5 P-V-T-dε/dt Materials Structure Science Project

– To bridge a gap between static- and shock-compression experiments –

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5-1 Introduction

In this project, we intend to organize a group of researchers specialized in static- and shock-compression experiments, develop measurement systems, and perform XRD, XAFS, and other measurements under static and shock compression (see CMRC annual report 2015 for the mission of the project). We mainly focus on phenomena, such as the collision of asteroids, mantle convection, seismic activity (in geophysics), and deformation and fracture of metals and ceramics (in material science). These phenomena require understanding of the time evolution and/or inhomogeneity. The project meeting was held at Osaka as a joint meeting with HERMES of Osaka University in March 2018.

5-2 Single-shot time-resolved X-ray diffraction system for shock compression

XRD under shock compression provides information on high strain rate (dε/dt) phenomena. Thanks to continuous upgrades in the past decade, we can now conduct high pressure in situ XRD measurements under shock compression with a 16 J Nd:glass laser at the NW14A beamline of PF-AR. To understand the Hugoniot elastic limit (HEL), we started the project in 2016 to measure Laue diffraction of Si under shock compression (Figure 1, see CMRC annual report 2015 and 2016 for more information regarding experimental details).

Figure 2 shows Laue diffraction images of a silicon single crystal with <100> orientation. The shock pressure was estimated to be 20 GPa, while the HEL of the sample is reported to be 9 GPa [1]. The 1 3 -1 spot was shifted to the high-angle side, indicating compression due to propagation of an elastic wave along the [100] direction. The elastic strain was about -5.5%. The 0 2 2

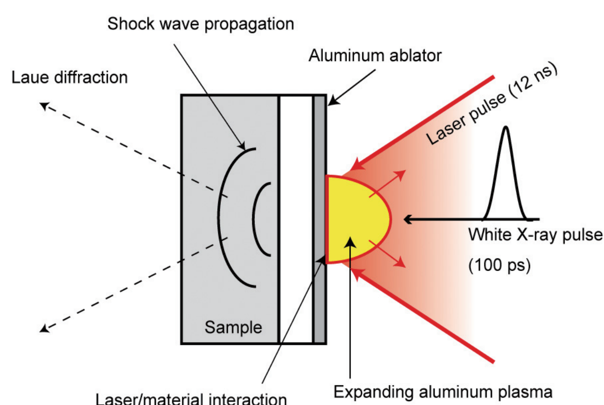

Fig. 1: Shock compression and Laue diffraction geometry at AR-NW14A. The sample was tilted 13 degrees from the incident X-rays to measure the 0 2 2 and 0 0 4 spots.

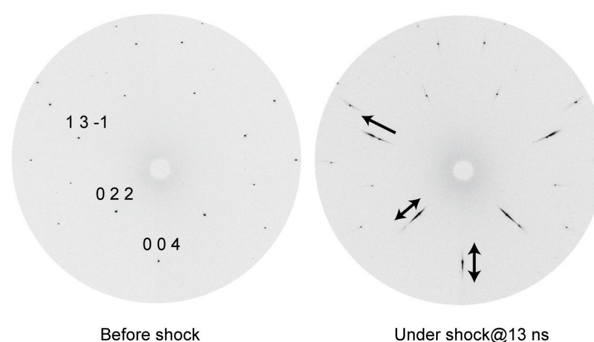

Fig. 2: Laue diffraction images of a silicon single crystal with <100> orientation before and under shock compression. The 1 3 -1 spot shifted to the high angle side, and the 0 2 2 and 0 0 4 were broadened without change in position.

and 0 0 4 spots were broadened without change in position, indicating increased mosaicity due to propagation of a plastic wave. The plastic wave, which follows the elastic wave, generates defects and collapses the crystallinity of the sample. We observed elastic compression and plastic deformation simultaneously, depending on the direction of the crystallographic planes.

This study is still in a preliminary stage. To clarify the dynamics at HEL, we continue to improve the system and/or gather more detailed measurements for various samples.

(This section is reported by K. Ichiyanagi and S. Takagi.)

5-3 X-ray absorption fine structure and X-ray diffraction measurement system for large-volume press

XAFS and XRD provide complementary information on the local structure around an absorbing atom and the average structure including all atoms, respectively. We developed a high pressure and high temperature in-situ XAFS-XRD system with a large volume cell by upgrading the NE5C beamline of PF-AR. Measurements on liquid iodine have been conducted up to 9 GPa with the new system [2]. We improved the energy resolution for XAFS measurements at high energies by introducing a Si(311) monochromator. Switching double crystal monochromators, Si(111) for low energies and Si(311) for high energies, allows transmission XAFS measurements to be conducted at 10-70 keV. The system is now used by several research groups.

Fluorescence XAFS is a powerful tool for probing the electronic state (e.g., valence) and short-range structure (e.g., bond length and coordination number) of an element dilutely contained in a sample. We set a Ge-SSD in the direction perpendicular to the incident monochromatic X-rays and performed some fluorescence XAFS tests (Figure 3). We obtained better spectra with the fluorescence system than with the transmission system from the sample containing <1000 ppm Ce at ambient conditions. Detection system and sample assembly improvements for high pressure experiments are ongoing. We will begin high pressure in-situ fluorescence XAFS measurements in the near future.

(This section is reported by D. Wakabayashi.)

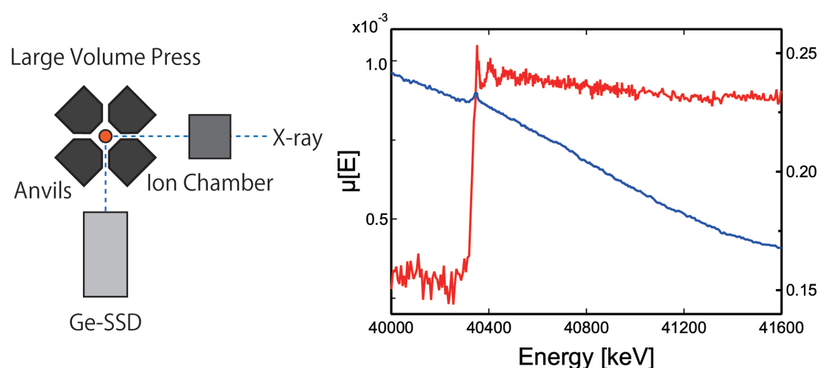

Fig. 3: Schematic illustration of the high pressure in-situ fluorescence XAFS system and Ce K-edge XAFS spectra measured at AR-NE5C. The sample is a CeO_2-NaCl mixture with Ce concentration below 1000 ppm. Red and blue lines represent the spectra measured in the fluorescence and transmission XAFS systems, respectively.

References

[1] S. J. Turneaure and Y. M. Gupta, Appl. Phys. Lett. **91**, 2101913 (2007).

[2] D. Wakabayashi, N. Funamori, T. Kikegawa, K. Watanabe, S. Kohara, H. Nitani, Y. Niwa, Y. Takeichi, H. Abe, and M. Kimura, Phys. Rev. B **96**, 024105 (2017).