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 have organized a group of researchers specialized in static- and shock-compression experiments. We are developing measurement systems, and are systematically performing XRD, XAFS, and other measurements under static and shock compression (see CMRC annual report 2015 for the mission of the project). We are mainly focusing on phenomena that need an understanding of time evolution and/or inhomogeneity, such as the collision of asteroids, mantle convection, and seismic activity (in geophysics), and the deformation and fracture of metals and ceramics (in material science). A project meeting was held in Kumamoto in March 2017 jointly with the Institute of Pulsed Power Science of Kumamoto University.

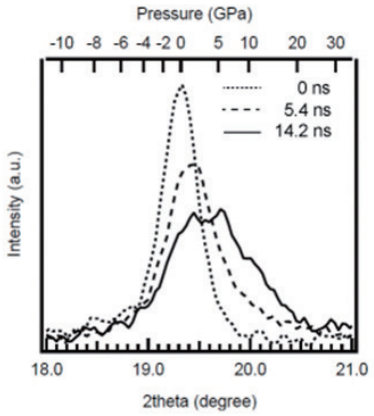

Fig. 1: Time evolution of the 111 diffraction peak of aluminum under shock compression. The shape of peaks reflects the pressure distribution within the sample.

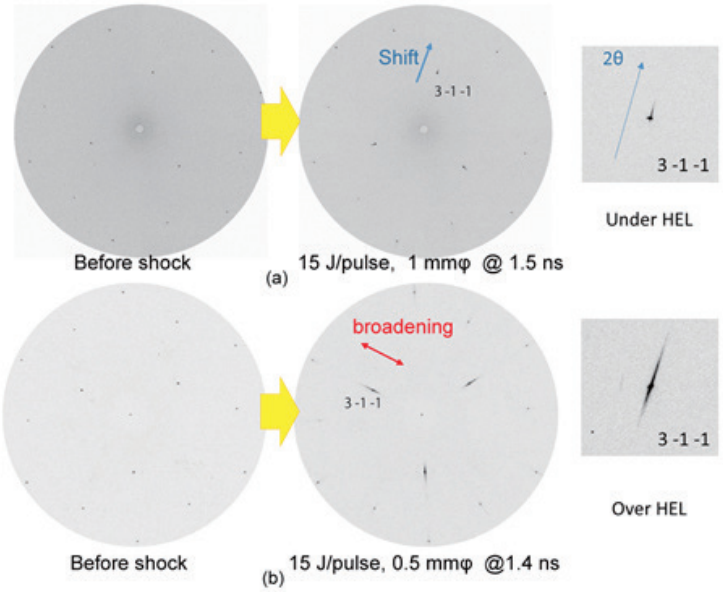

Fig. 2: Laue diffraction images of a silicon single crystal of <111> orientation, before and under shock compression. The focusing sizes of laser were φ1 mm in (a) and φ0.5 mm in (b), hence the shock pressure was higher in (b) than in (a).

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

XRD under shock compression provides information on phenomena that are characteristic of high strain rate (dε/dt). 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. Measurements to estimate shock pressure and to observe the Hugoniot Elastic Limit (HEL) of Si have been conducted this year. Under shock compression, materials yield above their HEL. We are interested in the change of microscopic structure (or state) at HEL.

Figure 1 shows the shift of the 111 diffraction peak of aluminum under shock compression. From this measurement, we confirmed that the present system can generate a maximum pressure of about 20 GPa. Figure 2 shows Laue diffraction images of a silicon single crystal of <111> orientation. The HEL of silicon at the strain rate of our system is about 9 GPa [1]. Laue spots shift to a higher angle below the HEL and they show broadening (without change in position, i.e., angle) above the HEL. This observation suggests that the sample is compressed uniaxially below the HEL and is compressed isotropically, accompanied by plastic deformation, above the HEL.

This study is still in a preliminary stage. To clarify the dynamics at HEL, we are continuing to improve the system and/or conduct 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. Thanks to upgrades in the last year, we can now conduct high-pressure and high-temperature in-situ XAFS-XRD measurements with a large-volume press installed at the NE5C beamline of PF-AR. Measurements on liquid iodine have been conducted up to 9 GPa with the new system [2]. This study may be the first to obtain both the XAFS spectrum and XRD profile in a single run with a large-volume press at high pressures and temperatures.

Iodine has attracted considerable attention as a model material to clarify the high-pressure behavior of diatomic molecules. Numerous studies have long been conducted on the metallization and molecular dissociation of solid iodine. As for liquid iodine, a possible molecular dissociation has been reported at 4 GPa by X-ray absorption fine structure (XAFS) measurements [3]. However, there is only one XAFS spectrum which could be evidence of molecular dissociation obtained at a single pressure point; there are no spectra at higher pressures. Moreover, no XRD measurements have been reported to support the molecular dissociation.

Figure 3 shows the EXAFS oscillation and structure factor obtained by XAFS and XRD measurements, respectively, and the atomic arrangement obtained by Reverse Monte Carlo (RMC)

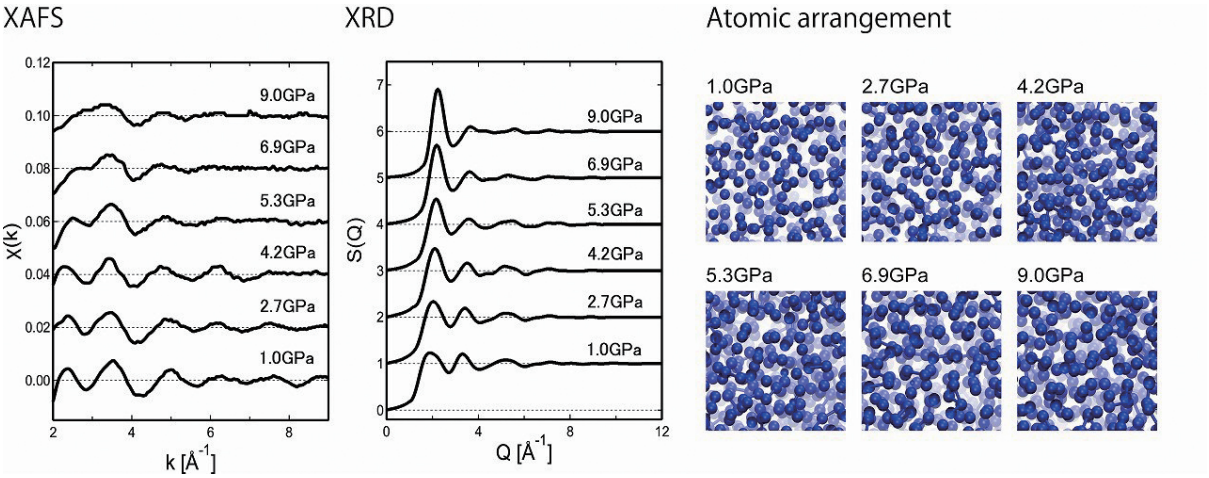

Fig. 3: EXAFS oscillation χ(k), structure factor S(Q), and the atomic arrangement of liquid iodine obtained by XAFS and XRD measurements and RMC modelings at high pressures. The modeling results can reproduce the two types of experimental data well.

modelings at high pressures [2]. The arrangements reproduce the two types of experimental data well. Detailed analyses clarify that the molecular bond persists up to 9 GPa and that liquid iodine undergoes the transformation at 4–5 GPa, accompanied by the onset (or drastic increase in the probability) of rebonding among adjacent molecules and the increase in electrical conductivity (possibly metallization) without molecular dissociation.

The Si(111) double crystal monochromator has been used for the above XAFS measurements. However, its resolution is not enough for XAFS measurements at high energies above 40 keV. Therefore, we now plan to upgrade the XAFS measurement system by setting up a Si(311) double crystal monochromator. We have already begun testing using synchrotron X-rays and have confirmed the generation of an X-ray beam at 40–60 keV. Improvements of the detection system and reduction in the time for changing the crystals of the monochromator are ongoing.
(This section is reported by D. Wakabayashi.)

References

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