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G. PETŐ
J. KANSKI
A. LOVAS
J. SASVÁRI

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BY PHOTOEMISSION

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THE INVESTIGATION OF AMORPHOUS-CRYSTALLINE
TRANSITION IN Fe-B METALLIC GLASSES BY PHOTOEMISSION

G. Pető, J. Kanski*, A. Lovas, J. Sasvári

Central Research Institute for Physics
H-1525 Budapest 114, P.O.B. 49, Hungary

*Chalmers University of Technology, Phys. Dep., S 41295 Sweden
Göteborg

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АННОТАЦИЯ

Измерялись ультрафиолетовые фотоэмиссионные спектры /UPS/ α -FeB, Fe₃B, Fe₂B+ α -Fe аморфных состояний и α -Fe для сравнения. Для контроля поверхностных примесей и кристаллической структуры те же образцы изучались как с помощью электронной Оже-спектроскопии /AES/, так и рентгеновских излучений. Наблюдалось отличие между структурами полос состояний α -Fe и α -Fe+Fe₂B относительно состояний α -FeB и Fe₃B, но последние два с точки зрения UPS² похожи друг на друга.

KIVONAT

Az ultraibolya fotoemissziós spektrumokat (UPS) mértük az α -FeB, Fe₃B, Fe₂B+ α -Fe állapotokban, és referenciaként α -Fe-ban. Auger elektron spektroszkópiával és röntgenvizsgálattal is tanulmányoztuk ugyanazon mintákat a felületi szennyezők és a kristályszerkezet ellenőrzése érdekében. Eltéréseket tapasztaltunk az α -Fe és az α -Fe+Fe₂B állapotok sáv szerkezetében az α -FeB és a Fe₃B állapotokhoz képest, de az utóbbi kettő hasonlít egymáshoz az UPS szempontjából.

ABSTRACT

The Ultraviolet Photoemission (UPS) spectra were measured in amorphous (α -FeB), Fe_3B , $\text{Fe}_2\text{B}+\alpha$ -Fe states together with α -Fe for reference. Auger electron spectroscopy (AES) and X-ray investigation were carried out on the same sample to check the surface contamination and the crystal structure. Differences are observed in the band structure of α -Fe and α -Fe+ Fe_2B in comparison with α -FeB and Fe_3B , but the last two are similar to each other from UPS point of view.

INTRODUCTION

The electronic structure of FeB metallic glass system is thoroughly investigated both, theoretically [1] and experimentally [2,3,4]. The electronic structure which is sensitive to the short range order may be different in amorphous and crystalline phases. It seems promising to investigate the electronic structure during the crystallization to detect the transition process and to measure the differences in the electronic structure more sensitively. Mössbauer spectroscopy indicates a similarity in the short range order of α -FeB at $C_B=25$ at% and Fe_3B [5] and the XPS and UPS data confirm this fact, too [2,3].

Our purpose is to deal with the band structure in the different stages of crystallization and compare them with the other experimental results.

SAMPLE PREPARATION AND EXPERIMENT

The samples were prepared by single roll melt quenching. The details are published elsewhere [7]. The samples were cleaned by ion-bombardment with a $5-7 \mu\text{A}/\text{cm}^2$ intensity 2 keV Ar^+ beam. The UPS spectra, were obtained by retarding field method, with $10,2 \text{ eV}$ exciting photon energy.

The surface compositions and contaminations were measured by AES, simultaneously with the UPS. The crystalline structures were investigated by X-ray diffraction, with $\text{Cr K}_{1\alpha}$ radiation, after the UPS-AES measurements.

The crystallization were carried out in-situ, in 10^{-6} Pa pressure, with the following heat-treatments. $2,5^{\text{h}}$ 250°C , at $C_{\text{B}}=16 \text{ at\%}$ and 1^{h} , 630°C at $C_{\text{B}}=25 \text{ at\%}$ for Fe_3B . 1^{h} , 700°C both at $C_{\text{B}}=16 \text{ at\%}$ and $C_{\text{B}}=25 \text{ at\%}$ for $\alpha\text{-Fe}+\text{Fe}_2\text{B}$ system.

RESULTS AND DISCUSSIONS

The AES spectra show that the surface contaminations are a few percent of C,O,Ar and the Fe/B ratio is nearly equal to the bulk composition (Fig. 1, Fig. 2).

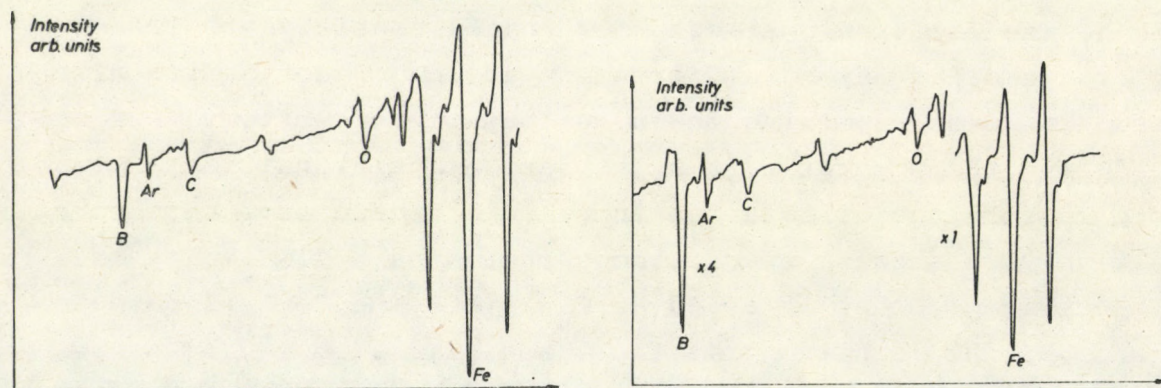


Fig. 1. Surface contaminations and composition of Fe-B $C_{\text{B}}=25 \text{ at\%}$

Fig. 2. Surface contaminations and composition of Fe-B $C_{\text{B}}=16 \text{ at\%}$

The surface contaminations of $\alpha\text{-Fe}$ were the same as they were on Fig. 1. and Fig. 2.

The UPS results are characterized by the secondary peak (SP) and the valence band emission (VBE) part of the electron distribution curve (EDC). The EDC is given by the photoelectron intensity versus photoelectron energy curve. The Fermi level was chosen as a zero point for the photoelectron energy.

The SP indicates the density of states (DOS) of empty levels above the E_F and the VBE shows DOS below the Fermi level in the amorphous state.

The general shape of the EDC is characterized by the ratio (R) of photoelectron intensity at the maximum of SP and -1 eV photoelectron energy in the V.B.E. region.

The EDC of a-FeB has very similar properties at 16 at% and 25 at% of B concentration (Fig. 3. and Fig. 4) with $R=2,70$ and $R=2,85$.

The Fe_3B samples has similar EDC characteristics as that of a-FeB system (Fig. 3. and Fig. 6.) at $C_B=16$ at% and $C_B=25$ at% as well (Fig. 5. and Fig. 6.) with $R=2,97$ and $R= 2,80$.

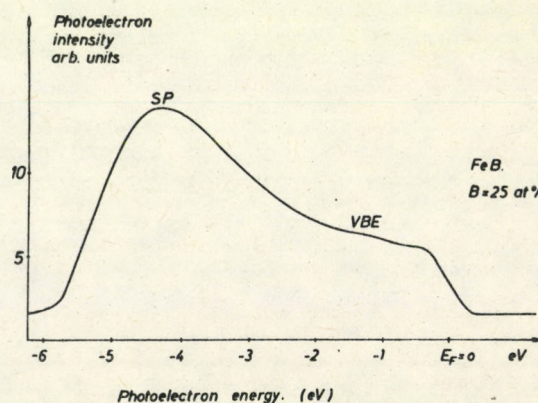
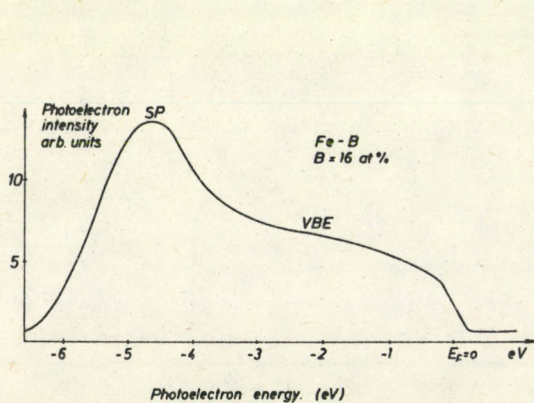


Fig. 3. EDC of UPS for amorphous state $C_B=16$ at%

Fig. 4. EDC of UPS for amorphous state $C_B=25$ at%

The EDC data of α -Fe+ Fe_2B and α -Fe systems are nearly equal to each other and they are different from the behaviour of a-FeB and Fe_3B . (Fig. 4. and Fig. 8). $R=2,0$ for α -Fe+ Fe_2B and α -Fe systems.

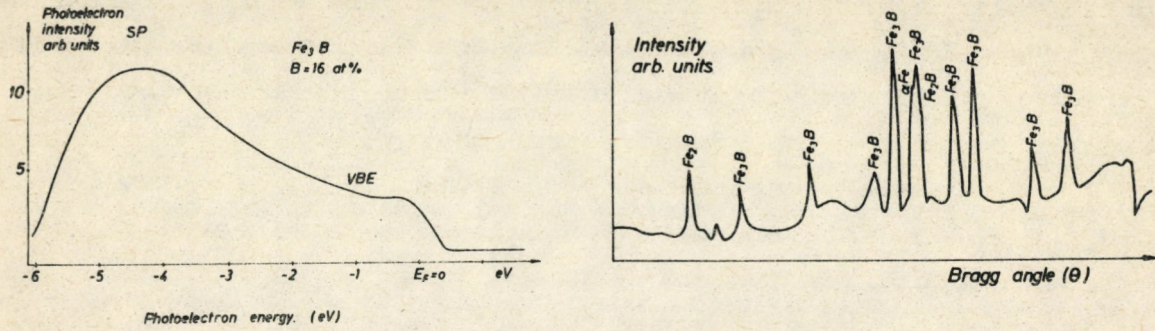


Fig. 5. EDC of UPS and X-ray diffraction of Fe_3B crystallized from $\alpha-FeB$ with $C_B=16$ at%

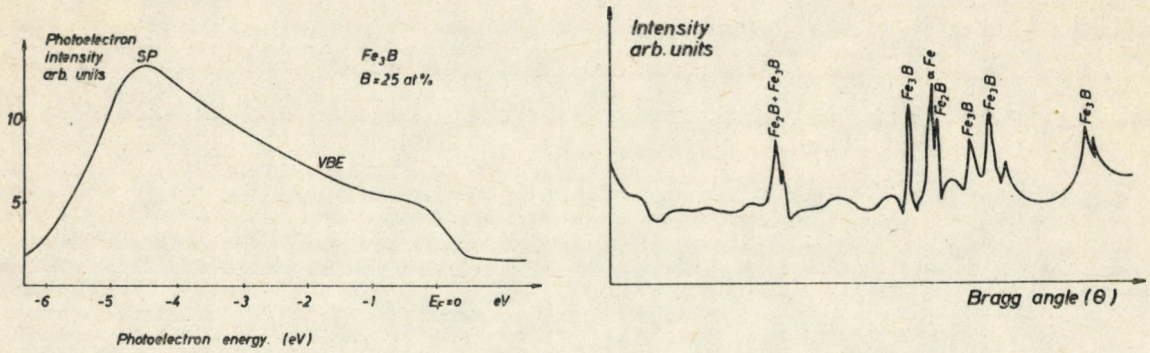


Fig. 6. EDC of UPS and X-ray diffraction for Fe_3B crystallized from $C_B=25$ at% amorphous sample.

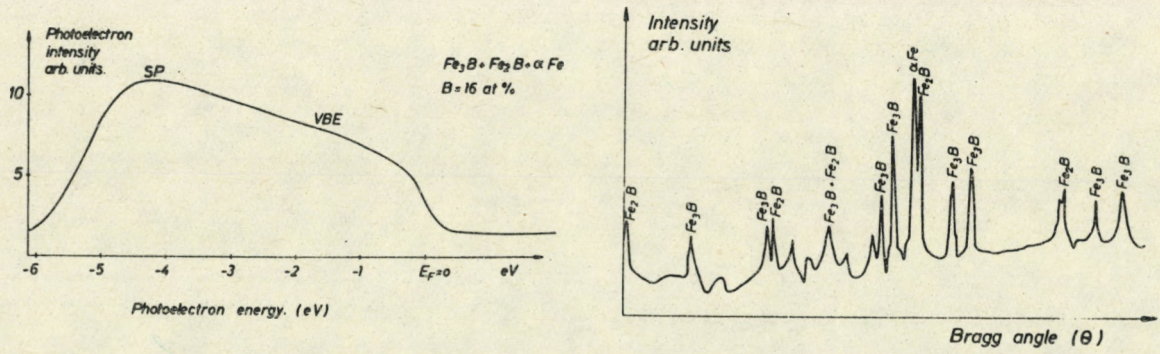


Fig. 7. EDC of UPS and X-ray diffraction for $\alpha-Fe+Fe_2B$. The initial concentration is $C_B=16$ at%

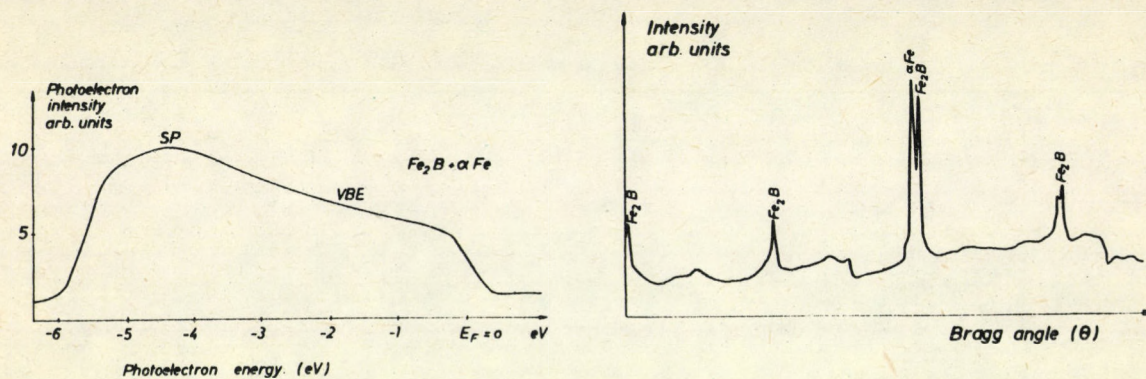


Fig. 8. EDC of UPS and X-ray diffraction for $\alpha\text{-Fe}+\text{Fe}_2\text{B}$ sample which was crystallized from $\alpha\text{-FeB}$ with 25 at% of Boron

The X-ray diffraction results show that in the $\alpha\text{-Fe}+\text{Fe}_2\text{B}$ sample the Fe_2B is tetragonal with $a=5,11 \text{ \AA}$ $c=4,25 \text{ \AA}$ [6]. The $\alpha\text{-Fe}$ sample shows the well known [8] EDC (Fig. 9).

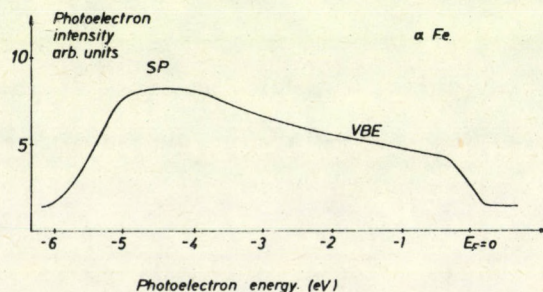


Fig. 9. EDC of UPS for $\alpha\text{-Fe}$

Comparing the UPS results for $\alpha\text{-FeB}$ and $\alpha\text{-Fe}$, it is seen that the differences are mainly concentrated at the S.P. region. There is a change at the VBE range too, but it is much smaller. The explanation of these observations is the increase of the DOS just above the Fe level, together with a change of the DOS also below the Fermi level. As it is known the $\alpha\text{-Fe}$ has large "d" peaks above and below the Fermi level. The deformation of these peaks mainly of the higher energy one, can result in the observed experimental facts. This deformation can be the shifting or a broadening of the "d" peaks. The similarity of the EDC for $\alpha\text{-FeB}$ and Fe_3B indicates that the band structure near the Fermi level and consequently the short range order should be identical for those structures, in agreement with the Mössbauer data [5].

The α -Fe+Fe₂B has nearly same EDC characteristics as α -Fe, because probably the band of the α -Fe dominates in the DOS near to the Fermi level for α -Fe+Fe₂B system.

The experimental results are very similar for the samples having 16 at% and 25 at% of B concentration.

The Fe₃B samples have some α -Fe and Fe₂B phases too, but they can not influence our results as they cause opposite effects than the Fe₃B. It is clear from our results that their relative contribution should be negligible in comparison with Fe₃B.

CONCLUSIONS

The UPS is a valuable method to follow the crystallization. The UPS results and the electronic structure near to the Fermi level of α -FeB samples at $C_B=16$ at% and $C_B=25$ at% are similar to each other and to Fe₃B. It differs from the band structure of α -Fe and the α -Fe+Fe₂B system.

The deformation of the iron "d" peaks is the main source of the difference in the electronic structures, in that energy range.

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