Polarization-dependent XAFS and DFT-based investigations of epitaxial GaMnN materials

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In this presentation, a correspondence between the results of the X-ray Near Edge Structure (XANES) spectroscopy and theoretical investigations within the density functional theory (DFT) for GaMnN materials is discussed [1,2]. The polarization-dependent XANES spectra of homogeneous GaMnN films exhibit characteristic features which are related to the local structure of particular samples. Namely, the shape of the experimental spectra may be reasonably resembled only with the model calculations for GaMnN systems with a nitrogen vacancy in the close vicinity of a Mn ion. Furthermore, the valence state of Mn ions (2+ or 3+) varies among samples of GaN materials, which is also reflected in XANES spectra and may be supported with the DFT-based calculations of the electronic structure for GaMnN systems.

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[2] E. Piskorska-Hommel, M.J. Winiarski, G. Kunert, D. Hommel, *J. Alloys Compd.* **725**, 632 (2017).