Crystal Structure Analyses of Solid Oxygen High-Pressure Phases and Research for Molecular Dissociation

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1. Introduction

Pressure-induced metallization and molecular dissociation of oxygen, O_2, with molecular magnetism have attracted special interest because of novel electronic and magnetic preperties of the high-pressure phases. Determination of the structural propertis the high-pressure phases is indispensable for understanding the electro-magnetic properties.

In this study, high-pressure powder diffraction experiments on the solid oxygen as well as other low-Z element, phosphorus, have been carried out including test of the BL10UX.

2. Experimental

The samples were loaded in DACs. Pwder diffraction images are collected by an angle dispersive method with the monochromated beam with a wavelength of 0.4374 Å. Exposure time was between 2 and 3 hrs. Obtained images were analyzed by PIP.

3. Results and Discussion

3.1. Oxygen(O_2)

In order to re-examine the structure of the ε-O_2 phase, powder patters at 10.3 and 11.3 GPa were measured. These patterns(shown in Fig.1) did not exhibit any extra peaks observed in the our previous experiment and were assigned by a monoclinic cell(C2/m) proposed by Johnson et al.[1]. Therefore, the previous extra peaks may come from certain extra phase such as H_2O or CO_2 impurities.

3.2. Phosphorus(P)

The presure-induced structural transition of phosphorus was studied up to 151 GPa at RT in order to reseach the post-simple cubic(SC) structure. A structural transition from the SC to the simple hexagonal(SH) by way of an intermediate phase was observed at 132 GPa. Typical diffraction patterns of these phases are shown in Fig.2. The fundamental transition is the first observation in the monoatomic system. The result suggests that phosphorus does not follow the systematics of the structure in other group Vb elements proposed by Iwasaki & Kikegawa[2].

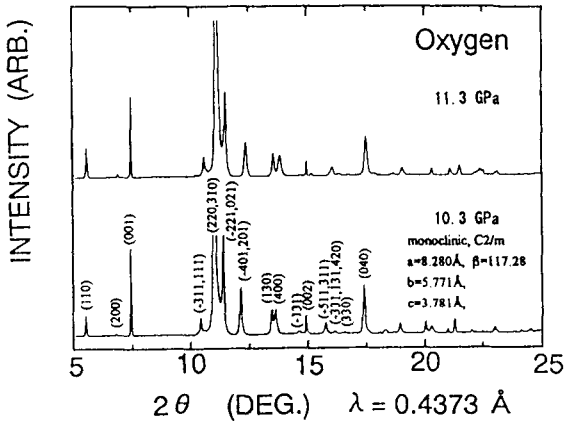

Fig.1. Powder patterns of e-O_2 phase at various pressre.

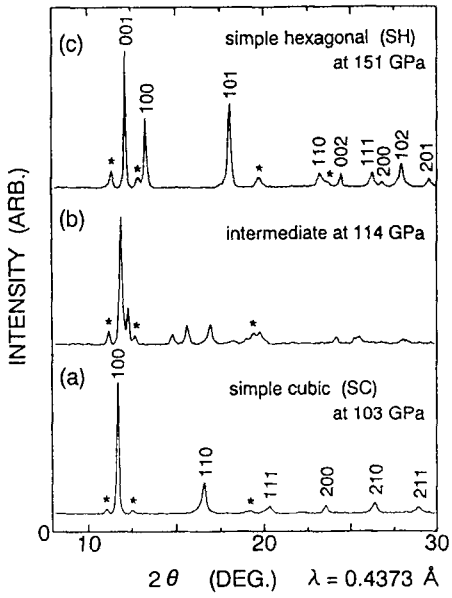

Fig.2 Typical powder patterns of high-pressure phases of phosphorus.

[1] S. W. Johnson et al., J. Appl. Crystallogr, **26**,320 (1993).
[2] H. Iwasaki & T. Kikegawa, Acta Cryst. **B53**,353(1997).