Contribution ID: **26** Type: **Poster**

X-Ray photoelectron spectral structure and chemical bonding in AmO2

Tuesday 20 May 2014 17:30 (4h 30m)

The quantitative analysis of the x-ray photoelectron spectral (XPS) structure of americium dioxide AmO2 was done in the valence electrons binding energy range taking into account binding energies and spectral structures of the core electronic levels (˜35 - 1250 eV) and the relativistic calculation data for the AmO812- (D4h) cluster reflecting americium close environment in AmO2. The experimental data suggest that the many-body processes and the multiplet splitting contribute to the valence XPS structure significantly less than the outer (0 - ˜15 eV) and the inner (˜15 - ˜35 eV) valence molecular orbitals formation does. The filled Am 5f electronic states were shown to appear in the valence band of AmO2. The atomic Am 6p electronic orbitals were shown to participate in formation of both inner and outer valence molecular orbitals (bands). The most part in the inner valence molecular orbitals formation were found to take the filled Am 6p3/2 and O 2s atomic shells. The composition and the sequent order of such orbitals in AmO2 were established in the binding energy range 0 - ˜35 eV. The obtained experimental and calculation data allowed for the first time a quantitative scheme of the molecular orbitals for AmO2. This scheme is essential and fundamental for understanding of the chemical bonding nature in AmO2 and for interpretation of the fine structures of other x-ray spectra.

The work was supported by the RFBR grant #13-03-00214.

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Session Classification: Poster

Track Classification: Solid State Chemistry and Physics of the Actinides