Pressure-Induced Phase Transitions of Scandium to 200 GPa

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1. Introduction

Scandium (Sc) is the lightest metal in the 3*d* transition elements and also belongs to rare-earth metals. For the pressure-induced phase transitions, a structural sequence of hcp-Sm type-dhcp-fcc, has been proposed. However, the x-ray diffraction study is limited in a lower pressure region because of the lower-Z number[1]. In order to clarify the proposed sequence of the structural transition, x-ray diffraction experiments have been carried out up to multi-megabar pressure at 300 K with a synchrotron radiation source.

2. Experimental

The powder x-ray diffraction profiles of scandium in a diamond anvil high-pressure cell were collected by the angle dispersive method using a monochromatic synchrotron radiation source (λ=0.4428 Å) on the BL10XU at the SPring-8. Beveled diamond anvils with a center flat size of 75 or 100 μm in diameter with a bevel angle of 8° to 300 μm in culet diameter were used for the ultra-high pressure generation. To obtain the detail of the first phase transition at 23 GPa, the anvils with 400μm were also used with helium pressure medium.

3. Results and Discussion

Upon loading to 200 GPa, Sc undergoes four structural phase transitions at 23, 80, 110 and 135 GPa as shown in Fig.1. Reproducibility of these transitions was confirmed in the second run. The starting phase of hcp is an anisotropic compressibility and the c/a decreases 1.553 at 21 GPa. Calculated atomic volumes at each pressure are illustrated in Fig.2 together with those of titanium(Ti) and vanadium(V). The first transition was proposed to be hcp to pseudo-bcc structure by previous study[1]. But the present diffraction data are not explained as the proposed structure. The diffraction patterns of other high-pressure phases are complicated and suggested that these phases do not follow the proposed structural sequence and have large unit cell with lower symmetry. The structural analysis of these phase is in progress.

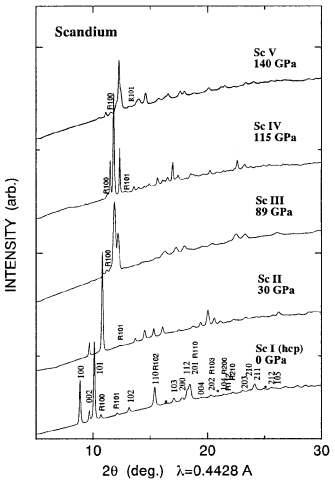

Fig.1 Pressure change of diffraction patterns of scandium (Sc) to 140 GPa at 300 K.

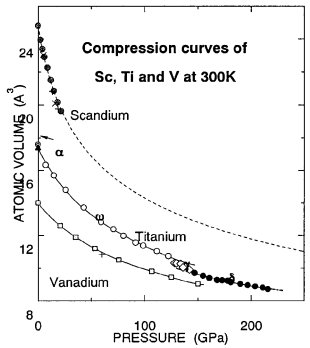

Fig.2. Compression curves of Sc, Ti, and V at 300K.

[1] Y.C.Zho *etal.*, Phys.Rev.B**54**,9715(1996).

Powder X-ray Diffraction Analysis of High-Pressure Phase of Solid Oxygen to 300 GPa

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1. Introduction

Recently, in the highly compressed solid oxygen, superconducting transition has been observed at low temperature[1], following the report of the metal-insulator transition[2]. Since the oxygen molecule, O_2, exhibits a simple and fundamental molecular magnetism, many attentions have focused on the phenomena relevant to its magnetism.

The detail feature of the transition is significant for understanding the metallization in the diatomic molecular solid such as H_2, O_2 and N_2. In this study, we perform the powder x-ray diffraction experiments of a low-*Z* elemental material, solid oxygen to multimegabar pressures and the structure of the metallic phase is proposed.

2. Experimental

The powder x-ray diffraction profiles of solid oxygen, in a diamond anvil high-pressure cell (DAC), were collected by the angle dispersive method using a monochromatic synchrotron radiation source (λ=0.4961 Å or 0.4246 Å) on the BL10XU at the Super Photon ring-8 GeV (SPring-8). Beveled diamond anvils with a center flat size of 75 or 100 μm in diameter with a bevel angle of 8° to 300 μm in culet diameter were used for the pressure generation. Liquid oxygen was loaded in a hole on a Re metal (or Ni alloy) gasket of a DAC, together with a ruby chip of the pressure marker. The powder profiles were measured up to 220 GPa with an x-ray beam reduced using a pinhole collimator of 20 μm diameter. Pressure was determined from the ruby fluorescence method or the equation of state of Re. One of their runs was carried out with a different gasket material, Udmet700 Ni alloy, in order to check the superposition of the diffraction lines from the Re gasket on those from the sample. The 2θ-intensity profiles were obtained by the integration of the recorded two-dimensional diffraction images[3].

3. Results and Discussion

The ε phase transformed into the ζ phase around 100 GPa. Corresponding to the transition, the 110 superlattice reflection of the ε phase vanishes and new reflections appear around 2θ=16° and 27.6° above 96 GPa. The transition pressure of structure transition well agrees with our previous report[4]. The pressure dependence of *d*-spacing shown in Fig. 1 is also suggestive of the transition at 96 GPa and consistent with our previous data[4]. The structure of the ζ phase could be explained as a monoclinic lattice with two O_2 molecules in the unit cell. The ε-ζ transition, which corresponded to the metal-insulator transition at 96 GPa, was sluggish and completed around 118 GPa with comparably large volume reduction of 6 %.

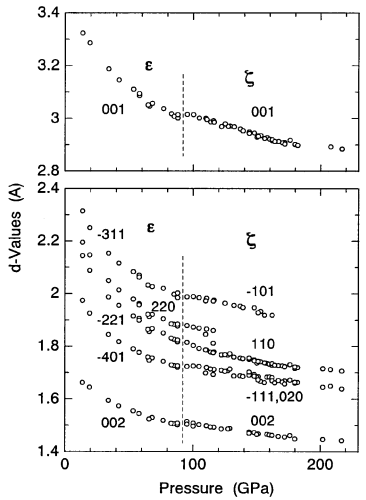

Fig.1 Pressure change of d-spacings of solid oxygen at 300 K.

[1] K.Shimizu etal: Nature **393** (1998)767.
[2] S.Desgreniers etal: J. Phys.Chem. **94**(1990)1117.
[3]O.Shimomura etal:Rev.Sci.Instrum.**63**(1992) 967.
[4] Y.Akahama etal: Phys. Rev. Lett. **74** (1995) 4690.