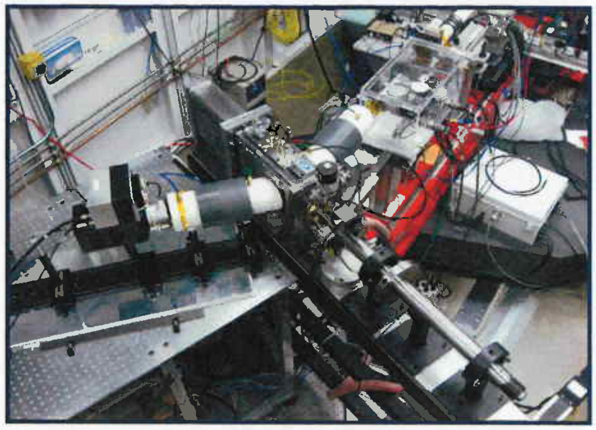

Fig. 1 *Synchrotron x-ray diffraction experiments on shocked LiF(111) at the HPCAT/APS*

Proposed Beamline Concepts

DC-CAT represents a unique opportunity for the DOE/NNSA Laboratories, while providing a research tool for a substantially broader basic science community at universities and national laboratories. Therefore, the participants of DC-CAT are expected to include scientists from those national laboratories, leading universities, and other research organizations.

DC-CAT will develop three beamlines, two double-undulator beamlines shared by a diamond monochromater and one high-energy bending magnet beamline, hosting (i) multi-bunch ns time-resolved x-ray diffraction to obtain the structural evolution of dynamically compressed solids, (ii) single-bunch high-resolution x-ray radiography to obtain a pristine look at shock fronts, interfaces, and materials in motion, and (iii) time-resolved white x-ray Laue diffraction of shocked single crystals. These beamlines will be optimized for dynamic experiments utilizing various dynamic compression drivers including gas- and powder-guns, lasers, and pulse power machines.

Shock wave experiments are destructive, and some data may have to be treated as sensitive information. In order to accommodate these safety and security concerns, the control rooms on the experimental floor will be enclosed with access controls, so that a part or all of the control rooms can be facilitated as a Temporary Access Controlled area when controlled experiments are conducted.

Broader Impact

The proposed DC-CAT will be a cornerstone for modern shock wave research in the 21st Century, utilizing the nation's unique and large-scale science facilities including APS, LCLS, SNS, NSLS-II, and ERL. Therefore, the experience and knowledge obtained from the present proposal will stimulate and benefit complementary experiments performed elsewhere including the fourth generation light sources ERL and LCLS. The DC-CAT will also develop large-scale collaborations with leading international organizations such as AWE in the UK and CEA in France. Finally, being at the center of a large-scale user facility, the DC-CAT will stimulate a substantially broader range of shock-wave research and developments for materials, medical, astrophysical, and national security applications and serve as a center for developing collaborations, training of students and junior scientists, and retaining scientists needed for nation's defense and basic science laboratories.

Team and Qualification

Professor **Yogendra Gupta** at Washington State University (WSU) will lead the proposed effort. He is a leader in the shock wave community and the director of the Institute for Shock Physics (ISP). WSU has a tradition of shock wave research, innovations, and educational excellence going back to the late 1950s. Professor Gupta has pioneered many time-resolved laser spectroscopies and x-ray diffraction experiments on shock-compressed materials and has trained an outstanding group of scientists who have gone on to become leaders in the field in academia and national laboratories. Other senior members of this team are as follows. Professor **Choong-Shik Yoo** at WSU is a leading expert in high-pressure materials research utilizing synchrotron x-rays. Prior to joining WSU, he was the High Pressure Physics Group Leader and one of four founding members of HPCAT beamlines at the APS. Dr. **Christian Mailhiot** a condensed matter physicist, who has held key leadership positions at LLNL, is currently on assignment at DOE/NNSA and will be the Project Coordinator for DC-CAT at NNSA. Drs**. Kim Budil and Gilbert Collins** at LLNL**, David Funk and Paulo Rigg** at LANL**, and Tom Mehlhorn and Dan Dolan** at SNL will represent DOE-NNSA Laboratories with world-leading expertise in dynamic experiments using high-power lasers, plate and explosive-driven impactors, and pulse power machines, respectively. Dr. **Russell Hemley** is the director of the Geophysical Laboratory at Carnegie Institution of Washington and has extensive experience in developments of several synchrotron beamlines in the US including the X17 and U2 beamlines at the NSLS and the GSECARS and HPCAT beamlines at the APS. Dr. **Chi-Chang Kao** is the chairman of NSLS and has extensive experience in designing synchrotron beamlines and developments of x-ray optics and detectors. He will participate in designing the DC-CAT beamlines and developments of x-ray diagnostics. Scientists at AWE and CEA will comprise the international partners in DC-CAT. The aforementioned scientists will make up the core group for development of the APS sector dedicated for dynamic high-pressure research.

Budget

The proposed project will cost ~ $20M for construction over 3 years. Annual operation costs will be approximately 15% of the construction costs. The funds will be provided by the Office of Defense Science at DOE/NNSA (Director, Dr. **Christopher Deeney**). During the construction period, we will utilize the HP-CAT beamline to test new and advanced experimental concepts that will be used at the DC-CAT. For these activities, we will seek additional funding from DOE-NNSA, DOE-BES, and participating institutions. Regarding dynamic compression drivers, we plan to acquire these from the NNSA Laboratories: LANL for gas and power-guns, LLNL for lasers, and SNL for a mini pulse-power accelerator.

Relevant Activities and Timetable

Scientific opportunities and needs of dynamic compression experiments were the central theme of the two DOE workshops mentioned above (Appendix A). Following the panel's recommendation, we submitted white paper to develop the DC-CAT to the DOE-NNSA (Appendix B), which received strong support at all levels. Furthermore, in Aug. 2007, a team of WSU researchers demonstrated the feasibility of synchrotron shock-wave experiments at the APS for single-bunch time-resolved single-crystal x-ray diffraction of oriented LiF, Al, and Cu under shock compression. These results were highly successful, not only to demonstrate experiments feasibility, but also to show how novel and in-depth materials information can be obtained from x-ray diffraction measurements at the APS. The main findings have been submitted for publication in Science (Feb. 2008).

The development of DC-CAT is summarized in the following timetable (tentative).

- Feb., 2007: DOE-NNSA workshop in Germantown, MD on *Use of BES User Facilities for NNSA Mission Needs*
- June, 2007: DOE-BES workshop in Bethesda, MD. on *Basic Research Needs for Materials under Extreme Environments* (http://www.sc.doe.gov/bes/reports/files/MUEErpt.pdf)
- June, 2007: Panel report on *Dynamic Response of Materials: Scientific Challenges and Opportunities*, submitted to the DOE-NNSA (**Appendix A**)

- Aug., 2007: White paper *Dynamic Compression Collaborative Access Team (DC-CAT) at the Advanced Photon Source*, submitted to NNSA (**Appendix B**)
- Feb., 2008: Letter of Intent for DC-CAT, submitted to APS
- Mar.-April, 2008: Visits to APS and NNSA National Laboratories for technical planning
- Apr., 2008: Formation of DC-CAT
- May, 2008: Workshop at APS on Dynamic Experiments at Unique DOE Facilities
- Sep., 2008: Full proposal for DC-CAT, submitted to the DOE-NNSA and APS

Jan 09 SAC →

- June, 2009: Construction begins
- Oct., 2012: Commission of beamlines

Appendix

A. DOE-NNSA panel report on *Dynamic Response of Materials: Scientific Challenges and Opportunities*

B. White paper *Dynamic Compression Collaborative Access Team (DC-CAT) at the Advanced Photon Source* submitted to the DOE-NNSA

Workshop ↔ Materials Under Extreme Environ.

- Shock compression
  - mechanical launcher / Harvard / CalTech
  - optical drivers / U of Rochester
  - acc. drivers / SNL (pulsed power) – WSU has such a driver