N *K*-edge XANES and XES Study of transition metal-doped AlN Films

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Heavy-doping of 3d-transition metals (TMs) to III-nitrides have attracted much interests for the last two decades because it can add new energy bands in their wide band gap, which can work as intermediate band (IB) for photoconversion of sunlight [1] or spin-polarized band for spintronics devices [2]. We have been exploring the possibility of heavy 3d-TM doping to AlN as IB materials [3-8]. One can have questions whether AlN is appropriate as a base for an IB material because the E_g of AlN is as wide as 6 eV. We thought, however, heavy-doping of 3d-TMs can cause not only IB formation but also reconstruction of the top of valence band (VB) and the bottom of conduction band (CB) of AlN, which has a wurtzite structure (C_{6v}), thorough hybridization of TM-*d* and N-*p* orbitals in non-centrosymmetric coordination structure such as T_d and C_{3v} when TMs occupy Al sites in AlN.

In this study, we carried out N *K*-edge X-ray absorption near edge structure and emission spectroscopies (XANES and XES, respectively) to reveal the detailed band structures of AlN doped with various 3d-TMs, such as Ti, V, and Cr at BL27SU of SPring-8. We will discuss the experimental spectra comparing with calculated spectra by FDMNES code [9] and calculated band structure by VASP code [10].

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