Structure analysis under non-ambient condition and dynamical observation

YAMANAKA, T., NAGAI, T., HATTORI, T. and TSUCHIYA, T.
Earth and Space Science, Graduate School of Science, Osaka University
1-1 Machikaneyama Toyonaka, Osaka, 560-0043 Japan

In order to comprehend the structure change of earth interiors, single-crystal structure analyses under non-ambient condition have been progressively undertaken. Kinetic studies become more significant subjects in order to elucidate phase transformation mechanisms under compression. Time-resolved and *in situ* diffraction studies using synchrotron radiation give a brilliant light to the dynamical observation of the pressure-induced structure change.

Since X-ray diffraction intensity measurement of single crystals with diamond anvil high-pressure cell has encountered many difficulties, possible structure analyses were often made at pressures lower than 30Gpa. We conquered those problems by using synchrotron radiation of 30~50keV (λ=0.25~0.4A) up to 50Gpa. A new backing plate of c-NB or sintered diamond instead of beryllium could give much larger load pressure, and He pressure media were applied for the hydrostatic compression at over 30Gpa. Crystals as small as 30μm in diameter could be used because of high brilliant incident beam.

This hydrostatic compression brings not only stable states but also intermediate states in the dynamical process. Plastic or elastic lattice deformation of the pressure-induce structure transformations causes coordination change, cation ordering, electronic state such as charge transfer and disproportionation, electron density of state, and spin-lattice interaction.

Molecular orbital calculation and molecular dynamics simulation of high-pressure phase are also effective methods to understand the structure and physical properties of earth interiors.