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Evidence for Polarised Boron in Co-B and Fe-B Alloys

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***Abstract*—By exploiting the tunability of synchrotron radiation in measurements of spin-resolved photoemission it has proved possible to obtain information on the polarisation of the valence electrons of Co-B and Fe-B amorphous magnetic alloys. Both the spin-integrated and spin-resolved energy distribution curves show a marked dependence on photon energy indicating that the *p* states of boron hybridise with the *d* states of the transition metals giving rise to mixed states in the binding energy range 1 to 5 eV. The observed polarisation and spin-resolved densities of states imply that in the above restricted energy range there is a net negative polarisation of the *boron* states.**

***Index Terms*—Amorphous alloys, magnetic glasses, spin-resolved photoemission, synchrotron radiation**

I. Introduction

IRON-boron and cobalt-boron amorphous alloys are archetypal transition metal-metalloid alloys and their magnetic, electronic and mechanical properties have been extensively studied over the last 20 years. Although much progress has been made in understanding the electronic and magnetic properties within an itinerant electron approach [1]-[5], precise details of the interactions depend on the atomic disorder in the system and on the electronic model used. The purpose of this paper is therefore to investigate the role of the *d* electrons of Co and Fe and the *p* electrons of boron by spin-polarised photoemission induced by synchrotron radiation. The crucial advantage of synchrotron radiation is its tuneability, leading to atom-specific information and in particular some knowledge of the polarisation of electrons in CoB and FeB alloys.

II Experimental

$Co_{77}B_{23}$ and $Fe_{75}B_{25}$alloys were prepared as 3 mm wide ribbons by melt-spinning in a helium atmosphere. The ribbons were formed into closed loops, shiny sides outermost, that could be magnetised by passing a small current through an insulated wire wrapped round the rear. (See[6] for a diagram of the arrangement.) Subsequent measurements of the Magneto-Optical Kerr Effect showed that they could be easily magnetised to saturation.

The surface areas of the ribbons facing the photon beam were cleaned *in situ* by argon ion bombardment until a sharp Fermi edge appeared. The compositions and impurity levels of the specimens were determined by *in situ* Auger electron spectroscopy and *ex situ* X-ray photoemission. The compositions were found to be close to their nominal values, and carbon and oxygen impurity levels of around 3% and 2% respectively were recorded. To prevent any tendency to re-crystallisation the samples were not annealed throughout the study; confirmation that the samples retained their amorphous structures following bakeout of the UHV system at about 135°C was confirmed by X-ray diffraction at the end of the measurements.

The photoemission measurements were made on Station 1.2 at the UK Synchrotron Radiation Source (SRS) with the experimental chamber at a pressure of 6×10^{-10} mbar. This station is dedicated to spin-polarised photoemission in the photon energy range 10-95 eV, and is described in detail in [7]. For these experiments the energy resolution was better than 0.2 eV and 0.4 eV for spin-integrated and spin-resolved measurements respectively.

III Results

In Fig. 1 we show spin-integrated energy distribution curves (EDCs) of $Fe_{75}B_{25}$ and $Co_{77}B_{23}$, each measured at photon energies of 15 eV and 35 eV. More detailed measurements show that there is very little change in the form of the spectra for photon energies between 30 eV and 40 eV, but that below 20 eV the spectral profiles are quite different. The reason for the changes is centred on the marked photon energy dependencies of the cross-sections of the Fe/Co *d* and the boron *p* electrons, with the former dominant at the higher energies and the latter comparable below 20 eV [8]. This is the key advantage of using photons generated by a synchrotron as distinct from a fixed frequency source.

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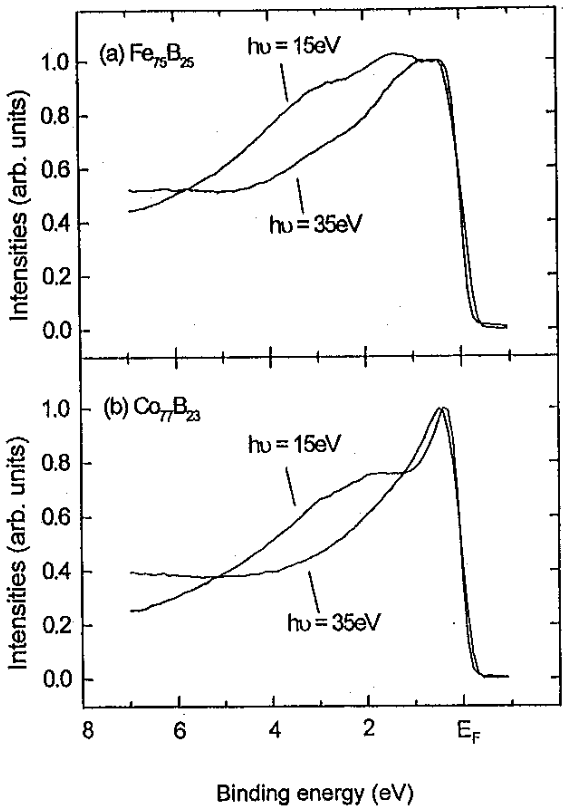

Fig. 1. Photoemission intensities at different binding energies for photon energies of 15 eV and 35 eV for (a) $Fe_{75}B_{25}$ and (b) $Co_{77}B_{23}$.

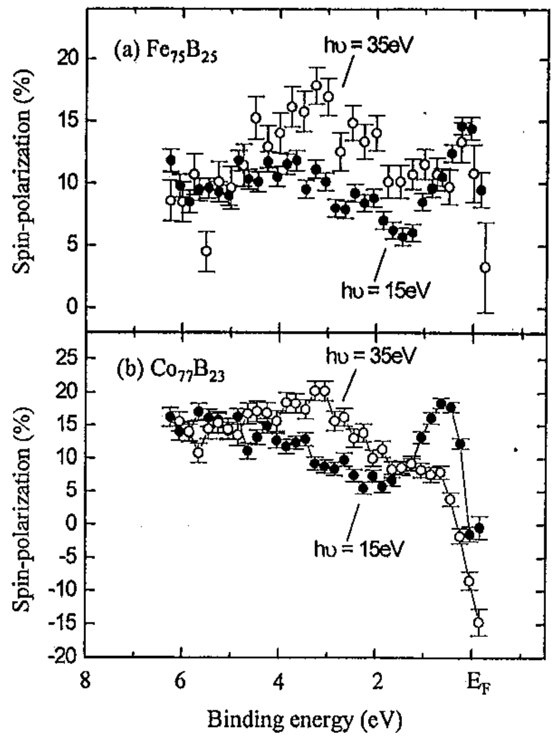

Fig. 2. Spin-polarisation at different binding energies for photon energies of 15 eV and 35 eV for (a) $Fe_{75}B_{25}$ and (b) $Co_{77}B_{23}$.

It is clear from Fig. 1 that the relative photoelectron intensity for both alloys increases strongly between 1 eV and 5 eV with decreasing photon energy, and the implication is that the *2p* electrons from boron contribute significantly to the total emission in this energy range. Previous measurements of this kind on amorphous $Fe_{75}B_{25}$ by Paul and Neddermeyer [9] using photons at 16.85 eV, 21.22 eV and 40.8 eV revealed a similar trend that was completely absent in polycrystalline Fe. Theoretical studies by Hafner *et al.* [4] have shown that the *p* states of boron interact strongly with the *d* states of iron to form a Fe/B complex that occupies a broad energy band roughly in this same range. Hybridisation is also predicted to play an important role in determining the magnetic properties of CoB alloys [5]. It is, of course, possible that the *2p* electrons from the C impurities play some role in this effect although the concentration is small and evidence from Auger spectra implies that the carbon is graphitic and unpolarised.

In Fig. 2 we show the spin-polarisation spectra of both alloys, again for photon energies of 15 eV and 35 eV. As with the spin-integrated EDCs there is a clear difference in the profiles at the two energies. For the photoelectrons resulting from radiation with 35 eV photons there are peaks in the polarisations between 3 eV and 4 eV, but these maxima decrease stongly as the photon energy is reduced.

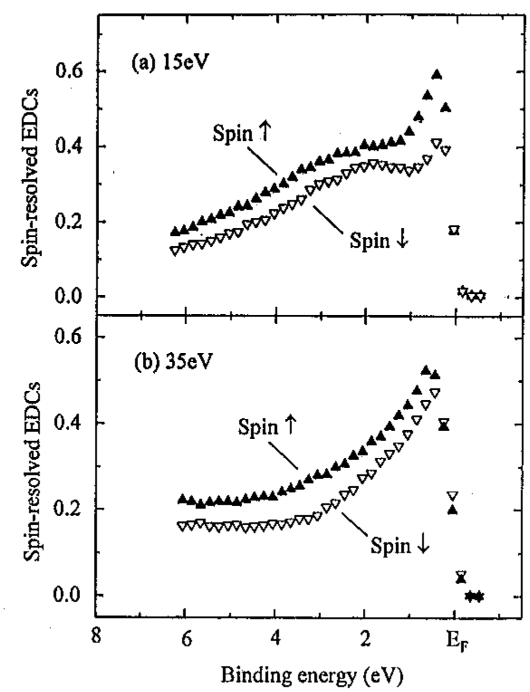

Fig. 3. Spin-resolved EDCs of $Co_{77}B_{23}$ for photon energies of (a) 15 eV and (b) 35 eV.

IV Discussion

A simple analysis of the spin-integrated and the polarisation data enables us to produce spin-resolved EDCs and the result for $Co_{77}B_{23}$ is shown in Fig. 3. The experimentally observed suppression of photoelectron polarisation exhibited by this CoB alloy in the binding energy range 2 - 4 eV (Fig. 2) is similar in pattern to the case of FeB, whose results have been compared with theory elsewhere [10]. The self-consistent calculations of Tanaka *et al.* [5] for $Co_{83}B_{17}$ (the closest composition for which theoretical predictions are available) show only a very small *net* negative polarisation (at most 2%), but a significant (≈ 25%) negative polarisation in the partial densities of boron *p* states between 2.5 eV and 5.5 eV (Fig. 4a), and indeed also between binding energies of 7 - 8 eV. However as the theoretical densities of *p* states of boron are significant only between binding energies 4 - 8.5 eV it is only over *this* energy range that they can affect a significant reduction in the observed polarisation (Fig. 4b); that is at energies above the 2 - 4 eV observed experimentally. Overall Tanaka *et al.* predict a much stronger separation of the boron *p* and cobalt *d* densities of states than is implied by experiment. Furthermore, the TM-B hybridisation is much weaker than in the FeB calculations [4]. Nevertheless the concept of negatively polarised *p* states of boron is supported by both theory and experiment.

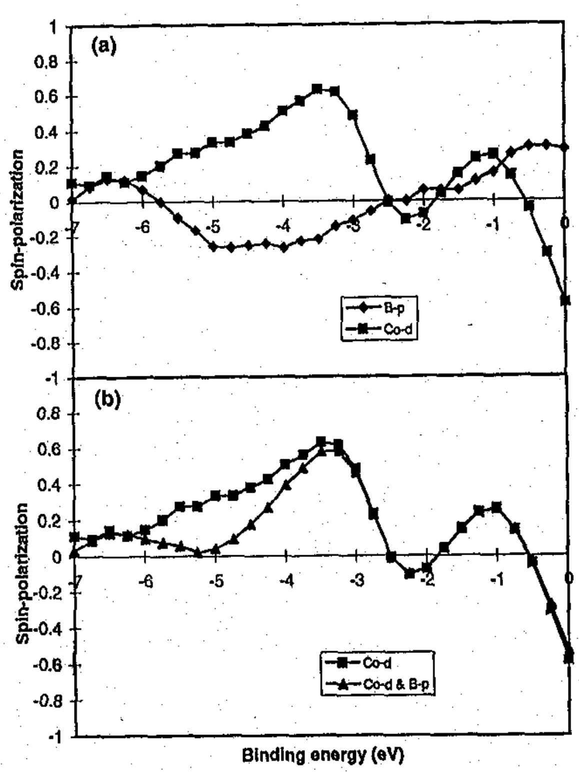

Fig.4. Variation with binding energy of the polarisation of *d* states of Co and *p* states of B estimated from Fig. 2 of [5]. (a) Shows the individual states while (b) is a comparison of the *d* states with a summation of the *d* and *p* components weighted by their *d* and *p* partial densities of states.

V Conclusions

In summary the observed systematic changes suggest that both the boron *2p* states and the transition metal *d* states are clearly polarised in energy and that the boron *2p* states make an increasingly important contribution to the total photoemission intensity as the photon energy is lowered below 20 eV. This coupled with the reduction in the polarisation and the spin-resolved densities of states at lower photon energies leads to the conclusion that these boron states carry a net polarisation in the *opposite direction* to that of the cobalt. A similar effect is observed in FeB.

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