

Phase Transformation of Zirconium under High P-T Conditions

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The behavior of zirconium metal under high pressures is important in the community of the high-pressure study, because changes in resistivity due to the phase transformations of zirconium (Zr) are used as pressure calibration points in the high-pressure experiments. Zirconium metal, which shows the hcp structure at ambient conditions, is known to transform to the bcc structure (beta phase) above 1135 K at ambient pressure. With increasing pressure, phase transformations to a hexagonal structure (omega phase), at the pressure around 5 GPa and to a bcc structure around 30 GPa have been observed at room temperature. The formation of the high-pressure phases is concerned with changes in the electronic structure. Recent investigations for the phase transformation from the hexagonal to the bcc structures at high temperatures (Zhang et al. 2005 and 2007) were inconsistent with previous study at temperatures around the room-T (Xia et al. 1991). Therefore, we reinvestigated the transformation pressure in zirconium metal.

The starting material used in this study was polycrystalline Zr. High-pressure X-ray diffraction experiments were carried out in an external heated diamond anvil cell. The small sample sandwiched between pellets of NaCl powder was loaded into a hole that had predrilled into a rhenium gasket. The heating temperature was up to 800 K, and was recorded using the R-type of thermocouples. The sample was probed using angle-dispersive X-ray diffraction, located on the synchrotron beam lines, at NE1A of the Photon Factory. Details of the synchrotron X-ray experiments have been described elsewhere (e.g., Ono et al. 2005). The angle-dispersive X-ray diffraction patterns were obtained on the imaging plate of an X-ray data collection system (Rigaku, RAXIS). The pressure was calculated from the NaCl unit cell volume using the equation of state (EOS) for NaCl, as developed by Ono (2010).

The boundary from the omega phase to the bcc phase was determined at high temperatures (300 - 800 K). Our results were in good agreement with those reported in previous room-temperature study. The gradient of dP/dT of the boundary was negative. However, the gradient observed in our experiments was 2-3 times more negative than that reported by previous high-temperature experiments (Zhang et al. 2005 and 2007). Our new data indicated that the difference in the stress conditions of the sample led to the discrepancy of the gradient of dP/dT slope in previous studies.

Keywords: Zirconium, Phase transition, High pressure and high temperature