Element specific spin-resolved densities of states in amorphous $Fe_{75}B_{25}$ probed with a synchrotron radiation source

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The partial spin-dependent densities of states (DOS) of both the iron and the boron in Fe–B amorphous magnetic alloys have been determined from spin-resolved photoemission using a synchrotron radiation source. The spin-integrated energy distribution curves (EDCs), polarization spectra and the spin-resolved EDCs show distinct differences between 15 and 40 eV photon energies due to strikingly different photon energy dependencies of the cross sections of Fe-*d* and B-*p* states. The B-*p* states were found to hybridize with Fe-*d* states and occupy a binding energy range of about 1–5.5 eV with a negative polarization; i.e., the *B* moment is ''antiferromagetically'' coupled with that of the Fe-*d* moment. © *2000 American Institute of Physics.* [S0021-8979(00)67408-X]

INTRODUCTION

The magnetism, electronic structures, and local atomic structures of amorphous alloys have been of interest for more than 20 years.[1,2] Recently there has been particular attention devoted to the spin-polarized density of states (DOS)[3–6] and the nature of the ferromagnetism in disordered metals.[7,8] Several first-principles electronic structure calculations have been made to obtain insight into the fundamental mechanisms of magnetism of the amorphous magnetic alloys.[3–6] The electronic states close to the Fermi level are predicted to be dominated by the TM-*d* band that is strongly hybridized with the metalloid to form a $p-d$ band complex. A decrease of the magnetic moment with increasing metalloid content is also predicted and attributed to a dilution effect; polarizable $d-d$ bonds are replaced by magnetically inert $p-d$ bonds.

In contrast with the significant progress in theoretical studies, experimental investigations of spin-dependent electronic structures are relatively rare in magnetic amorphous alloys[9,10] and, indeed, in magnetic alloys in general. In our previous work,[10] we measured the spin-resolved energy distribution curves (EDCs) of the Fe-*d* band in amorphous $Fe_{80}B_{20}$ and compared the results with three theoretical predictions. It is however, essential, to probe experimentally the element specific density of states in the alloys. As we discussed above, a key feature of these DOS calculations[3–6] is that the TM-*d* band interacts with the metalloid $2p$ band and forms a $p-d$ band complex. A polarized boron state due to this $p-d$ hybridization was predicted in α-$Fe_{80}B_{20}$ by Ching and Xu,[3] and in α-$Fe_{100-x}B_x$ with a composition range of $x=10-50$ by Bratkovsky and Smirnov[5] and $x=5-50$ by Hafner *et al.*[6]

There is an important experimental reason why the amorphous Fe–B system may offer an ideal opportunity to probe the spin-polarized density of states of both Fe states and B states. The inset of Fig. 1 shows the photon energy dependence of the cross sections of Fe and B.[11] The cross sections of the B-$2s$ and $2p$ states are much smaller than that of the Fe $3d$ states for photons with energy larger than ~25 eV. Using higher energy photons, the photoelectrons are therefore essentially due to the $3d$ states of Fe in these alloys. However, the figure also suggests that for photons with energy lower than about 20 eV the cross section of the boron-*p* states are comparable with those of Fe-*d* and could

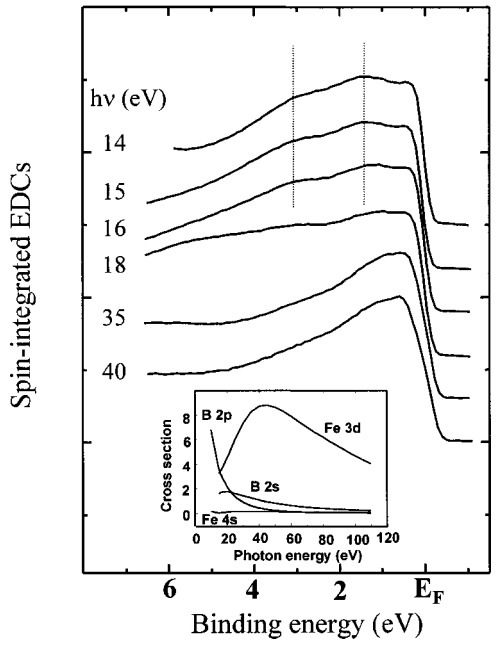

FIG. 1. Spin-integrated EDCs of $Fe_{75}B_{25}$ with different photon energies. (Inset) Cross sections of Fe and B.

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even be larger. That is to say the boron will contribute significantly to the total photoelectron emission if excited with low-energy photons. Furthermore, there is no concept of *k*-space in amorphous states in the absence of translational symmetry and band dispersion is not expected. The different cross sections therefore play a dominant role in determining the photoelectron intensity. This is crucial in separating the different states using a range of photon energies.

In this paper, we report spin-resolved photoemission studies of magnetic amorphous Fe–B alloys using a synchrotron radiation source. A similar study on Co–B alloys has been presented in a previous report,[12] and polarized boron states were found. One great advantage of the synchrotron radiation source is its tunability. With spin-detectors, the photoelectrons can further be separated into two spin channels. We show that the spin-resolved EDCs of both Fe-*d* and B-*p* states have been observed and a negative spin-polarization of the B-*p* states are found.

EXPERIMENTS

The experiment was performed using station 1.2, beamline 1, on the SRS at the UK Daresbury Laboratory. The photon energy range was 5–90 eV with a resolution better than 0.2 eV for the spin-integrated and 0.4 eV for the spin-resolved measurements. The base pressure of the main chamber was better than 4×10^{-10} mbar. A conventional high-energy Mott-polarimeter operated at 100 kV consists of nine detectors, four forward detectors, four backward detectors, and one straight-through detector. Magnetic amorphous ribbons were prepared by melt spinning in a helium atmosphere. The samples were formed into a closed loop with an insulated wire wrapped around the rear for magnetization. The magnetic properties of the ribbon were assessed by surface magneto-optical Kerr effect (SMOKE) measurements. The samples with 100% remanence ratio were used for the spin-resolved photoemission measurements and were cleaned by argon ion bombardment at ~1.6 kV until a sharp Fermi edge appeared and the contamination was reduced to a minimum level. The composition and contamination were monitored by *in situ* Auger electron spectroscopy and analyzed quantitatively by XPS in the RUSTI Scienta spectrometer at Daresbury Laboratory. The compositions of the samples determined from XPS were close to the nominal values quoted here (within about 6%), and the contamination of C and O were estimated to be C:~3% and O:~2%, respectively.

RESULTS AND DISCUSSIONS

Figure 1 shows the spin-integrated energy distribution curves (EDCs) of amorphous $Fe_{75}B_{25}$ with the photon energies varying from 14 to 40 eV. The particular alloy composition $Fe_{75}B_{25}$ was chosen to give a relatively large boron contribution while retaining the ferromagnetic phase. The spectra were collected under the same photon and electron energy resolution, and normalized to the maximum near the Fermi edge. The spectra at 35 eV and 40 eV show little difference with the intensity decreasing monotonically from the maximum around the Fermi level. As the cross section of the Fe-*d* band is much larger than that of B states for photon energies of 35 eV and 40 eV, the EDCs should be a representative of the Fe partial density of states in Fe–B amorphous alloys. The spectra at lower photon energies (<18 eV) show different profiles from those at higher photon energies. The curves show two broad peaks around 1.4 eV and 3 eV. The relative photoelectron intensity between 1 eV and 5 eV increases with decreasing photon energies. As shown clearly in the inset of Fig. 1, the cross section of B-2*p* states increases sharply with decreasing photon energies below about 20 eV. This suggests that the B:2*p* electrons in the TM-B alloys contribute significantly to the total photoelectron intensity in the 1–5 eV binding energy range.

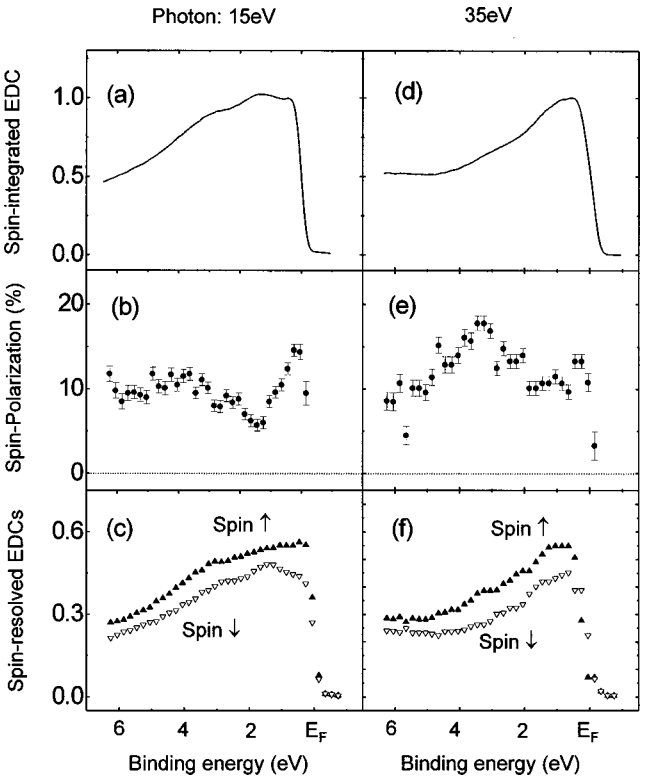

FIG. 2. Spin-integrated EDCs (a and d), polarization spectra (b and e), and spin-resolved EDCs (c and f) of $Fe_{75}B_{25}$ at photon energies of 35 eV and 15 eV, respectively.

The spin-integrated photoemission of amorphous $Fe_{75}B_{25}$ has been studied by Paul and Neddermeyer[13] for photon energies of 16.85 eV, 21.22 eV, and 40.8 eV. They also found that the photoemission intensity between 0.5 eV and 5 eV increases with decreasing photon energy. They further studied polycrystalline Fe and pure B and this effect was not observed in polycrystalline Fe. The partial density of states of $Fe_{75}B_{25}$ has been calculated by Hafner *et al.*[3] They found that B-*s* states interact only weakly with the Fe-*d* band, lying about 8 eV below the Fermi level. However, B-*p* states interact strongly with the Fe-*d* band and form a Fe-*d*–B-*p* band complex, which occupies a broad energy range from about 1.5 eV to 6.0 eV.

Figure 2 shows the spin-integrated EDCs, spin-polarization spectra, and the spin-resolved EDCs of amorphous $Fe_{75}B_{25}$ for photon energies of 15 and 35 eV, respectively. These were chosen to give large counting rates in the

detectors and reflect the features of the spin-integrated EDCs shown in Fig. 1. The spectra collected at 35 eV are mainly due to Fe-*d* states as we discussed above. The polarization is positive around the Fermi level and there is a broad peak around 3.4 eV, similar to that observed in $Fe_{80}B_{20}$.[10] This may be due to the fact that their compositions are rather close. The positive spin-polarization of the Fe-*d* band at Fermi level is in good agreement with the models of Ching and Xu[3] and Hafner *et al.*[5]

The polarization spectra of $Fe_{75}B_{25}$ collected at 15 eV show a distinct feature—a broad minimum around 2 eV, not observed at higher photon energies. This minimum in the spin-polarization yields a broad local maximum in the minority spin states as shown in Fig. 2(c). From the spin-integrated measurements discussed above, the B-*p* states contribute significantly to the total photoemission intensity at low photon energies. The binding energy range (~1–5 eV) of the B-2*p* states coincides with the minimum of the spin-polarization spectra. This suggests that *B*-p states carry a net spin-polarization with a direction opposite to that of Fe-*d* states.

In order to eliminate an alternative explanation we consider the possibility of a ''spin filter'' effect. A strong spin dependence of mean free paths at low kinetic energies has been observed in all the transition metal ferromagnets studied so far.[14,15] Although for amorphous materials the polarization typically shows an enhancement below kinetic energy of about 10 eV, above that value it is more or less constant. In the course of these experiments we have therefore measured the secondary electron polarization in the kinetic energy range of 0–30 eV and found it to be constant above about 8 eV but increasing monotonically by as much as 60% at lower energies. The *minimum* in the spin-polarization shown in Fig. 2(b) cannot therefore be explained by this effect.

To estimate qualitatively the B density of states, we assume that the photoelectrons at 35 eV are due to contributions from the Fe-*d* band only, but that at 15 eV there is an equal contribution from the Fe-*d* and B-bands, as suggested by the their cross sections. Figure 3(c) shows the spin-resolved EDCs of boron obtained by subtracting the curves in Figs. 2(c) and 2(f). The spin-integrated EDC and polarization spectra calculated from the spin-resolved EDCs in Fig. 3(c) are shown in Figs. 3(a) and 3(b), respectively. The spin-integrated intensity curve in Fig. 3(a) shows that the B-*p* band occupies an energy range of about 1–5.5 eV with a broad peak around 3.2 eV. The key observation of this work is negatively polarized B-*p* states in the binding energy range of about 1–4 eV as shown clearly in Figs. 3(b) and 3(c). This negative polarization is in agreement with theoretical predictions.[3,5,6] A detailed comparison of the experimental spin-resolved DOS with the theoretical results will be published later.

CONCLUSION

In summary, the spin-dependent density of states (DOS) of both Fe and boron in an Fe–B amorphous magnetic alloy has been successfully measured with spin-resolved photoemission using a synchrotron radiation source. The B-*p* states were shown to hybridize with Fe-*d* states and to occupy a binding energy range of 1–5.5 eV with a net negative spin-polarization. We have shown that spin-resolved photoemission from an amorphous Fe–B alloy can be used to extract element specific spin-resolved density of states.

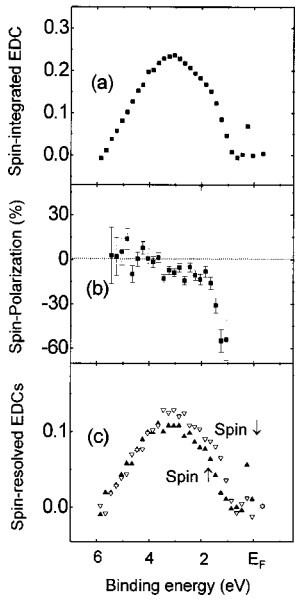

FIG. 3. (a) Spin-integrated EDC, (b) polarization spectra, and (c) spin-resolved EDC of B-*p* states in $Fe_{75}B_{25}$.

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