## X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism of Novel Materials for Spintronics, Nanoelectronics and Advanced Devices

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Our work seeks to design and control the magnetic and electronic properties of materials, which allow the discovery of new physics and enable future device applications. X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) are powerful techniques that can be used to probe the magnetic and electronic states in materials. They are utilized extensively in our group to probe bulk, thin film and nanostructures of Heusler compounds and transition metal oxides with strongly correlated electrons.

#### Simple Rules for Designing Mn-based Heusler Compounds for Spintronics<sup>1</sup>

Mn-based Heusler compounds are perhaps some of the most attractive compounds for future spintronics applications. For instance, Mn<sub>3</sub>Ga has been proposed as a potential material for spin transfer torque devices.<sup>2</sup> Here, Mn is present on multiple sublattices, and the magnetic moments are antiparallel, guaranteeing a low total moment with a high Curie temperature. <sup>2</sup> Additionally, Mn when coordinated octahedrally by Si in Co<sub>2</sub>MnSi leads to full spinpolarization of the charge carriers<sup>3</sup> and consequently widespread applicability as an electrode material in tunneling magnetoresistance (TMR) devices.<sup>4</sup>



Fig. 1: Mn L-edge absorption for selected Heusler compounds.

These materials are highly tunable, due in part to the large number of different elements that can be used to form the ternary compounds on a relatively simple lattice with high symmetry, which, in the chemical sense, contains multiple sublattices. Designing new materials for future device applications necessitates a general understanding of how Mn behaves on the individual chemical sublattices. We therefore probed the electronic and magnetic properties of Mn as a function of coordination with respect to Z in full and half Heusler compounds experimentally using X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) and theoretically with ab initio calculations (Fig. 1). Both theory and experiment show that the Mn oxidation state indicates delocalized metallic-like behavior in the full and half Heusler compounds. However, the magnetic moment in the octahedral sites is large and localized (atomiclike), but the moment in the tetrahedral sites is reduced. These general rules can be used to tailor the magnetic and electronic properties for future applications in Mn-based Heusler compounds by carefully controlling the individual sublattices.

### Mn<sub>x</sub>Ga<sub>1-x</sub> Thin Films and Nanodots with High Coercivity and Perpendicular Magnetic Anisotropy<sup>5</sup>

 $Mn_xGa_{1-x}$  thin films (x=0.70, 0.75) were grown at different temperatures and thicknesses on SrTiO<sub>3</sub> substrates. Samples grown at 300 - 350°C evidently lead to polycrystalline films with a significant fraction exhibiting the tetragonal c-axis in the film plane (Fig. 2a), which subsequently results in a secondary magnetic component in the out of plane M(H) curve as well as an in-plane hysteresis (Fig. 2a). Reducing the film thickness or Mn concentration improves the film quality. Additionally, a self-assembly nanolithography approach was used to pattern 550 nm nanostructures in a Mn<sub>70</sub>Ga<sub>30</sub> epitaxial thin film (Fig. 2b). The resultant nanodots exhibited similar features to the parent film i.e. PMA and a large coercivity. A kink was evidenced in the magnetic hysteresis loop near H=0 in the nanostructured material and attributed to chemical disorder induced during the lithography procedure (Fig. 2b). Chemical order was recovered in the nanostructures after annealing (Fig 2b). Our results suggest Mn<sub>x</sub>Ga<sub>1-x</sub> as a promising material for spin valve devices.

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Fig. 2: (a) Cross sectional HRTEM image from the x=0.75,  $350^{\circ}C$  sample. The bottom inset shows a portion of the FFT in the film region. The top inset shows in-plane (dashed) and out-of-plane (solid) magnetization. (b) M(H) for  $Mn_{70}Ga_{30}$  film and nanodots before and after annealing. The bottom inset shows an XRD pattern of the same samples. The top inset shows an SEM image of the nanodots.

# Single Phase Co<sub>2</sub>NiGa Nanoparticles for Nanoscale Devices<sup>6</sup>

We fabricated for the first time Co<sub>2</sub>NiGa nanoparticles (NPs) of a single  $\gamma$ -phase ( $\gamma$ -Co<sub>2</sub>NiGa). The NPs were prepared by impregnation in colloidal silica followed by high temperature annealing. Energy dispersive X-ray spectroscopy mapping and X-ray absorption near edge structure data provided evidence for the successful preparation of the intermetallic NPs and the absence of impurity phases. Extended X-ray absorption fine structure spectroscopy data confirm the formation of the  $\gamma$ -Co<sub>2</sub>NiGa phase by examining the atomic environments surrounding Co, Ni, and Ga (Fig. 3). The Co<sub>2</sub>NiGa NPs were ferromagnetic with a high saturation magnetization.  $\gamma$ -Co<sub>2</sub>NiGa NPs exhibited a very high Curie temperature ( $\approx 1139$  K), which make them promising candidates for high temperature magnetically activated nanoscale devices.



Fig. 3: XANES data for the  $\gamma$ -Co<sub>2</sub>NiGa nanoparticles at the absorption edges of Co (a), Ni (b), and Ga (c).

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