Insights into doped magnetic semiconductors from soft x-ray spectroscopy

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Introduction

Semiconductors doped with magnetic ions are of enormous interest for their potential ability to generate and manipulate spin currents. In these materials, magnetic dopants provide a localized magnetic moment and a hole, leading to a polarization of valence band states, which mediates the interaction between the dopants. At the same time, defects in the material may play a strong role in determining where the dopants reside in the lattice, which has a strong influence on the magnetic ordering.

Methods and Materials

Since these questions involve all of the elemental constituents in the material, chemically specific x-ray techniques such as soft x-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD), coupled with theoretical calculations based on realistic defect structures, have proven to be very useful for understanding the origin of magnetism in doped systems. We have used these techniques at sector 4 of the Advanced Photon Source to examine Mn-doped GaAs and GaN, in combination with density functional theory (DFT) calculations.

Results and Discussion

In Mn:GaAs, XMCD revealed magnetic moments on the Ga and As atoms which are consistent with the predictions of density functional theory calculations.[1] However, in Mn:GaN, the Ga moment is opposite to that predicted, suggesting that the ordering mechanism may be different than in GaAs. Further analysis of the local Mn environment in both materials via the Mn XAS and XMCD lineshapes provides additional insight into the magnetic ordering of the Mn. In GaAs, a single component lineshape was observed which indicated divalent Mn, but were best reproduced with a DFT model combining simple Mn substitutions and Mn interstitials. In GaN, a more complicated two-site spectrum was observed (c.f., Fig. 1). Both the Mn lineshape and the Ga spin direction could only be reproduced by introducing a certain type of N interstitial defect. In this model, two N atoms occupy a N site, and Mn is preferentially bound to neighboring sites,[2] as in Fig. 2. These results show that defect states can drive the Mn site occupancy and strongly influence the magnetism, and that their role can be strikingly different even between two closely related materials.

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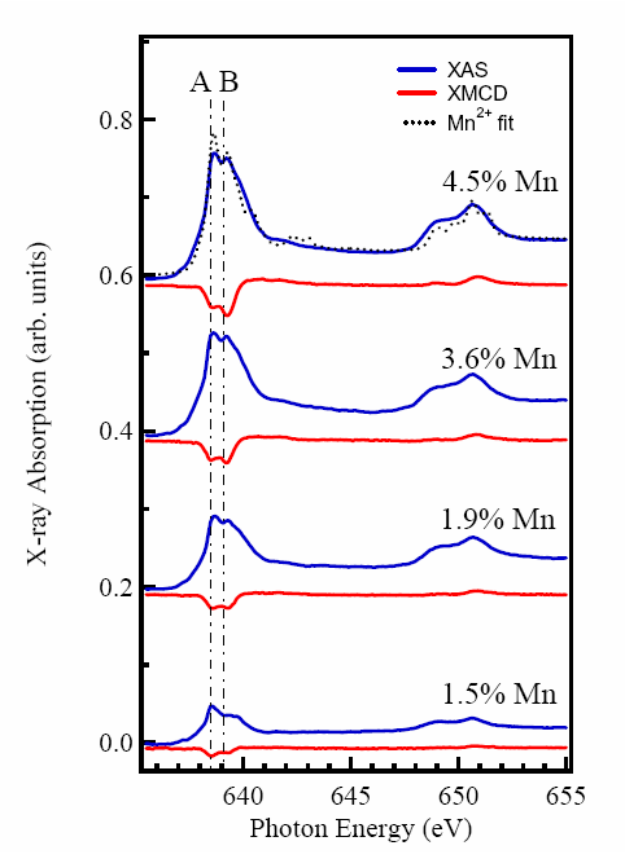

Fig. 1. XAS (blue) and XMCD (red) data for Mn-doped GaN with varying Mn concentration. The dotted curve is a it to a two-site divalent Mn model.

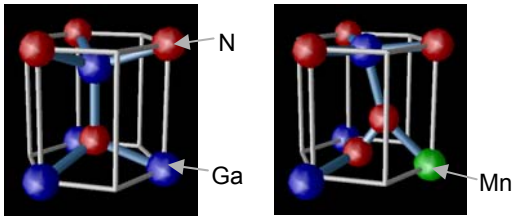

Fig. 2. Models showing the relative atomic positions for ideal GaN (left) and in the presence of a N split interstitial. The Ga sites neighboring the split interstitials are more energetically favorable for Mn occupancy and reproduce the XAS spectra observed in Fig. 1.

References

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[2] D. J. Keavney, S. H. Cheung, S. T. King, M. Weinert, and L. Li, Phys. Rev. Lett. **95**, 257201 (2005).