Electronic structure and surface morphology of nanoscale crystal structures of iron-based complex alloys

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Introduction

Since amorphous metal alloy‘s discovery, they have been the subject of increased scientific interest due to their unique mechanical and magnetic properties, enhanced biocompatibility, and high corrosion resistance [1]. However, the widespread use of amorphous alloys is significantly limited by their high-cost production.

Aims

Scanning tunneling microscopy and photoelectron spectroscopy was used to study the surface morphology and electronic structure of iron-based bulk metal alloys (BMGs) $Fe_{61.37}Cr_{3.78}Co_{6.84}V_{0.85}W_{0.82}Mo_{1.06}Nb_{0.85}B_{19.87}C_{1.99}Si_{2.57}$(HB-4) and $Fe_{55}Ni_8Co_6Mo_4Cr_2V_1Al_2P_9C_6B_5Si_2$ (NHRP-6).

Method

X-ray spectrometer:”JEOL” JSPM-4610 with scanning tunneling microscope. Work pressure no less then 10^{-7} Pa.

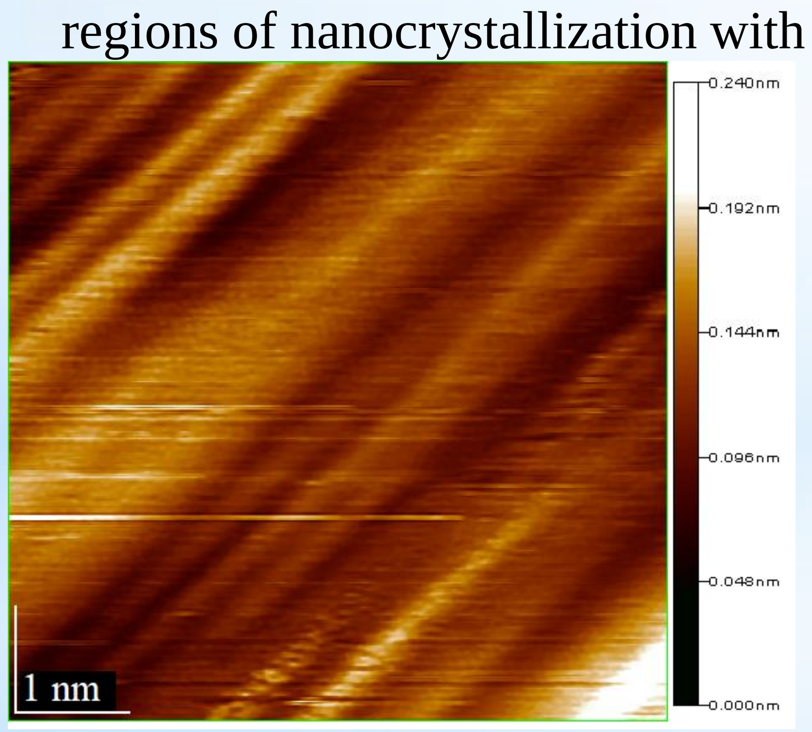
X-ray source Mg K_α 1253.6 eV. Energy resolution 0.1 eV.

Result

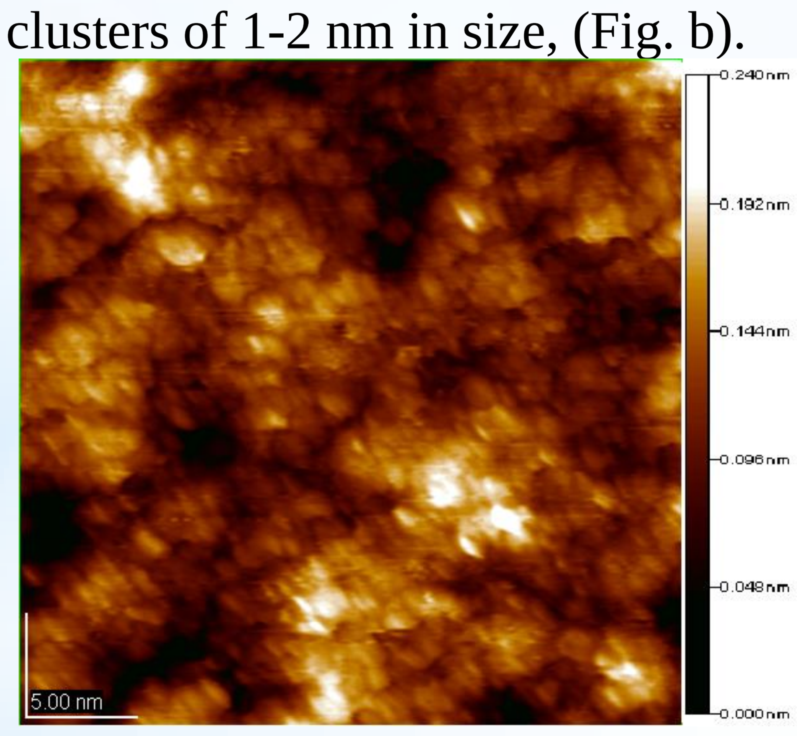
Taking into account that the mechanism of obtaining the studied BMGs consists of controlled nanocrystallization from the initial amorphous state, the "mother" base of the nanocrystalline alloy is an amorphous alloy. So the morphology of such alloys must contain both amorphous and crystalline components.

NHRP-6

Areas of the amorphous component of the alloy are observed, atomically ordered along the current lines (Fig. a), and regions of nanocrystallization with clusters of 1-2 nm in size, (Fig. b).



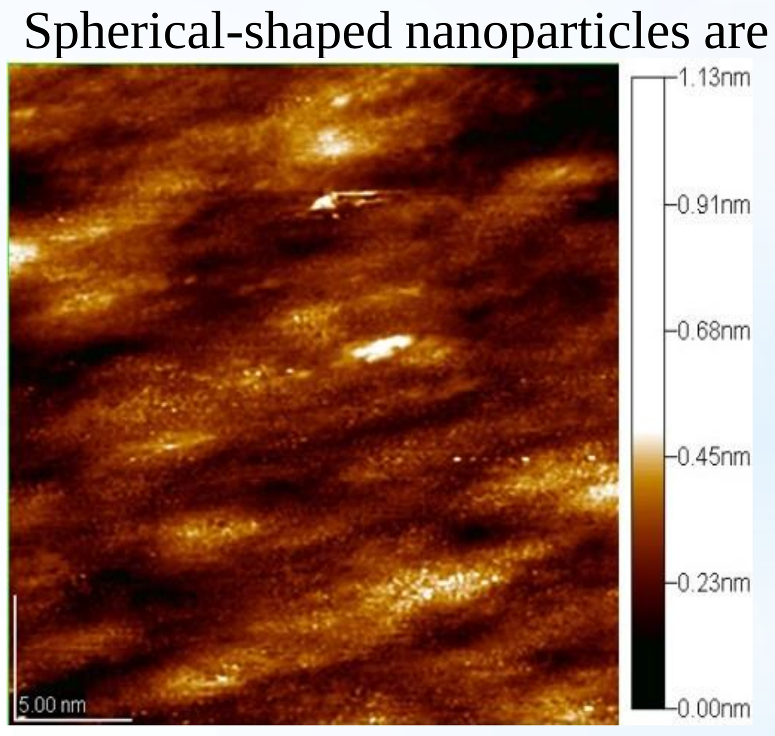
(a)



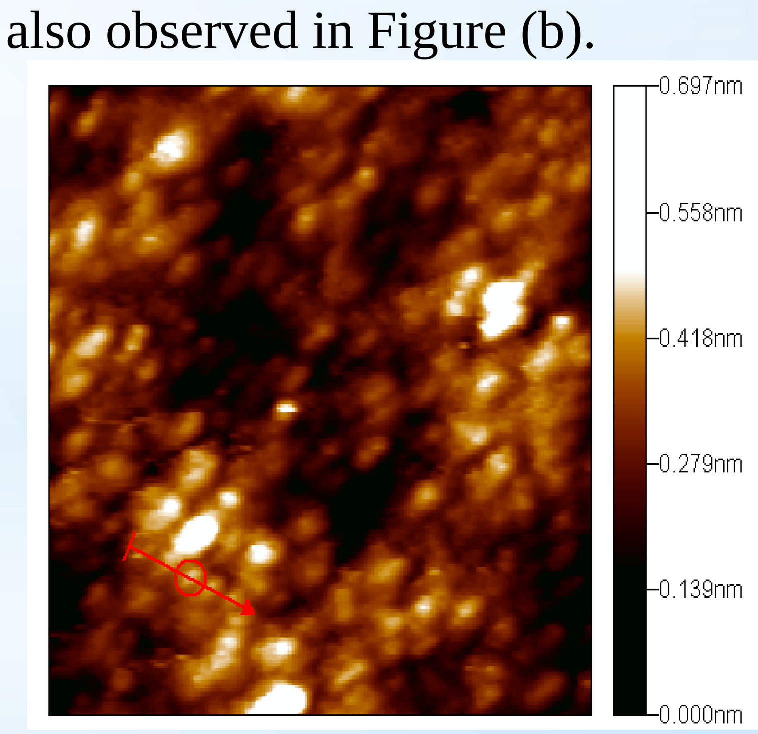
(b)

HB-4

No areas of a pure amorphous matrix are observed; instead, the formation of needle-shaped clusters immediately occurs Figure (a). Spherical-shaped nanoparticles are also observed in Figure (b).



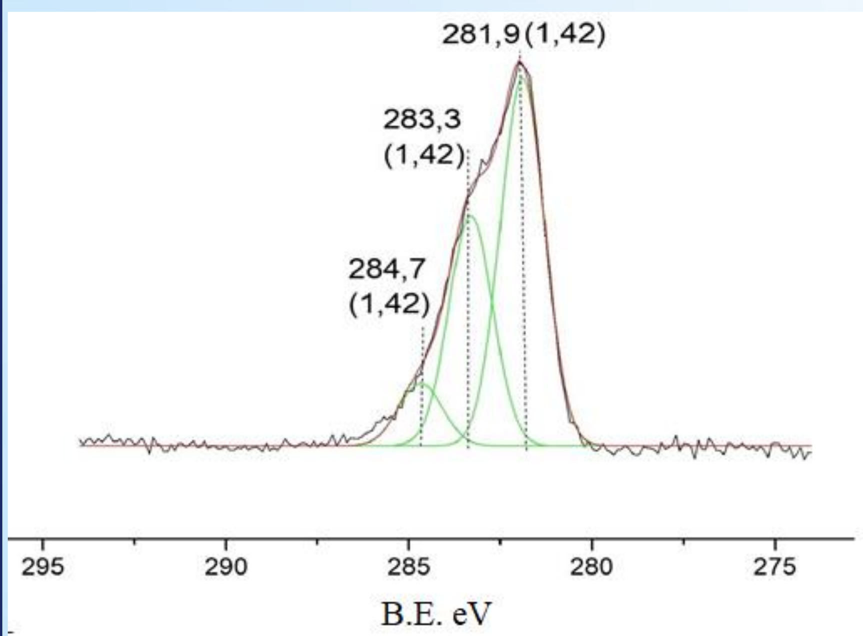
(a)

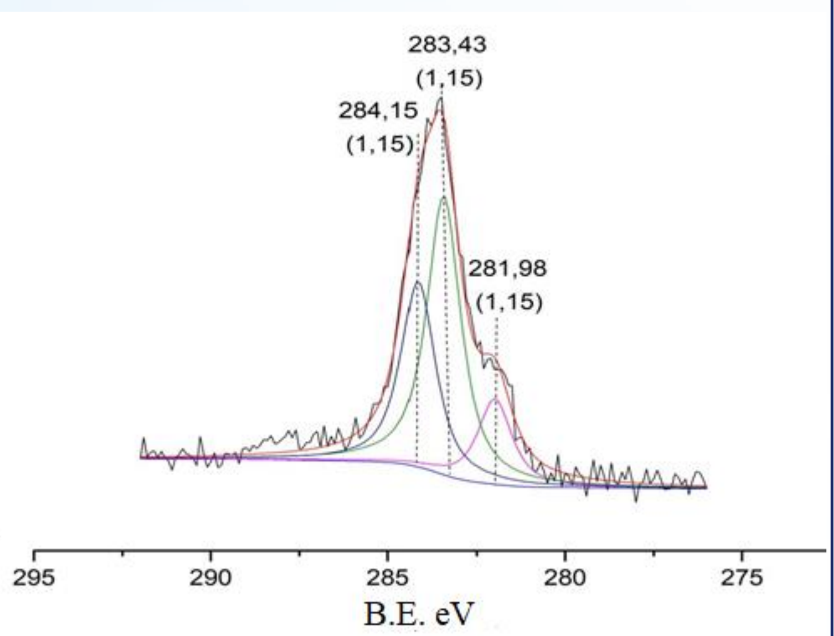


(b)

Electronic structure

C1s



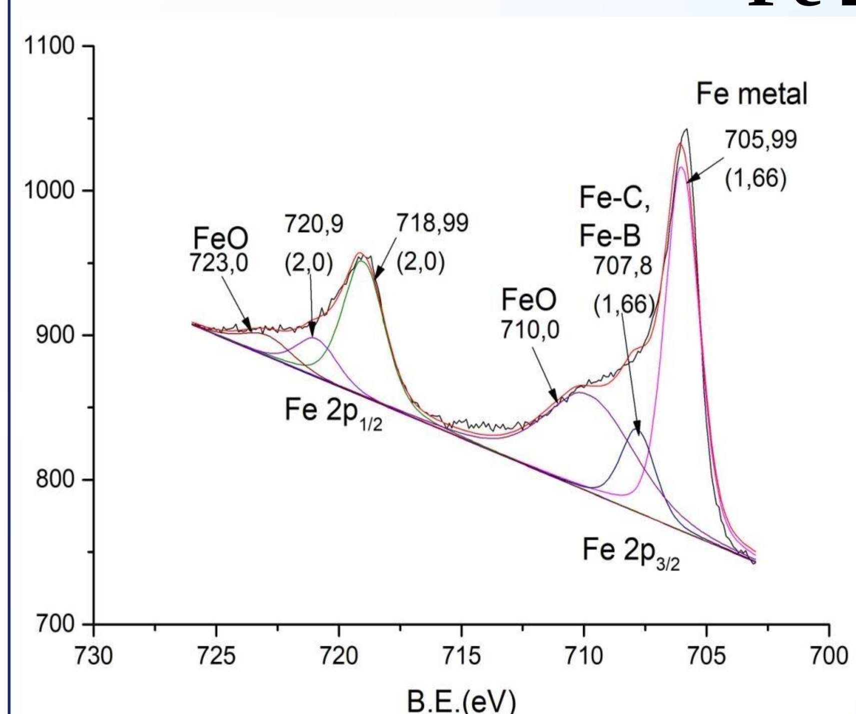


HB-4: 281,9 eV - C-Me; 283,3 eV C-C; 284,7 eV - C-O

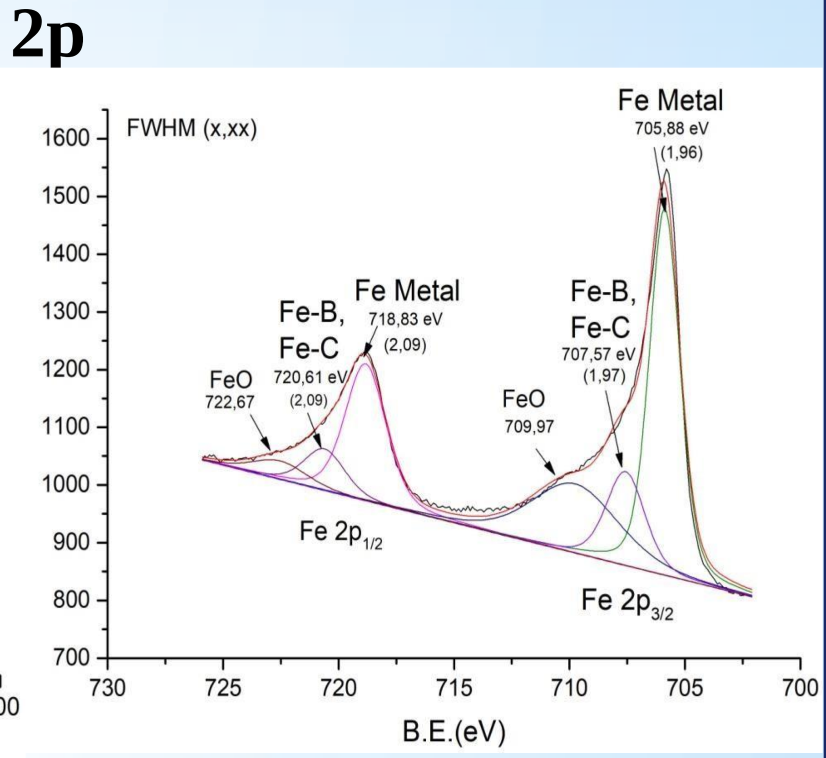
NHRP-6: 281,98 eV C-Me; 283,4 eV C-C; 284,15 eV - C-O

This difference in the nature of the distribution of the balance of the electron density of carbon atoms is explained by higher carbon content in the NHRP-6 alloy (C_6 versus $C_{1.99}$), and the significantly lower content of iron (Fe_{55} versus $Fe_{61.37}$) and boron (B_5 versus $B_{19.87}$).

Fe 2p



NHRP-6



HB-4

The formation of morphological features of the surface of the amorphous film in the process of rapid hardening is accompanied by the formation of different phases [2,3]. Fe_2B and Fe_3C immersion phases are observed in the studied BMGs.

CONCLUSIONS: It was found that the structure of nanocrystalline alloy is a two-phase system, one of the phases is nanocrystals and the second is a final amorphous matrix. In the study of surface morphology, both areas of atomic ordering along the current lines and areas of clustering with clusters of size 3-5 nm are observed.

The presence of iron carbide and iron borides as well as small amounts of oxygen is detected in the ribbon volume. Carbon on the surface of the alloys is mainly in an oxidized state, while in the volume it exists in the form of compounds with boron and iron.

[1] Inoue A. Bulk Amorphous Alloys - Practical Characteristics and Applications. *Trans Tech Publications*, Switzerland. 1999. 148 P

[2] Arch. Mater. Sci. Eng. – 2008. – V. 34 (1). – P. 9–13.

[3] Handbook of X-ray photoelectron spectroscopy (Tokyo: Japan: JEOL Ltd: 1991)