XANES and the electronic state of Americium oxides

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Am is notable from the view point of reducing the environmental burden in the disposal of high level radioactive waste, and transmutation of Am in the form of mixed oxide (MOX) fuel is considered to be an important option for the future nuclear fuel cycle. The local and electronic structures around Am atom in MOX fuel are indispensable information to design the fuel and to evaluate the irradiation behavior. X-ray absorption near edge structure (XANES) is an excellent method for examining the local and electronic structures.

We measured Am L_{III} XANES spectra of AmO_2 and Am_2O_3 and found the peak structures such as the white line, the tail structure, and the high-energy broad peak structure in these spectra. In order to characterize XANES in aspect of the electronic structures for the Am_2O_3 and AmO_2, the theoretical assignments were performed with Wine2k code, which is based on the all-electron full potential linearized augmented plane wave (FP-LAPW) method. The XANES spectra of Am_2O_3 and AmO_2 were calculated, and the experimental spectra were well reproduced in these calculations. In addition, it was found that the white line peak was created due to the interaction between Am-d and O-p components, and the broad peak and the tail peak were created due to the interaction between Am-d and O-d component. Besides, these spectra were evaluated by the analysis in the view points of the exited electron behavior in the electron density, and the difference between XANES spectra of AmO_2 and Am_2O_3 was clarified by the analysis in these view points. In addition, XANES of (Am, U) mixed oxides were evaluated in these view points.