Charge Transfer at the Fe-GaAs Interface

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Introduction

Intermixing at metal-semiconductor interfaces is of vital importance in semiconductor device physics. Formation of Schottky barriers, as well as metallic interconnects on semiconductor-based electronics, are strongly influenced by the structure and disorder of the interface. With the recent explosion of magnetic-based electronics,[1] there is a growing need to efficiently integrate magnetic and semiconductor-based electronic structures. In this way, one can use the spin degree of freedom as an additional handle for the modification of electron transport to produce spin-based electronics.[2-4] However, the integration process is fraught with several barriers that must be overcome. First is the reduction of interfacial intermixing commonly found at metal-semiconductor interfaces, which degrades the spin transport performance. Second, to tailor magnetic device properties for specific tasks requires an understanding of the detailed chemistry and physics at the interface.

Iron on GaAs was one of the first ferromagnetic-semiconductor systems studied due to the lattice match for epitaxial growth. Studies have focused on the GaAs surface structure to determine if the unique magnetic properties of the overlayer are related to the wide variety of possible surface reconstructions.[5-8] For thicknesses less than 5 monolayers (ML), all systems are found to be magnetically inactive, while thicker films ferromagnetically order and display a strong uniaxial magnetic anisotropy along the (110) direction in contrast to bulk Fe.

We present evidence for the formation of a Fe-As local bonding environment at the interface between Fe thin films and GaAs surfaces of differing orientation and preparation.[9] Changes in the unoccupied electronic states of Fe thin films on sputtered GaAs(100) and cleaved GaAs(110) display a similar amount of 3d charge transfer into the GaAs substrate even though the mode of surface preparation leads to reduced intermixing in the (100) case.

Methods and Materials

Experiments were performed at the high-resolution spectroscopy beamline (2-ID-C) at the Advanced Photon Source, which operates in the intermediate x-ray range of 500 - 3000 eV. At all absorption edges studied, beamline resolution was sufficient that the measured absorption was limited only by the natural linewidth. X-ray photoelectron spectroscopy (XPS) was performed using a hemispherical energy analyzer with 100 meV resolution. Absorption measurements were acquired in total electron yield (TEY) and fluorescence yield (TFY) modes by monitoring the sample current and using a photodiode, respectively. Iron was deposited at room temperature (300K) at a growth rate of ~1 Å/min from a high-purity Fe wire heated resistively. For the (100) orientation, polished GaAs wafers were cleaned with 1 keV Ar^+ ion sputtering until the core level spectra showed no traces of oxygen and carbon. The (110) surfaces were achieved by {in situ} cleaving of notched GaAs blocks. In both cases the GaAs substrates were n^+ doped to promote the necessary conductivity required for spectroscopy measurements. Core level spectra were used to confirm that the surface was free of contamination after each deposition cycle. Fe overlayer thickness was determined from both a quartz crystal oscillator and from a combination of the absorption edge jumps and XPS intensities.

Results and Discussion

First, we examine the intermixing of Ga and As with the Fe over layer using XPS. By tracking the intensities of the Ga and As 3d levels and comparing with the results expect for not intermixing, it is clearly seen that the two surface preparations lead to quite distinct behavior (see Figs. 1 and 2). For the (100) case there is almost no intermixing, while the (110) case shows significant

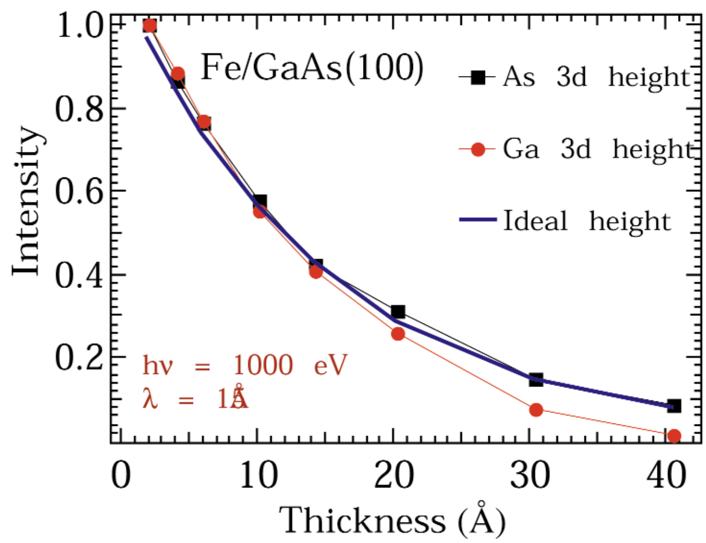

FIG. 1. Ga and As 3d XPS intensities vs. Fe overlayer coverage.

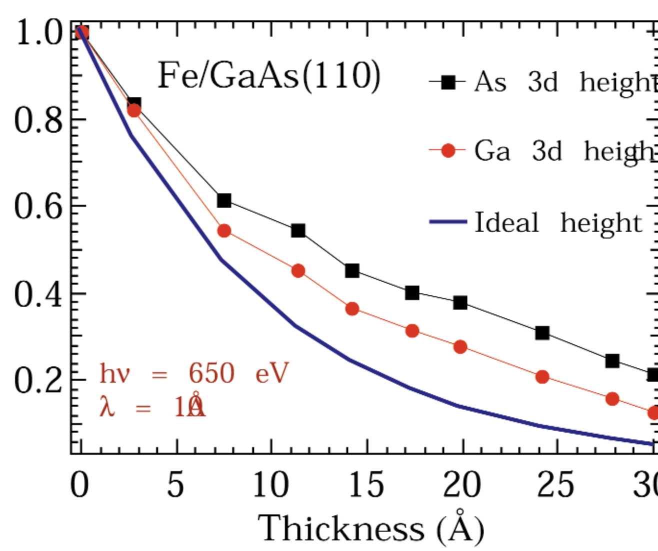

FIG. 2. Ga and As 3d XPS intensities vs. Fe overlayer coverage.

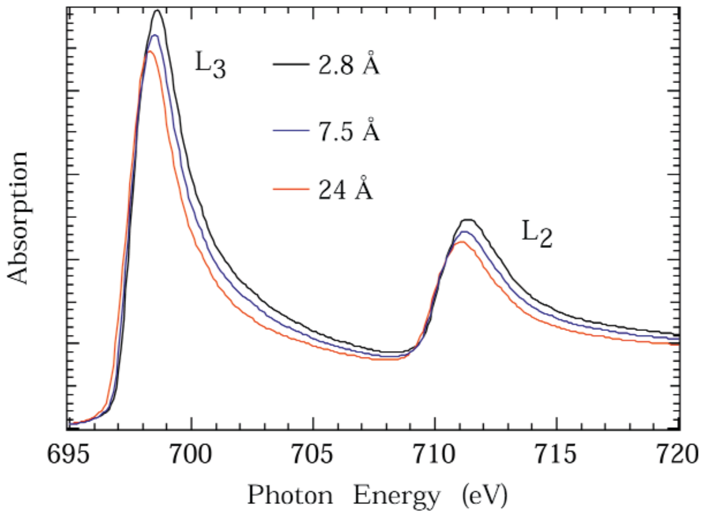

FIG. 3. Fe L-edge absorption vs. Fe overlayer thickness.

outdiffusion of Ga and As into the Fe overlayer. This is shown by comparing the behavior of the intensities to the exponential decay expect for an ideal uniform layer with no intermixing.

Of most interest though in the study of magnetic materials on semiconductors is the change in the Fe overlayer. Since the 3d electrons of Fe carry the magnetic moment, any intermixing or charge transfer at the interface will alter the 3d band occupancy and directly influence the magnetic order. To determine the amount of charge transfer at the interface, Fe L edge absorption spectra were measured as a function of overlayer coverage (see Fig. 3). Changes in the white line intensity are directly related to the number of 3d holes that show major changes with increasing coverage. Most important is the dramatic change in the width of the absorption line. This change must be associated with an increase in the density of 3d unoccupied states as is consistent with significant transfer of charge from Fe into the GaAs substrate.

After correction of saturation effects, removal of the background from excitation into the continuum, and integration of the white line intensity, the transfer of 3d charge from the Fe into the substrate can be constructed as shown in Fig. 4. Most importantly though, as a function of ML coverage, the two systems show a similar amount of charge transfer even though preparation occurred on two uniquely different surfaces. While extrapolation of the data to 1 ML coverage cannot be done accurately, it does indicate that the Fe overlayer is in a configuration in the neighborhood of 3d for both substrate orientations. The charge transfer is consistent with a local Fe-As bonding configuration at the interface and a resultant balancing of the Fermi levels in the two materials. Due to the large difference in electronegativities, As will tend to draw charge away from Fe. Ga has an electronegativity close to Fe, which implies that Ga could not be responsible for such a large transfer. For the (110) system, the Fe-As interface is formed using an intermixing reaction to create the desired interface with the extra surface components migrating into the Fe layer. For (100) even though no diffusion is observed, it is possible that the Ga at the interface is displaced but lacks sufficient energy to move farther than a few monolayers into the overlayer. Another interesting facet of this result is that intermixing and surface roughness do not dramatically affect the 3d charge transfer. Typically intermixing is the one of the key factors in modification of material properties.

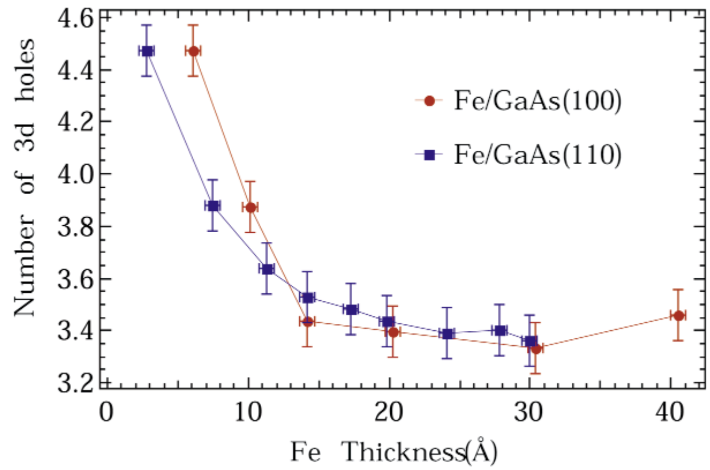

FIG. 4. Number of 3d holes vs. Fe overlayer thickness.

Acknowledgments

Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38.

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