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 low-Z elements, nitrogen and 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 between 25-27 KeV. Exposure time was between 2 and 8 hrs. Obtained images were analyzed by PIP.

3. Results and Discussion

3.1. Oxygen(O_2)

Figure 1 shows the pressure change of powder patterns of the solid oxygen ε phase up to 25 GPa. Observe strong reflections were assigned by a monoclinic cell(C2/m) proposed by Johnson et al.[1]. The patterns at 10.5 and 12.5 GPa indicate 4 new reflections with weak intensity, which could not be explained by the proposed structure, while a strong preferred orientation occurs with pressure. The result suggests a super-lattice structure of the monoclinic cell to the ε phase and is consistent with recent our IR absorption experiment[2].

3.2. Nitrogen(N_2)

Powder pattern of the solid nitrogen was obtained as a function of pressure to 68 GPa. The result did not indicate any structural phase tansition at 66 GPa previously proposed by Raman study[3]. Recent our result of Raman study has not also suggested the transition. It was found that remarkable broadening of the diffraction lines was observed above 40 GPa.

3.3. Phosphorus(P)

The simple cubic(SC) structure, which occurs at 10 GPa at RT, was studied up to 113 GPa in order to reseach its structural stability and the post-SC structure. A phase transition from the SC to a low symmetric structure was observed at 107 GPa shown in Fig. 2. The post-SC structure was not explained by the proposed structure(distorted-bcc)[4].

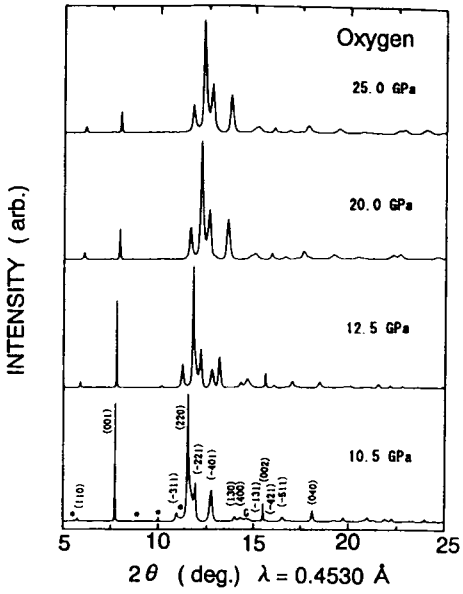

Fig.1. Powder patterns of e-O_2 phase at various pressre.

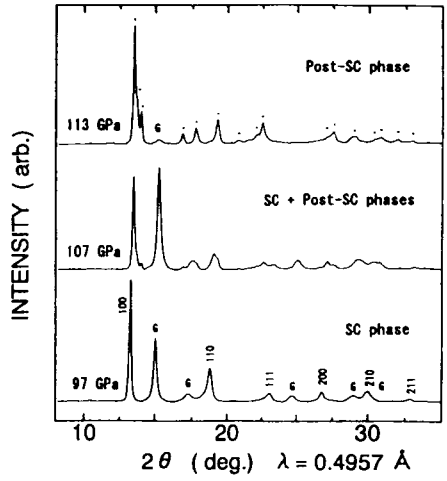

Fig.2 Powder patterns of phosphorus around a phase transition at 107 GPa.

[1] S. W. Johnson et al., J. Appl. Crystallogr, **26**,320 (1993).
[2] Y. Akahama et al., in *Proc. AIRAPT Int. Conf.* Kyoto, (1997)p.781.
[3] R. Rreichlin et al., Phys. Rev. Lett. **55**, 1464(1985).
[4] H. Iwasaki & T. Kikegawa, Acta Cryst. **B53**,353(1997).