XANES Spectroscopic Studies of the Phase Transition in $Gd_2Zr_2O_7$

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The structural phase transition from the fluorite to pyrochlore and the strength of the coordination bond of Zr–O in $Gd_2Zr_2O_7$ were investigated by XANES spectra of both O and Zr *K*-edge. Energy difference of the O *K*-edge absorption spectra at 532 and 536 eV was assigned to the crystal field splitting energy of 4d orbital ($\Delta E_{4d,}$ t_{2g} and e_g) of Zr ion. Besides, the samples prepared at higher temperatures, the 536 eV peak moves slightly to higher energy, whereas the absorption energy of 532 eV peak does not shift. The correlation between ΔE_{4d} and the strength of interaction between Zr (4d) and O (2p) orbitals have been found. Furthermore, two Zr *K*-edge absorptions at 18020 and 18030 eV of $Gd_2Zr_2O_7$ have been observed, the splitting energy (ΔE), peak intensity ratio (I_{18030}/I_{18020}), and FWHM of the first derivative of the absorption curve depend on the preparation temperatures. The effect of crystal symmetry and Zr–O bonding character on the XANES spectral profile was discussed.