ESRF	Experiment title: Reitveld Refinement of Solid Oxygen High-Pressure Phases and Research for Molecular Dissociation	Experiment number: HS-342
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Report:

Pressure-induced metallization and molecular dissociation of oxygen, 0,, with molecular magnetism have attracted special interest because of novel electronic and magnetic properties of the h&h-pressure phases. Determination of the structural properties of these phases is indispensable for understanding the electro-magnetic properties, Recently, by using a high-brilliance beam of ESRF, we have observed a new structural transition from the ε to ζ phase at 96 GPa corresponding to metallization[1]. Further studies on high-pressure phases of solid oxygen were carried out as follow.

1.Research for molecular dissociation

Powder X-ray diffraction expeiment to 182 GPa was accomplished for solid oxygen by an angle-dispersive method with λ=0.4223Å. Obtained patterns are showned in Fig. 1. The transition to the ζ phase at 96 GPa reappeared. Figure 2 shows the pressure dependence of the d-values of the diffraction peaks. The present data well agree with previous ones[1]. These results above 96 GPa indicate none of sign for a structural transition. To determine and refine the structure of the ζ phase, the lines from a metal gasket ought to be removed from the patterns. Further experiments at higher pressure are needed for observation of molecular dissociation.

2.Reitveld refinement of the ε phase

For the ε phase, the space group of C2/m has been proposed but the atomic positional parameter are not determined. The present Reitveld refinement has suggested a possible arrangement of oxygen molecules in the unit cell; the molecular axis of 0, is orientated to c-axis. But strong preferred-orientation of the sample powder made further refinement difficult.

3.Single-crystal analysis of the ε phase

Single crystals of the ε phase was grown under a condition 20 GPa and 650 K in a DAC for the crystal structure analysis. Obtained oscillation photograph showed that the single crystal analysis is feasible. We could determined the c-axis direction of the crystal. Polarization property of infrared spectra of this crystal supported our suggestion of the molecular arrangement.

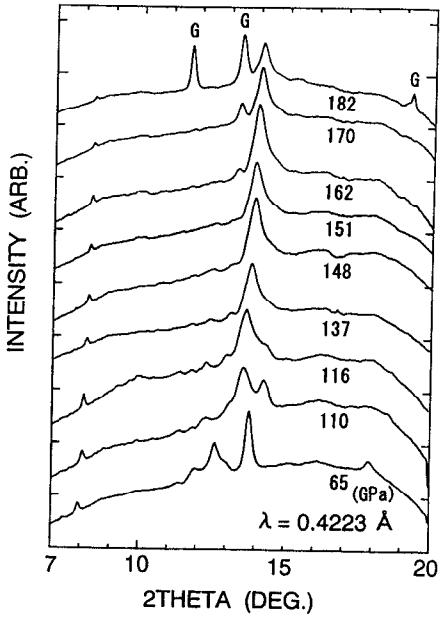

Fig.1 Diffraction patterns of solid O_2.

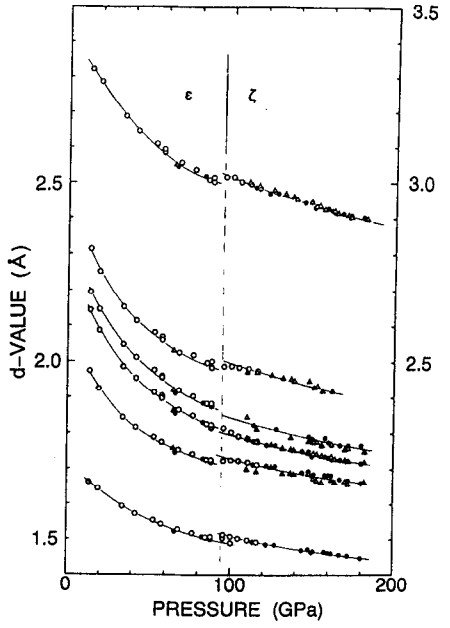

Fig.2 Pressure dependence of d-values. Open circles show the previous data[1].

[1] Y.Akahama et al. Phys. Rev.Lett. 74(1995)4690.