# 5 P-V-T-$d\varepsilon/dt$ Materials Structure Science Project

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

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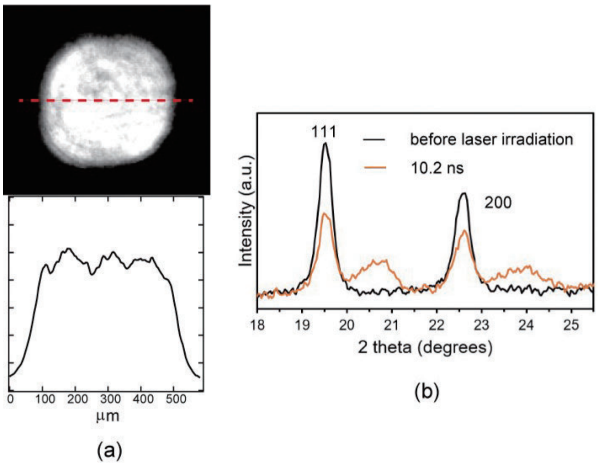
### 5-1 Introduction

In this project, we organize a group of researchers specialized in static- and shock-compression experiments, and develop the measurement systems and make XRD, XAFS, and other measurements systematically under static and shock compression (kindly view the CMRC annual report, 2015, to understand the mission of the project). This project is focused on the phenomena, which require an understanding of the 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). Because the project leader dedicated himself to reconstructing the Photon Factory (as the new director, starting April 2019), the project meeting with researchers from other institutes was skipped this academic year.



(a)

(b)

**Fig. 1**: (a) Intensity profile of Nd:Glass laser at the sample position. The diameter of flat-top region is about 0.4 mm. (b) XRD patterns of polycrystalline aluminum foil of thickness 100 μm. It is seen that the diffraction peaks of 111 and 200 (of compressed sample) are shifted at 10.2 sec after firing the laser.

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

X-ray diffraction (XRD) performed under shock compression provides information on the phenomenon characteristic for high strain rate ($d\varepsilon/dt$). Owing to continuous developments in the past decade, conduction of high-pressure in situ XRD measurements under shock compression with a 16 J Nd:glass laser at NW14A beamline of PF-AR is now possible. In addition, we have improved the glass laser system, converting the spatial profile from Gaussian to flat-top (Figure 1) [1]. The flat-top beam provides a uniform spatial-pressure distribution. Figure 1 shows the XRD pattern of the improved system at approximately 15 GPa .

Here we report dynamic grain refinement of the polycrystalline-aluminum foil under shock compression [2]. Figure 2 shows the typical Debye-Scherrer rings from the foil under ambient pressure at 30 ns, after laser irradiation (upto a pressure of approximately 5 GPa). The Debye-

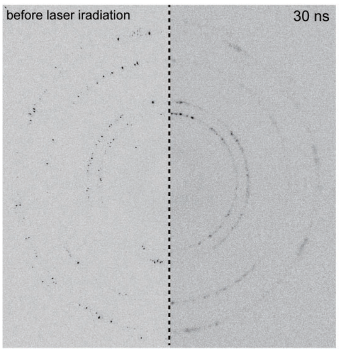


**Fig. 2**: Two-dimensional X-ray image of polycrystalline aluminum foil.

Scherrer ring at 30 ns appears smoothened and broadened because of shock-wave-induced plastic deformation accompanied by the fragmentation of micrometer-scale grains.

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

### 5-3 Small-angle X-ray scattering system for diamond-anvil cell

Small-angle X-ray scattering (SAXS) provides information on the inhomogeneity of materials in nanometer or larger scale. We developed a high-pressure SAXS system for diamond-anvil cell at BL-18C beamline of PF (Figure 3), and studied the intermediate state of the pressure-induced phase transformation in $SiO_2$ glass [3]. This system has been made available for the community, and some outputs have already been obtained [4, 5].

$SiO_2$ glass is one of the most studied non-crystalline materials. Despite its simple chemical composition, this material exhibits some interesting behaviors such as anomalous elasticity, permanent densification, and gradual structural changes in short-range order, which occur between 20 GPa and 35 GPa, accompanied by an approximately 30% increase in density. In spite of such large changes in density, the glass remains optically homogeneous during the transformation. XRD reveals that the average silicon coordination number gradually increases from 4 to 6 as the transformation proceeds.

Figure 4 shows the pressure dependence of the scattering intensity averaged over the low-Q range ($I_{av}$). From Figure 4, it is clear that $I_{av}$ reaches the maximum during the phase transition between fourfold- and sixfold- coordinated amorphous polymorphs. This is a definitive evidence of a heterogeneous intermediate state during the transformation. Detailed analyses suggest that the intermediate state consists of sub-nanometer-scale domains (~6 Å) for the two amorphous polymorphs and the boundary region between them. This study is the first to experimentally prove the existence of such domains.

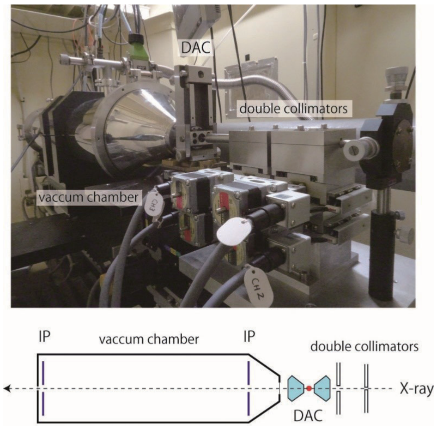


**Fig. 3:** High-pressure small-angle X-ray scattering system at BL-18C of PF.

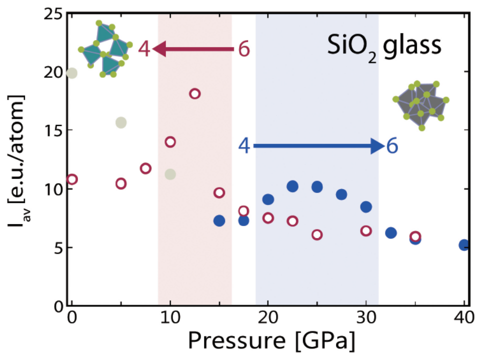


**Fig. 4:** Pressure dependence of $I_{av}$, the average scattering intensity at Q = 0.14-0.60 $Å^{-1}$, of $SiO_2$ glass.

The result well explains the lack of heterogeneous features such as grain boundaries and cracks in optical microscopy, although the two structures coexist in $SiO_2$ glass during the transformation. First, optical microscopy cannot identify the domains that are smaller than the wavelength of visible light. Second, the broad boundary region with an intermediate structure likely works as a buffer.

(This section has been reported by D. Wakabayashi, with assistance from T. Sato)

## References

[1] S. Takagi et al., in preparation.

[2] K. Ichiyanagi, S. Takagi, N. Kawai, R. Fukaya, S. Nozawa, K. G. Nakamura, K. D. Liss, M. Kimura, S. Adachi, Sci. Rep. **9**, 7604 (2019).

[3] T. Sato, N. Funamori, D. Wakabayashi, K. Nishida, and T. Kikegawa, Phys. Rev. B **98**, 144111 (2018).

[4] Y. Yoshimura, Y. Takekiyo, Y. Koyama, M. Takaku, N. Kikuchi, D. Wakabayashi, N. Funamori, K. Matsuishi, H. Abe, and N. Hamaya, Phys. Chem. Chem. Phys. **20**, 199 (2018).

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