Induced Ge Spin Polarization at the Fe/Ge Interface

J.W. Freeland,[1] R.H. Kodama,[2] M. Vedpathak,[2] S.C. Erwin,[3] D.J. Keavney,[1]
R. Winarski,[1] P. Ryan,[1] R.A. Rosenberg[1]

[1]Advanced Photon Source (APS), Argonne National Laboratory, Argonne, IL, U.S.A.
[2]Department of Physics, University of Illinois at Chicago, IL, U.S.A.
[3]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, U.S.A.

Introduction

Understanding the transport of spins across the ferromagnet/semiconductor interface poses many fundamental questions but has wide implications for spin-based electronics [1]. A key area is understanding how spin-polarized electrons or holes are injected from a magnetic material into a semiconductor [2, 3]. If the spins are injected from a ferromagnet, then one needs to consider the influence of the magnetic component on the semiconductor electronic structure. Induced moments have been observed in all metal ferromagnet/nonmagnet systems [4-6] but never directly in the ferromagnet/semiconductor system. Electronic structure calculations have predicted an induced moment (~0.05 μ_B) and modified density of states at the boundary [7-9], but to date, there has been no direct evidence for these induced interface moments. This issue is central to the tunneling of spins into a semiconductor. After a theoretical prediction [10], recent results have demonstrated high spin-injection efficiencies by tunneling through the Schottky barrier formed at the metal/semiconductor interface [11]. For the tunneling process, one needs to consider the behavior of s electrons in the system, which have sufficient overlap across the tunnel barrier and make up the majority of tunneling current. The 4s spin polarization in Fe corresponds to a total moment of ~0.05 μ_B [12], which is on the same order of magnitude as the predicted induced semiconductor moments. Thus, the characterization and understanding of these moments are keys to assessing the potential impact of a possible spin-scattering center due to the induced moment.

This report presents direct evidence of spin-polarized Ge at the interface with a magnetic transition metal. X-ray magnetic circular dichroism at the Ge L edge in an Fe/Ge multilayer provided unambiguous evidence for induced spin on Ge [13]. A comparison with single-crystal results enables the identification of the spin polarization into an s moment close to the Fermi level and a d component at higher energy. The data are consistent with an antiparallel induced moment on Ge. Layer-resolved electronic structure calculations show the induced moment is localized around the interface with the s and d moments ~0.01 μ_B that are antiparallel to the Fe 3d moment.

Methods and Materials

Element-selective magnetic measurements were made by using x-ray magnetic circular dichroism (XMCD), which arises from the coupling of the magnetic orientation to the x-ray polarization. These experiments were performed at sector 4 at the APS. Beamline station 4-ID-C provides high-resolution polarized x-rays in the intermediate x-ray range of 500 to 3000 eV. The x-rays are generated by a novel circularly polarized undulator that provides left- and right-circular polarization switchable on demand at a polarization of 96%. The samples were studied by measurement of total fluorescence yield (TFY) by using a microchannel plate detector. Fluorescence yield was used because of both its bulk sensitivity and its ability to measure in an applied magnetic field. The measurement involves changing the magnetization direction at each energy point of the absorption curve in order to measure the absorption with photon helicity and magnetization parallel (Γ^+) and antiparallel (Γ^-). The sum ($\Gamma^+ + \Gamma^-$) provides chemical information, while the XMCD ($\Gamma^+ - \Gamma^-$) is magnetic in origin. Since the XMCD signal is very small, it was confirmed that the XMCD changed sign upon reversal of the photon helicity.

Results

Measurement of the polarization-dependent absorption at the Ge L edge (see Fig. 1) provides direct access to the electronic and magnetic order of Ge. Because of the dipole selection rules for x-ray absorption, this excitation details the d and s contributions to the spin-polarized density of unoccupied states. The presence of a nonzero XMCD provides direct evidence of the spin-polarized Ge. A more detailed analysis of the data, however, requires an understanding of the electronic character of the unoccupied states contributing to the XMCD. As is shown below, the XMCD can be considered as consisting of three fundamental components: (1) a negative peak close to the Fermi level ascribed to spin-polarized s states, (2) higher-lying spin-polarized d states, and (3) an extended component that may be attributed to magnetic extended absorption fine structure.
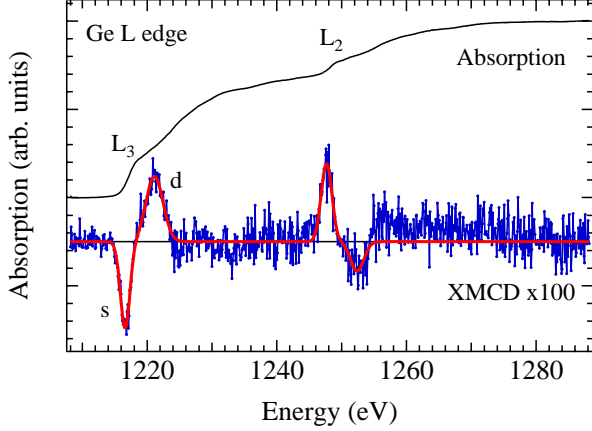
FIG. 1. *Average absorption ($I^+ + I^-$) XMCD (= $I^+ - I^-$) at the Ge L edge for the Fe/amorphous Ge multilayer. Nonzero XMCD gives a clear indication of an induced magnetic moment on Ge. The structure in the XMCD is attributed to spin-polarized s and d states as well as a small magnetic signal in the extended signal, which might be due to magnetic extended absorption fine structure.*

Discussion

To assign the XMCD to particular electronic states, first consider the results for bulk Ge, which will provide an initial framework. Calculations for amorphous Ge (a-Ge) show the density of unoccupied states are nearly the same as crystalline Ge (c-Ge) with only small modifications. The peaks in the c-Ge case result from the *s* and *d* density of unoccupied states as well as from multiple scattering from the highly ordered crystal. The edge for the c-Ge case was described by an initial peak due to *s* states followed by a double-peak feature due to *d* states. Results for the a-Ge system could be reproduced by the same density of states simply by varying the degree of coherent multiple scattering to simulate the disordered amorphous state. The first XMCD peak (labeled s in Fig. 1) lies in the pre-edge region close to the Fermi level, which may have an important impact on spin-dependent transport. Bulk electronic structure in this region is predominately *s* in character. The second XMCD peak coincides with the doublet assigned to *d* states. This provides an initial assignment, as shown in Fig. 1, which is consistent with the analysis of the experimental data and the layer-resolved density of state calculations, both of which are discussed below.

With an assignment of features, the dipole selection rules enable the determination of orientation between the Fe and Ge moments. The XMCD selection rules for *p* to *d* versus *p* to *s* transitions allow *s* and *d* contributions to the spin moment $<S_Z>$ to be written as:

$$<S_Z> = <S_Z^d> - 2 <S_Z^s> \frac{P_s}{P_d} + \frac{7}{2} <T_Z>$$

where P_s/P_d is the probability ratio for *s* versus *d* excitation and $<T_Z>$ is the magnetic dipole term. The important point is that the selection rules result in a minus sign between the *d* versus *s* XMCD for the same magnetic moment direction. Since the initial L_3 XMCD is negative for Fe (not shown), this is direct evidence of the antiparallel orientation of the Ge *s* moment and the 3*d* transition metal moment. The *d* component has a positive signal, indicating that the *d* component of the induced Ge moment is antiparallel to that of Fe as well. These results are in agreement with the electronic structure calculations presented below.

To interpret these results theoretically, we turn to density-functional theory calculations. Two sets of calculations were performed to elucidate different aspects of induced Ge moments in Fe: (1) two specific Fe/Ge interface models representing the ideal structure and the structure with Fe-Ge intermixing and (2) fixed-spin-moment calculations for bulk Ge, for the purpose of estimating the ratio between induced *p* moments (which are the largest) to *s* and *d* moments (which are measured by the L-edge XMCD). The calculations were performed within the generalized-gradient approximation, by using projector-augmented-wave potentials [14, 15]. The plane-wave cutoff and k-point sampling were sufficient to converge all quantities to the precision given.

To study Fe/Ge interfaces, we used three models introduced previously for Fe/GaAs interfaces [9]. All are 1×1 interfaces between crystalline Ge and Fe, with the interface boundary either ideal (i.e., atomically abrupt) or rough (with 1.0 monolayer of Ge in the Fe host). The isolated interfaces were modeled by supercells containing seven layers each of Ge and Fe, with atomic coordinates completely relaxed within two layers of the interface. The induced Ge moments for the ideal structure are shown in Fig. 2; the results for the other two models are qualitatively similar. The interfacial Ge layer has a moment of 0.06 μ_B antiparallel to the Fe magnetization. Although small, this is roughly half the value obtained for isolated Ge in an Fe matrix and thus appears reasonable. Ge atoms one layer away from the interface are less polarized (in the Fe direction), and further layers are essentially nonmagnetic. From these results, it can be inferred that the induced *s* and *d* moments on Ge atoms near the Fe/Ge interface are ~0.01 μ_B. There is also a consistency between the average moment orientation and the experimental results showing anti-alignment of the Ge *s* and *d* moments with respect to the Fe 3*d* moment.
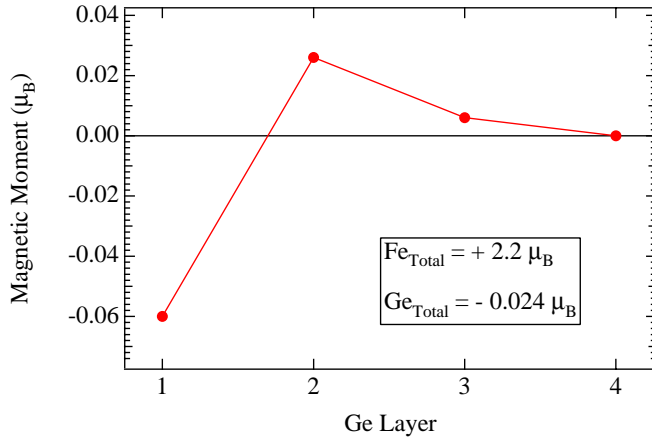
FIG. 2. Layer-resolved calculated moments for an ideal Fe/Ge interface. The inset shows the average total moment for the structure, since XMCD in absorption is an average over all layers that contribute a magnetic signal.

Acknowledgments

References

[1] S.A. Wolf et al., Science **294**, 1488 (2001).
[2] R. Fiederling et al., Nature **402**, 787 (1999).
[3] Y. Ohno et al., Nature **402**, 790 (1999).
[4] S. Pizzini et al., Phys. Rev. Lett. **74**, 170 (1995).
[5] G. Harp et al., Phys. Rev. B **51**, 12037 (1995).
[6] M. Samant et al., Phys. Rev. Lett. **72**, 1112 (1994).
[7] W.E. Pickett and D.A. Papaconstantopoulos, Phys. Rev. B **34**, 8372 (1986).
[8] I. Cabria, A. Perlov, and H. Ebert, Phys. Rev. B **63**, 104424 (2001).
[9] S.C. Erwin, S.-H. Lee, and M. Scheffler, Phys. Rev. B **65**, 205422 (2002).
[10] E. Rashba, Phys. Rev. B **62**, R16267 (2000).
[11] A.T. Hanbicki et al., Appl. Phys. Lett. **80**, 1240 (2002).
[12] W.L. O'Brien and B. Tonner, Phys. Rev. B **50**, 12672 (1994).
[13] J.W. Freeland et al., Phys. Rev. Lett. (submitted, 2002).
[14] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[15] G. Kresse and J. Furthmuller, Phys. Rev. B **54**, 11169 (1996).