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The phase transition of BeO under high pressure

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Introduction

BeO is an interesting ceramic because of its electrical, thermal and crystal properties. BeO crystallizes the hexagonal wurtzite structure (B4) under ambient conditions although the other BeX (X=S, Se, and Te) crystallizes the cubic zinc-blend (B3). The experimental reports of the high pressure x-ray diffraction study show that the phase transition occurs for the BeS, BeSe, and BeTe at 51 GPa, 56 GPa and 35 GPa, respectively, and transforms to the sixfold-coordinated hexagonal nickel-arsenide structure (B8). On the other hand, there is still no experimental report of the pressure induced phase transition to the sixfold-coordinated phase for BeO because of the low atomic number [1]. The theoretical report on BeO under high pressure shows a calculated phase transition from the four-fold coordinated hexagonal phase to six-fold coordinated NaCl (B1) phase [2-5].

In this research, we carried out the powder x-ray diffraction studies by using the synchrotron radiation source of this low Z material under high pressure to find the phase transition from the four-fold coordinated phase to the six-fold coordinated phase.

Experiment

The pressure was generated using a diamond anvil cell with a 150 μm culet diamond. A Re-W alloy was used as a gasket. The pressures were determined using the ruby fluorescence method below 100 GPa and the Raman shift of the diamond beyond 100 GPa. High pressure x-ray studies were carried out to 175 GPa using the angle dispersive x-ray diffraction at BL-18C and BL-13A beam line in Photon Factory and at BL10XU beam line in SPring-8. The collimated x-ray beam with 15 ∝m in diameter exposed on the sample and the diffraction from the sample was recorded on an imaging plate.

The x-ray diffraction data were analysed by the Rietveld method (RIETAN-2000 [6]).

Results and discussions

By increasing the pressure, all peaks shifted to the higher angle positions, however the phase transition did not occur to 126 GPa which is different from other BeX. The pressure dependences of the lattice constant a and c were calculated with these diffractions. These lattice parameters continuously decrease with increasing pressure. Moreover the ratio of c/a increases with increasing pressure with the pressure coefficient of 4×10^{-5} GPa^{-1}. The bulk modulus at zero pressure was 232 GPa calculated by the Birch equation, similar to the value of the previous report [1]. The x-ray diffraction pattern of BeO at 137 GPa is shown in Fig. 1. The phase transition was found at this pressure. The diffraction lines denoted plus sign (+) are due to the high pressure phase. The
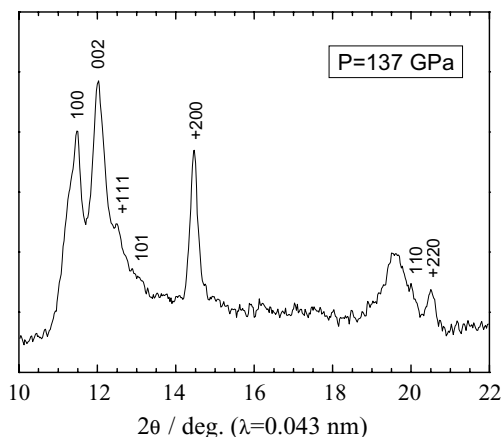

Fig.1 X-ray diffraction of BeO at 137 GPa.

value of the transition pressure is similar to the theoretical report [2]. The ratio of the cation to the anion radius of BeO (0.244) at ambient pressure is much larger than for other BeX chalcogenides (0.172-0.196). The linear correlation between the logarithm of the transition pressure and the cation radius to anion radius ratio for the BeO and BeX are found. With increasing pressure, the B4 phase disappeared, and the diffraction was totally from the high pressure phase at 175 GPa. The crystal structure of the high pressure phase was determined to be the NaCl (B1) phase using the Rietveld analysis. In this case, the R-factors were 0.31%, 0.24%, 0.25% and 1.23 for R_{wp}, R_p, R_e and S respectively. The color of the sample before phase transition was still transparency. The dielectric theory of Phillips and Van Vechten shows that the tetrahedral compound with the lower Phillips ionicity (f_i) than 0.35 as BeX transforms to a metallic phase directly with increasing pressure. On the other hand, the case of the higher ionicity than 0.35 as BeO (f_i =0.602), the phase transforms to an ionic six-fold structure and then to a metallic phase. It is considered the transparent color is cause by the ionic phase and the higher metallic phase is expected under the higher pressure.

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