ESRF	**Experiment title:** Reitveld Refinement of Solid Oxygen High-Pressure Phases and Research for Molecular Dissociation	**Experiment number:** HS-128
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Report:

Pressure-induced metallization and molecular dissociation of oxygen, O_2, with molecular magnetism have attracted special interest because of novel electronic and magnetic properties of the high-pressure phases. Determination of the structural properties of these phases is indispensable for understanding the electromagnetic 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 difiaction patterns, which were obtained at pressure up to 15 1 GPa by an angle-dispersive method with λ=0.4249Å, are shown in Fig. 1. The transition to the ζ phase at 96 GPa reappears in the figure. Figure 2 shows the pressure dependence of the d-values of the diffaction peaks. The present data well agree with previous ones[1]. Both 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 pattern. Further experiments at higher pressure are needed for observation of molecular dissociation.

2. Reitveld refinement of the ε phase

The space group of C2/m has been proposed for the ε phase but the atomic positional parameter are not determined. For Reitveld refinement of the ε phase, a high-quality powder diffraction patterns were obtained at 13.7,17 and 2 1 GPa and a structural analysis was done. A possible arrangement of oxygen molecules in the unit cell shown in Fig. 3 was proposed. Then the intermolecular distance of O_2 was fixed at 1.2Å. But strong preferred-orientation of the sample was difficult to further reline the structure.

3. Single-crystal analysis of the ε phase

The single crystal of the ε phase was grown under a condition of 20 GPa and 650 K in a DAC for the crystal structure analysis. A preliminary experiment was carried out by oscillating the sample and Bragg reflections from the single crystal were observed. It is clear now that the single-crystal analysis of the ε phase is feasible.

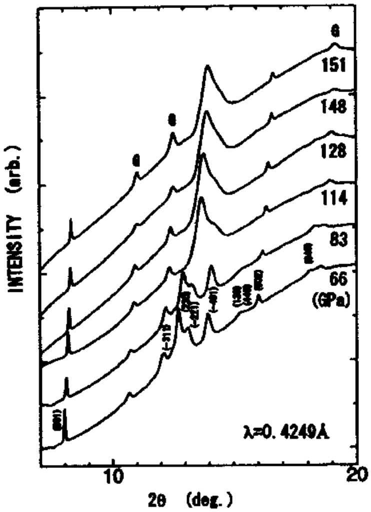

Fig.1 Diffraction patterns of solid O_2.

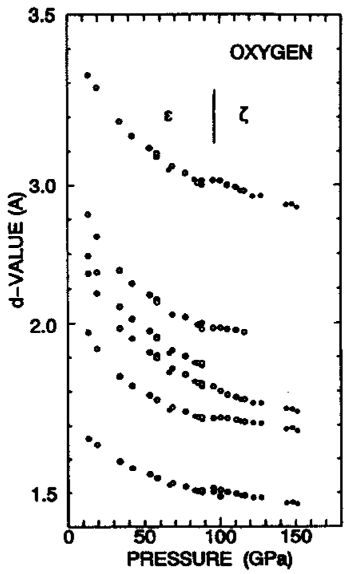

Fig.2 Pressure dependence of d-values. Open circles show the previous data[1].

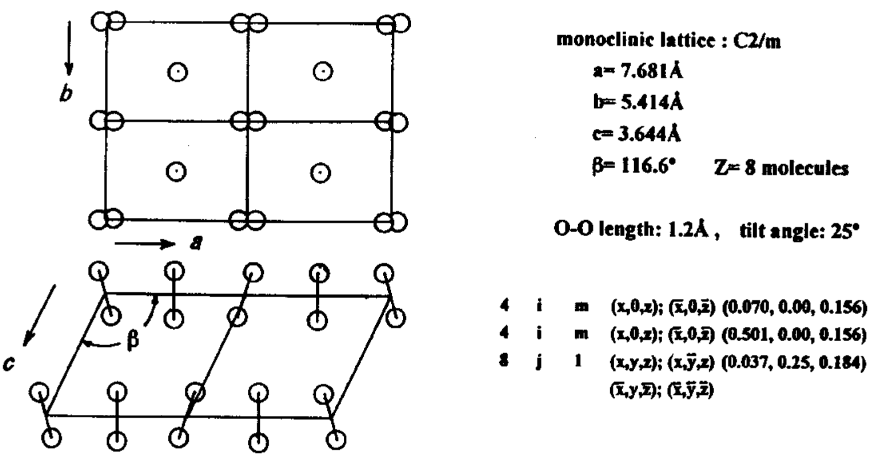

Fig.3 A possible model of the structure for the ε O_2 phase at 22.6 GPa.

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