XAFS study of ZrO$_2$ nano particles under high pressure

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XAFS spectra measurements near the Zr K-edge for the $P2_1/c$ and $Pbca$ ZrO$_2$ phases with particle size of 62 nm and 0.50 µm were performed under pressure up to 7.8 GPa using a multi-anvil high-pressure device and synchrotron radiation at BL14B1, SPring-8, Hyogo. XANES spectra change gradually near the phase transition region of 3.0-4.8 and 4.8-7.8 for bulk and nano particles (Fig. 1). The second-nearest Zr-Zr distance in nano particle is 0.02 Å longer than that in bulk particle. It was found that the nano particle is more compressible comparing with the bulk particle and transforms to the $Pbca$ phase at certain specific Zr-O and Zr-Zr distances (Fig. 2). The decrease rate of EXAFS Debye-Waller factor $\sigma^2$ by pressure is the same for both bulk and nano size particles. The magnitudes of $\sigma^2$ for Zr-Zr distance in the nano particle are significantly larger because of the static disorder near the surface (Fig3).

Figure 1. Experimental Zr K-edge XANES spectra of the bulk and nano size ZrO$_2$ particles under pressures. The shape of XANES changes gradually around 3.5-4.8 and 4.8-7.8 GPa for the bulk and nano particles, respectively.

Figure 2. Variation of second nearest Zr-Zr distance in bulk and nano ZrO$_2$ particles by compression.

Figure 3. Pressure dependence of $\sigma^2$ for Zr-Zr distances in nano and bulk ZrO$_2$ particles.