Single Crystal Analyses of ε-O_2 High-Pressure Phase of Solid Oxygen

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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 the novel electronic and magnetic preperties of the high-pressure phases[1]. Determination of the structural properties of the high-pressure phases is indispensable for understanding the electro-magnetic properties.

In this study, the high-pressure single-crystal analysis of β-O_2 and ε-O_2 of low-Z element has been carried out including setup of the diffractometer on the BL02B1.

2. Experimental

The rhombohedral β-O_2 ($R\bar{3}m$) and monoclinic ε-O_2 crystals were grown under high pressure and temperature conditions at 5.5 GPa and 300 K and at 20 GPa and 600 K, respectively, in a Merrill-Bassett type DAC[2] which had a conical window of 70° (2θ=35°) to insident and scattering sides. The DAC was placed on a Huber diffractometor and the monochromated beam with an energy of 30 KeV(λ=0.4133 Å) was exposed to the sample through a 0.5 mm diameter pin-hole.

3. Results and Discussion

For the β-O_2 sample, the UB parameter and the lattice constants of the hexagonal cell, a=2.806(2) and c=10.28(2) Å, were determined from a least-squares fitting of 13 reflections. The values are listed in table I together with previous results[3].The c-axis was unfortunately vertical to the top-surface of the diamond anvil. The typical reflection profile is shown in Fig.1. The almost reflections splitted into two or more peaks. Intensity data could be measured for 39 symmetry-independent reflections which were reduced to 12 nonequivalent reflections. Structure refinement is in progress.

Two polycrystal ε-O_2 samples with several crystals were tested with the oscillation photographs taken by using a vacuum camera and it was found that the single crystal analysis is feasible.

Table I. Structure parameters for β-O_2 phase together with the previous results[3].

		This work	Schiferl[3]
Pressure	P(GPa)	5.7	5.5
Temperature	T(K)	297	299
Lattice constant	a(Å)	2.806(2)	2.846
	c(Å)	10.285(2)	10.224
Volume	V(Å^3)	70.2(2)	71.76
Atomic parameter	z		0.0577(2)
Thermal parameter	$\beta_{11}=\beta_{22}=2\beta_{12}$		0.1647(7)
	$\beta_{13}=\beta_{23}$		0
	β_{33}		0.0055(3)
Internuclear distance	S(Å)		1.202(2)
R factor	R_w		0.050

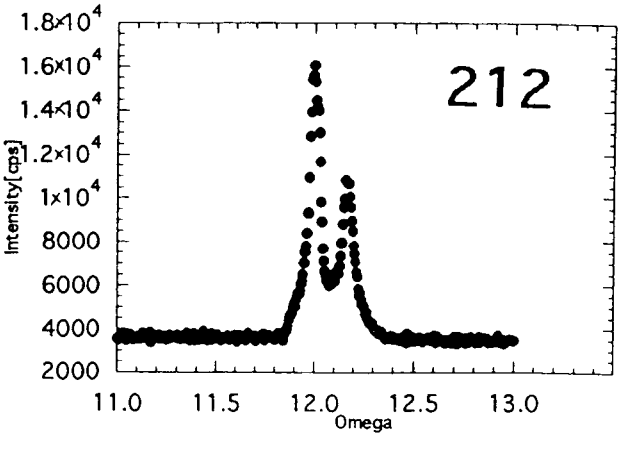

Fig.1 Typical reflection profile of β-O_2 phase.

[1]Y. Akahama et al., Phys. Rev. Lett. **74**, 4690 (1995).
[2]Y. Akahama et al., in *Proc. AIRAPT Int.Conf.* Kyoto, (1997)p.781.
[3] D. Schiferl et al., Acta Cryst. **B37**, 1329 (1981).