Journal of Alloys and Compounds 747 (2018) 636–639

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Structures and physical properties of two magnetic Fe-based metallic glasses

Jiliang Zhang [a, b], Guangcun Shan [a, b, *], Jiong Li [c], Yingmin Wang [d], Chan Hung Shek [b, **]

[a] School of Instrument Science and Opto-electronics Engineering, Institute of Precision Instrument and Quantum Sensing, Beihang University, Beijing 100191, China
[b] Department of Physics and Materials Science, City University of Hong Kong, Kowloon Tong, Hong Kong Special Administrative Region
[c] Shanghai Synchrotron Radiation Facility, Shanghai Institute of Applied Physics, Shanghai 200624, PR China
[d] Key Laboratory of Materials Modification by Laser, Ion, and Electron Beams, Ministry of Education, School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, PR China

ARTICLE INFO

Article history:
Received 10 January 2018
Received in revised form
6 March 2018
Accepted 8 March 2018
Available online 9 March 2018

Keywords:
Metallic glass
Magnetic
Atomic cluster
Structure
EXAFS

ABSTRACT

Significant differences in structural, thermal, mechanical and magnetic properties were observed between traditional FeSiB metallic glass and newly developed FeMB (M = mixture of Zr, Nb and Y) metallic glass. The origin of the differences is attributed to the more negative heat of mixing between boron and the metallic alloying elements. This leads to the transition of local structure and bonding nature of Fe–B elucidated by the measured extended X-ray absorption fine structure (EXAFS) spectra functions that were analyzed employing *ab initio* multiple scattering calculations using the FEFF8.4 code and by the electronic structures of Fe as well. Such dramatic change sheds light on the understanding of the correlations between structure and physical properties in metallic glasses. The results were discussed based on electronic structures and they provide a new route to design magnetic Fe-based metallic glasses.

1. Introduction

FeB-based metallic glass were extensively investigated because of the wide applications in electrical transformers, magnetic sensors and radio-frequency inductive devices, etc. due to their many advantages compared with traditional silicon steels [1–3]. In recent years, several families of Fe-based metallic glasses with high glass forming ability (GFA) were developed [4–6]. Nevertheless, most of these new members exhibit poor soft magnetic behaviors and some even show no ferromagnetic behavior at room temperature. It is therefore vital to understand the structural nature which gives rise to their magnetic properties.

The stereochemically defined model stipulates that local unit with nearest neighbors in metal-metalloid metallic glasses has the same type of structure and composition as their crystalline counterparts [7], which provides a good description of the structural properties of tradition metals-metalloid metallic glasses. Recently, Zhang et al. [8,9] developed two kinds of CoSiB metallic glasses with distinct magnetic properties based on different local unit in intermetallics, despite their similar compositions. The newly developed metallic glasses of large GFA show dominant unit of icosahedral clusters bridged by minor clusters or atoms [10–13]. Such different local structures likely gave rise to different magnetic behaviors in Fe-based metallic glasses, since magnetic moment is predominantly a localized phenomenon. In this study, we investigated the structure and properties of two FeB-based metallic glasses with significantly different GFA, namely $Fe_{71}B_{17}Si_{12}$ (FeBSi) and $Fe_{71}B_{17}Nb_4Y_4Zr_4$ (FeBM) respectively, and explored the correlations among the local order and properties.

2. Experiments

Master ingots of the two nominal compositions as well as $Fe_{80}B_{20}$ were prepared by arc melting the mixtures of pure constituent elements Fe (99.99 wt%), B (99.9 wt%), Si (99.99 wt%), Nb (99.9 wt%), Y (99.9 wt%) and Zr (99.9 wt%) under a Ti-gettered argon atmosphere. Using these master ingots, ribbon samples

* Corresponding author. School of Instrument Science and Opto-electronics Engineering & Institute of Precision Instrument and Quantum Sensing, Beihang University, Beijing 100191, China.
** Corresponding author.
E-mail addresses: gshan2-c@my.cityu.edu.hk (G. Shan), apchshek@cityu.edu.hk (C.H. Shek).

https://doi.org/10.1016/j.jallcom.2018.03.085
0925-8388/

with thickness of ~30 μm and width of ~2 mm were produced by a single roller melt-spinning apparatus. Structural identification was conducted on a Philips X'pert X-ray diffractometer (Cu Kα, λ = 0.15406 nm). Thermal stability was measured with a Perkin Elmer Diamond differential scanning calorimeter (DSC) at a heating rate of 20 K/min. Magnetic measurements were carried out using a Cryogenic vibrating sample magnetometer with a maximum field of up to 50000 Oe. Domain structures of ribbons were observed with a Vecco magnetic force microscope (MFM) operated in the tapping/lift scanning mode. Electronic structure was measured using x-ray photoelectron spectroscopy (XPS) with a monochromatized Al K_α radiation (1486.6 eV) in an ULVAC-PHI 5802 system (Kanagawa, Japan). The atomic-scale structures of these metallic glasses were investigated by EXAFS spectroscopy at beam line BL14W of the Shanghai synchrotron radiation facility, Shanghai, China. EXAFS spectra of Fe–K edge was measured in transmission mode at temperature 300 ± 2 K. The thicknesses of the samples were optimized to obtain suitable absorption jumps at each K-absorption edge. The experimental EXAFS signals were extracted by a standard data-reduction procedure using the Athena program [14]. Note that the EXAFS spectra model of the simulated atomic configurations were fitted using an *ab initio* multiple scattering calculation implemented in FEFF8.4 [15].

3. Results and discussions

XRD patterns in Fig. 1 confirmed the glassy nature of both samples. A side-by-side comparison of XRD patterns for the two metallic glasses shows that the diffuse hump in the FeBM metallic glasses is not only broadened, but shifted towards smaller angle as well. The difference is made evident by the Gaussian fitting on the peaks (see solid lines in Fig. 1). It suggests more variation of the local structure in FeBM metallic glasses. Because pair distribution function (PDF) is a Fourier sine transform of powder XRD (after the corrections of instrumental sources and backgrounds), the shift of the amorphous hump towards low angle in the XRD pattern of the FeBM metallic glass indicates that it has a larger dominant nearest neighboring distance, while the broadening profile suggests more different atomic clusters from the dominant nearest neighboring distances in the FeBM metallic glass. Like most FeBSi metallic glasses, the present FeBSi metallic glass did not exhibit a detectable glass transition in the DSC scans [16]. Its crystallization temperature T_x was 851 K, which was typical for traditional FeBSi metallic glasses [1]. The FeBM metallic glasses show high thermal stability with $T_g = 873$ K and $T_x = 922$ K, which were the same as the reported values [7]. The addition of transition metals yields high GFA and high thermal stability, viz., 71 K higher than FeBSi in crystallization temperature. Such large difference of thermal stability is not common in metallic glasses based on one primary element. In Zr–Al-TM systems, there is only 30 K difference in crystallization temperature when the concentration of Zr changes from less than 55% to more than 65% [2,13]. Such obvious change can be explained in terms of local structures, as discussed previously for CoBSi metallic glasses [8]. Significant differences should be expected in its properties, especially in magnetic behaviors.

The nanoindentation load-penetration curves revealed distinctive mechanical behaviors of the two types of metallic glasses (see Fig. 2). The FeBSi metallic glass shows a higher hardness and larger elastic modulus, despite its lower thermal stability. Such mechanical behaviors are different from that expected normally, and this may suggest that the local structural units in these two metallic glasses are completely different. The dramatic change of such mechanical properties is not common in minor alloyed metallic glasses [1,2,13]. This supports that the difference should be related to distinctive structural change and even the change in bonding nature.

The magnetization curves in Fig. 3 show the magnetic behaviors of the two metallic glasses. Both metallic glasses show high initial magnetic susceptibility and small magnetic hysteresis, which are favorable for soft magnetic materials. It seems that these soft magnetic characters including high initial susceptibility and low coercive force are not affected significantly by the change of local structure but related to the amorphous state. The main difference is the much smaller saturation magnetization of the FeBM compared with that of FeBSi. The large initial susceptibility and small saturation field suggest that the small saturation moment in the latter should not be an indication of antiferromagnetic order but from reduced net spin per atom due to the local structure.

To clarify such change from the perspective of local structures, the EXAFS technique was employed. The Fourier transform of the experimental EXAFS spectra $K^2\chi(K)$ of FeBSi and FeBM glassy alloys, i.e., $\chi(R)$, at Fe–K edges exhibit evident differences, as shown in Fig. 4. The parameter K is the wave number of the photoelectron in XAFS process, which has dimensions of 1/distance, and is defined as

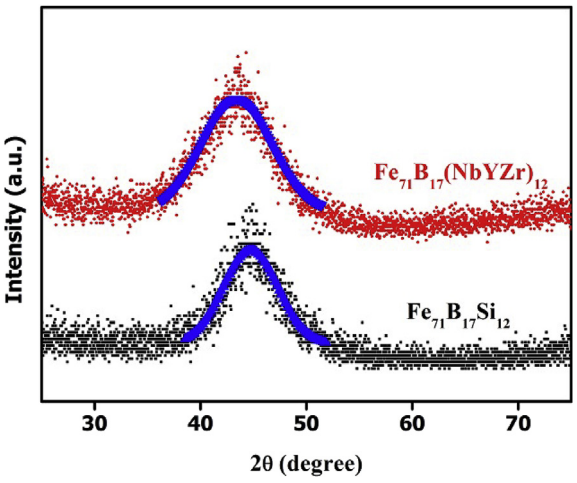

Fig. 1. XRD patterns of two Fe-based metallic glasses. The solid lines show the Gaussian fittings.

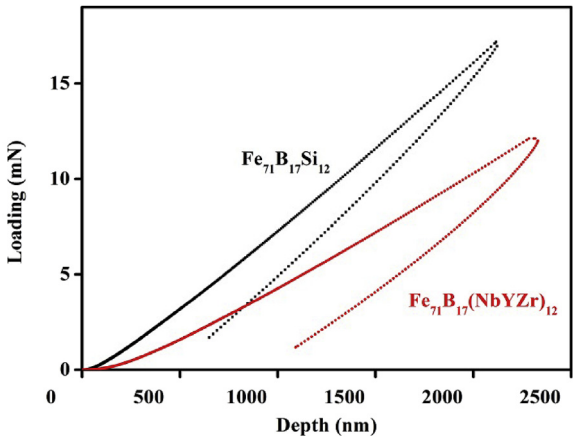

Fig. 2. Load-penetration curves of two Fe-based metallic glasses obtained with nanoindentation.