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DAC 実験における選択配向性および格子ひずみの解析手法の開発
Texture and strain analyses using 2-dimensional X-ray diffraction patterns under DAC experiments

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Angle dispersive X-ray diffraction experiments using area detectors (CCD and CMOS cameras and image-plate recorders) provide wide opportunity for the determination of lattice preferred crystallite orientation (LPO) and lattice strain under stress condition in polycrystalline materials. LPO is reflected in circumferential oscillations along Debye rings, while the effect of lattice strain appears in elliptic distortions of the each ring and a deviation of the original crystallographic geometry among rings. These are substantial factors of bulk physical properties in polycrystalline materials, including seismic velocity, thermal/electric conductivity and so on. Diamond anvil cell (DAC) is the only technique that can create at extreme pressures corresponding to the Earth’s core, and it simultaneously involves non-hydrostatic, uniaxial stress in the sample. Although such non-hydrostatic effects under DAC experiments has been reported many previous studies, in many cases the quantitative treatments have not yet been developed into a standard technique.

In order to examine quantitative stress conditions under DAC experiments, high pressure experiments were carried out in a symmetrical DAC in the present study. Two stating materials, Al2O3 (˜1um in diameter) and MgO (<0.1 um), were used as stating materials, and no pressure media were loaded. Each runs were performed at the pressures from 0 GPa to 70 GPa by 10 GPa step under room temperatures, and synchrotron X-ray diffraction patterns were collected using a flat imag-plate at BL10XU at SPring-8. A software code was also developed by the author, which simulates a two-dimensional diffraction pattern based on given experimental parameters and (poly)crystalline properties. A fitting procedure was also incorporated into the code, where the orientation distribution and stress condition were iteratively modified according to a residual value of the simulated/observed patterns.

In runs of Al2O3 experiments, the diffraction peaks became distinctly broad and asymmetric shapes with increasing pressures, whereas the scattering angles (2theta) were apparently almost constant. This means that lattice compression involved by pressures was cancelled out by deviatoric stress. Nonetheless, the stress conditions could be derived mainly from the shapes of the peaks using the fitting procedure; e.g. at the highest pressure condition in the present study, maximum and minimum principal stresses could be estimated as 73GPa (parallel to compression axis) and 25 GPa, respectively, corresponding to the deviatoric stress of 50 GPa. The maximum principal stress was consistent with the estimated pressure by the diamond Raman pressure scale. On the other hand, MgO experiments maintained pseudo-hydrostatic conditions with small deviatoric stress only up to ˜1GPa under all performed pressures. A whole pattern fitting method such as the code developed in the present study may help us understand the stress conditions under DAC experiments

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