# The spin-dependent electronic structure of amorphous magnetic alloys

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Spin-resolved photoemission from FeB and CoB binary amorphous alloys has been measured using, for the first time, a synchrotron radiation source. A comparison of the experimental results with several *ab initio* calculations on two model systems $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ shows that the spin-resolved photoemission provided a critical test of theoretical models, and gives insight into the spin-dependent electronic structures of these materials.  [S0021-8979(97)17908-7]

## I. INTRODUCTION

Ferromagnetic transition metal binary amorphous alloys continue to be of interest both as model systems to understand the electronic structure and magnetism in amorphous metals and as prototypes of these technically important magnetic materials. Their physical properties such as electronic specific heat, magnetic susceptibility, and even glass-forming ability are directly related to their electronic structure. There have recently been a number of theoretical studies on the spin-dependent electronic structure of these binary amorphous alloy systems, e.g., FeB,[1–4] CoB,[5] and FeY,[6] but only limited experimental tests of their predictions have been made.

Photoemission spectroscopy is the most direct technique to probe electronic structure. There have previously been a number of ultraviolet photoemission spectroscopy (UPS) and x-ray photoemission spectroscopy (XPS) measurements in magnetic amorphous alloys,[7] but it is difficult to obtain an insight into the electronic structure from the spin-integrated measurements as sharp features are not expected in the amorphous state. The valence band is split into two subbands of majority and minority spin states, and it is extremely valuable to separate the density of states into two spin channels using spin-resolved photoemission measurements. There is, however, a very limited range of spin-resolved photoemission measurements on amorphous magnetic metals currently available. Hopster *et al.*[8] have studied the spin-resolved densities of states of $Fe_xB_yX_z$ ($X$=Ni or Si) using UPS ($h\nu$ =21.2 eV) and See and Klebanoff[9] have studied a commercial ribbon $Co_{66}Fe_4Ni_1B_{14}Si_{15}$ using spin-resolved XPS. Recently, we have made extensive spin-resolved photoemission studies on the binary amorphous alloys, FeB and CoB systems, using a synchrotron radiation source. In this article, the results on two model systems $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ are presented, and compared with several *ab initio* spin-resolved electronic structure calculations.[1–5]

## II. EXPERIMENTAL DETAILS

The experimental work reported here was performed in station 1.2 at the SRS Daresbury Laboratory. The photon energy range is 5–90 eV with 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 is better than $4\times10^{-10}$ mbar. A conventional high energy Mott polarimeter operated at 100 kV has recently been established at this station, and has been described in detail in a previous article.[10] The system consists of nine detectors, four forward detectors, four backward detectors, and one straight-through detector. The forward detectors are used to monitor the instrumental asymmetry. The system was carefully aligned during the experiment to make sure only spin-dependent asymmetry was measured. The effective Sherman function was estimated to be 0.18 from the secondary electron polarization of a $Co_{66}Fe_4Ni_1B_{14}Si_{15}$ ribbon.[11]

$Fe_{1-x}B_x$ ($x$=15, 20, and 25) and $Co_{1-x}B_x$ ($x$=20, 23, and 32) amorphous alloys were prepared by melt spinning in a helium atmosphere. The ribbons were formed into a closed loop with an insulated wire wrapped around the rear of the sample in order to magnetize them. Magneto-optical Kerr effect measurements showed that the ribbons could be magnetized to saturation with 100% remanence. The samples were cleaned by argon ion bombardment at ~1.6 kV until a sharp Fermi edge appeared. 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 composition of the samples is very close to the nominal value, and the contamination of C and O was estimated to be C: ~3% and O: ~2%, respectively. The only heat treatment received by the ribbon was during the chamber bakeouts when it was heated to a temperature of around 150 °C. The amorphous states were confirmed by x-ray diffraction after both the initial melt spinning and at the end of the measurements.

## III. RESULTS AND DISCUSSIONS

Figure 1(a) shows the spin-integrated energy distribution curves (EDCs) of $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ amorphous alloys using 35 eV photons. The EDC of $Fe_{80}B_{20}$ shows a sharp Fermi edge, a maximum intensity just below the Fermi level $E_f$ and a shoulder at binding energy $E_b$~1 eV, results which agree very well with those reported by Paul and Neddermeyer.[12] This agreement is encouraging from an experimental point of

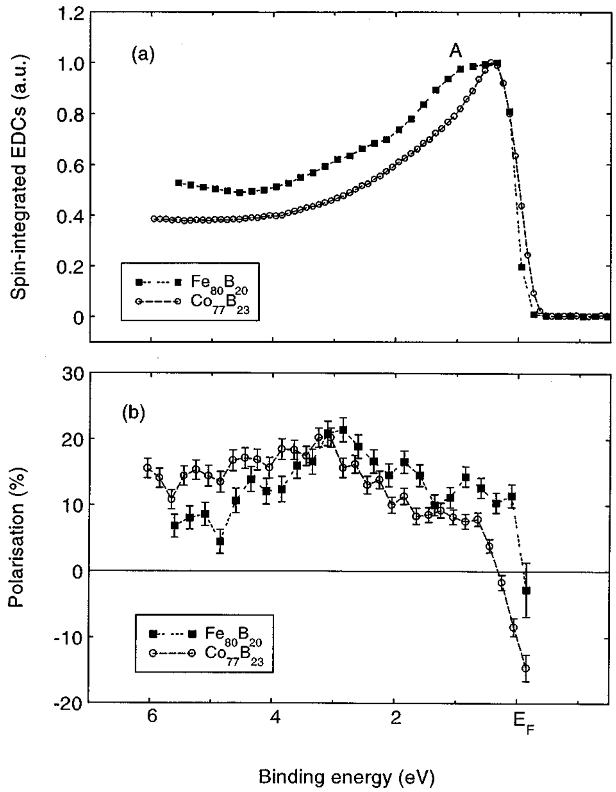


FIG. 1. (a) Spin-integrated photoemission energy distribution curves (EDCs) and (b) the photoelectron spin-polarization spectra of $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ amorphous alloys with photon energy 35 eV.

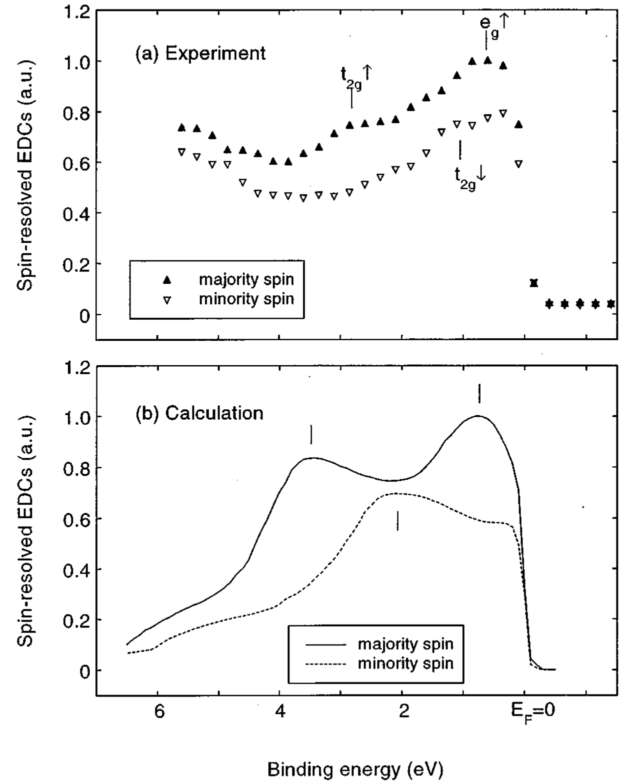


FIG. 2. (a) Experimental spin-resolved EDCs of an $Fe_{80}B_{20}$ amorphous alloy and (b) theoretical spin-resolved bulk density of states (DOS) calculated by Hafner *et al.* (Ref. 4).

view, as it suggests that reproducible and reliable experimental results can be obtained even in such amorphous materials, provided the samples were well prepared and cleaned in a good UHV environment. The spin-integrated EDC of amorphous $Co_{77}B_{23}$ in Fig. 1(a) shows a maximum just below the Fermi level, and then decreases smoothly with increasing binding energy, showing essentially the same profile as earlier UPS results on crystalline $Co_3B$ and amorphous $Co_{77}P_{14}B_8$.[13]

The spin-polarization spectra of amorphous $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ are shown in Fig. 1(b). Both spectra show a similar profile with a broad hump around 3 eV binding energy. The spin-polarization $P$ around the Fermi level is of special interest: in $Fe_{80}B_{20}$ $P$ is positive at and below $E_f$, while for $Co_{77}B_{23}$ $P$ changes sign at $E_b=0.4\pm0.1$ eV and a clear negative polarization $\sim$14% was observed around the Fermi level.

The spin-resolved EDCs (SREDCs) of $Fe_{80}B_{20}$ are shown in Fig. 2(a), where we can see clearly the electronic structure for both spin channels. The majority and minority spin spectra are well resolved with errors comparable to the size of the data points. As the cross sections of B: $2p$ and $2s$ are very small compared with that of Fe $3d$ ($\sigma_B/\sigma_{\mathrm{Fe}}=\sim0.06$)[14] at 35 eV photon energy, the photoelectrons are essentially from the Fe $d$ band.

One significant feature is the two-peak structure. Two humps were observed previously in $Fe_{80}B_{20}$ using spin-resolved soft x-ray photoemission,[15] but with the photoelectron kinetic energy of 25–30 eV the resolution is much better here. It is well known that the density of states (DOS) of elemental bcc Fe shows two peaks originating from the atomic arrangement in the bcc lattice with eight nearest neighbors arranged on a cube and six next-nearest neighbors arranged on an octahedron. The band splitting in the amorphous $Fe_{80}B_{20}$ alloy indicates that very short range local order exists in the amorphous phase and plays an important role in the electronic structure. It is useful to retain the labelling of states in the cubic environment even although the local symmetry is only roughly retained in the amorphous material. The band splitting $\sim$2 eV, defined as the separation between the peaks labelled $e_g\uparrow$ and $t_{2g}\uparrow$, is close to that of pure Fe.[9,16] Similarly, the exchange splitting $\sim$2 eV of the $t_{2g}$ states, the separation between $t_{2g}\uparrow$ and $t_{2g}\downarrow$, is also comparable to that of Fe.[9,16]

There are several spin-dependent DOS calculations of the model system $Fe_{80}B_{20}$. Recent computations by Hafner *et al.*[4] have combined improved structural modeling using molecular dynamics with enhanced self-consistency based on a supercell linear-muffin-tin-orbit approach. Theoretical SREDCs, shown in Fig. 2(b), have been convoluted with an instrumental resolution function of breadth 0.3 eV. The experimental and calculated SREDCs show very similar profiles and the agreement around Fermi edge is especially good. The experiment confirmed the two-peak structure predicted theoretically. Both experiment and theory suggest that the Fermi level falls in a region of rapidly decreasing DOS, but with majority spin states remaining dominant towards $E_f$. On the other hand, according to the predictions by Brat-

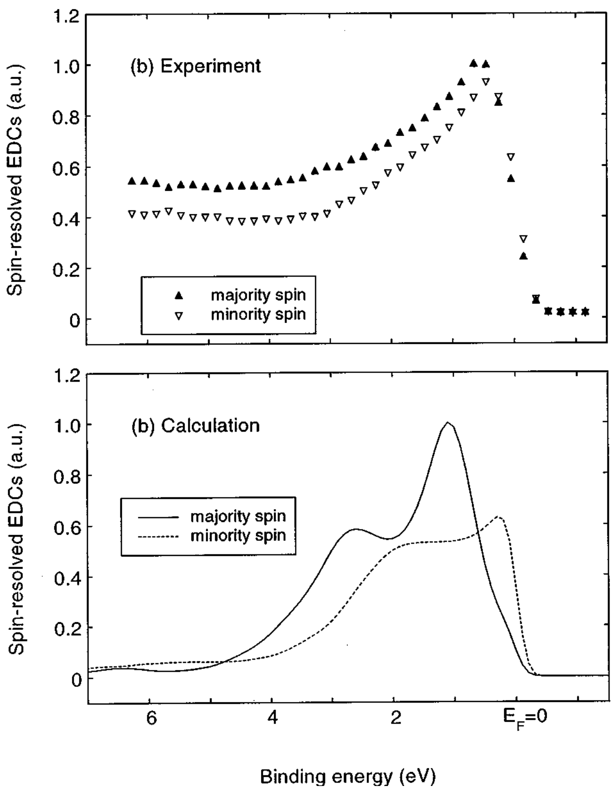


FIG. 3. (a) Experimental spin-resolved EDCs of a $Co_{77}B_{23}$ amorphous alloy and (b) theoretical spin-resolved bulk DOS calculated by Tanaka *et al.* (Ref. 5).

kovsky *et al.*,[3] and Nowak *et al.*,[1] the minority spin states are dominant around $E_f$, which is not in agreement with our experimental results. The predicted spin-resolved DOS (SRDOS) by Hafner *et al.*[4] gives the best agreement with experiment near the Fermi edge, but the binding energy of the $t_{2g}\uparrow$ states is clearly larger than the experimental value and that of other predictions.[1–3]

Figure 3 shows the spin-resolved EDCs of an amorphous $Co_{77}B_{23}$ alloy using photons of 35 eV. In contrast to the measurements on $Fe_{80}B_{20}$, no band splitting behavior was observed. There is only one peak near the Fermi edge for both spin channels. The existence of band splitting in FeB, but not in CoB, may indicate that their local structure is different even in the amorphous state. The spin-resolved EDCs of pure Co and $Co_{66}Fe_4Ni_1B_{14}Si_{15}$ ribbon reported by See and Klebanoff[9] showed a profile similar to that of amorphous $Co_{77}B_{23}$ alloy, but the negative polarization at $E_f$ is well resolved here due to much better resolution in this study.

Figure 3(b) shows the theoretical spin-resolved EDCs of $Co_{77}B_{23}$, which were convoluted from the SRDOS calculated by Tanaka *et al.*[5] At low binding energy, the minority-spin state density is much larger than that of the majority-spin state, suggesting a negative polarization at Fermi edge. This is in qualitative agreement with experimental results. However, the calculated SREDCs predicted a two peak band structure. As shown in Fig. 3(a), no clear experimental evidence was observed to support this prediction.

In the results presented here, we have compared spin-resolved photoemission intensities with spin resolved *bulk* densities of states of amorphous $Fe_{1-x}B_x$ and $Co_{1-x}B_x$ alloys. Two important effects have not been considered: first, with $h\upsilon$=35 eV photoemission is highly surface sensitive and so should mainly reflect the surface density of states, which, in the case of transition metals, differs significantly from the bulk.[17] Second, we have assumed the same constant $3d$ photoelectron cross section throughout the band for both spin-up and spin-down states. Significant differences in the cross sections may indeed exist across the band, but are likely to be similar in $Fe_{1-x}B_x$ and $Co_{1-x}B_x$.

In conclusion, the electronic and magnetic properties of amorphous FeB and CoB have been investigated using spin-resolved photoemission. A detailed comparison of the experimental results with several bulk band structure calculations on the two model systems $Fe_{80}B_{20}$ and $Co_{77}B_{23}$ shows broad agreement, although a number of significant discrepancies remain. Further understanding of the spin resolved surface densities of states of magnetic amorphous alloys is needed to resolve these issues.

## ACKNOWLEDGMENTS

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