NRIXS Investigation of a-MgFe and a-ScFe Alloy Thin Films

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Introduction

Nuclear resonant inelastic x-ray scattering (NRIXS) is an efficient technique for the direct measurement of the partial vibrational density of states [VDOS, g(E)] of solids. The low-energy part of the VDOS of amorphous (a-) systems is interesting, because it shows an "excess" VDOS as compared with the Debye behavior [$g(E) \propto E^2$]. This excess VDOS is known as the "boson peak." The boson peak is a characteristics of all amorphous systems. According to our previous results for the partial VDOS of a-FeTb and a-FeY [1, 2] alloy thin films, the boson peak is found to be pronounced for higher Tb or Y concentrations. This vibrational softening is also indicated by the concentration dependence of the Lamb-Mössbauer factor.

In the literature, the behavior of the boson peak is widely investigated by neutron inelastic scattering on many complex bulk materials. However, studies on simple binary metallic systems are rare. In this experiment, we observed the boson peak on amorphous binary metallic alloy thin films by NRIXS.

Methods and Materials

The samples we studied include a-Mg_xFe_{1-x} (x = 0.30, 0.70) and a-Sc_xFe_{1-x} (x = 0.33, 0.75). All these amorphous alloy thin films were prepared in ultrahigh vacuum at a base pressure of about 5×10^{-10} mbar and $<10^{-9}$ mbar during deposition. The preparation was done by thermal co-evaporation of the elements deposited onto oxidized Si(100) substrates at -140°C. For the thermal evaporation of Mg and ^{57}Fe (95.5% enriched), we used two different Knudsen cells, and for Sc, an electron gun was employed. All samples were 800-Å thick and covered by 60 Å of Cr for protection.

The amorphous nature of the films was characterized by x-ray diffraction (XRD) and conversion electron Mössbauer spectroscopy (CEMS). Figures 1 and 2 show the XRD and CEMS results, respectively. No sharp Bragg peaks of the films are observed in Fig. 1, indicating their amorphous structure. Considering the many different local environments of ^{57}Fe atoms in an amorphous alloy, the spectra in Fig. 2 were fitted by a distribution of quadrupole splittings, being typical for amorphous metallic systems [1, 2].

For the determination of the VDOS of these amorphous alloy films, we performed NRIXS at SRI-CAT beamline 3-ID at the APS. All experiments

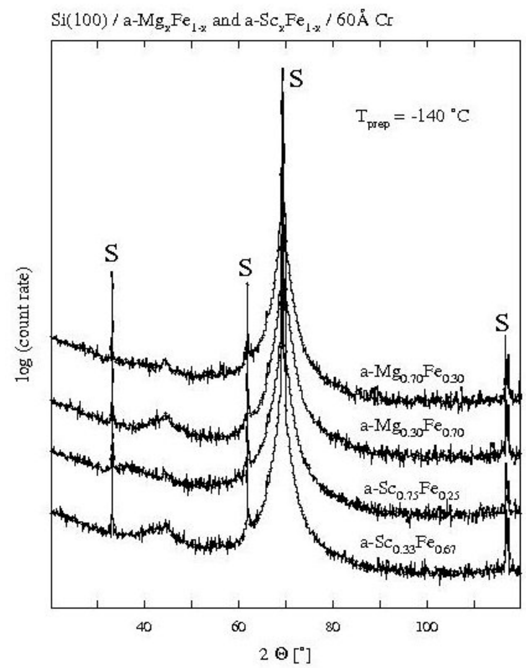

FIG. 1. XRD of a-Mg_xFe_{1-x} and a-Sc_xFe_{1-x} alloy thin films. The peaks marked S are the Bragg reflections from the substrate [Si(100)].

SRI-CAT beamline 3-ID at the APS. All experiments were done at room temperature. The white beam from the undulator was monochromatized to 14.4125-keV energy by two separate monochromators. The final monochromatic beam left the high-resolution monochromator with an energy resolution of 1 meV. The pulsed nature of the synchrotron beam helped us to count the delayed photons originating from the nuclear de-excitations of ^{57}Fe nuclei. The count rate of the incoherent 6.4-keV fluorescent x-rays of Fe was measured by avalanche photo diode (APD) detectors. The details of this technique are given in Refs. 3-5. The measurements were carried out until similar statistics in all the spectra were achieved. These data were then normalized and taken for the removal of the elastic peak and then for the determination of the VDOS. Other related quantities (like the Lamb-Mössbauer factor and average force constant) were also determined.

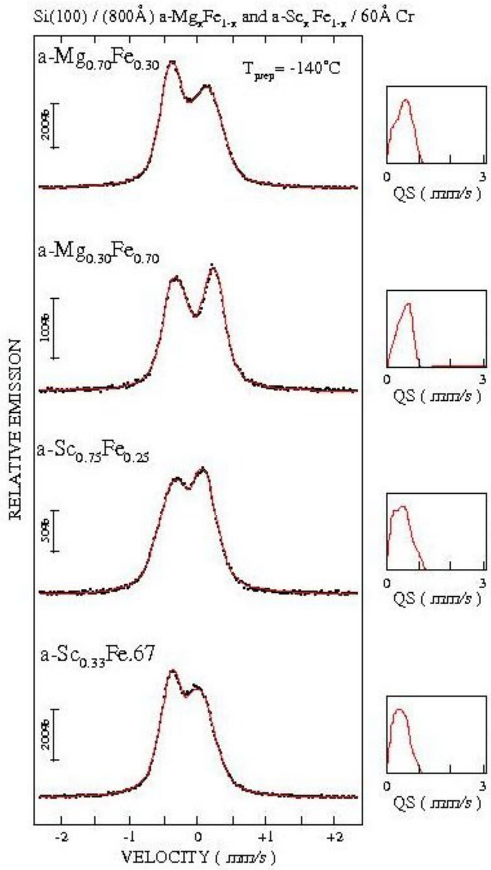

FIG. 2. CEM spectra of a-Mg_xFe_{1-x} and a-Sc_xFe_{1-x} alloy thin film at room temperature. The spectra are fitted with a distribution of quadrupole splittings, P(QS).

Results and Discussion

The measured and normalized NRIX spectra are shown in Fig. 3. For clarity, the spectra are vertically displaced. Each spectrum shows the common features of inelastic scattering (i.e., the elastically scattered intense peak at the nuclear resonance energy along with the side bands). The features on the right and left side of the elastic peak are due to phonon creation and annihilation, respectively. The instrumental resolution function (the dotted curve in Fig. 3) has a full width at half maximum (FWHM) of 1 meV.

Figure 4 shows the VDOS of the measured a-MgFe and a-ScFe alloy films. The VDOSs were obtained from the normalized vibrational excitation probabilities by the use of the computer program PHOENIX. The insert in Fig. 4 is the magnified view of the low-energy part of the VDOS. The low-energy part is clearly different for different concentrations of the amorphous alloy. The clear differences of this part can be visualized by

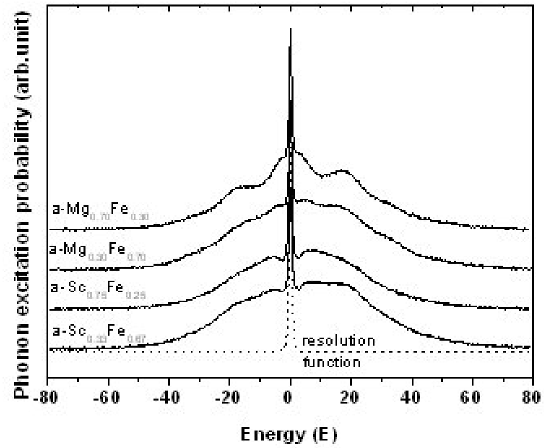

FIG. 3. Normalized vibrational excitation probability for a-MgFe and a-ScFe alloy films.

plotting $g(E)/E^2$ versus E, which should be a constant (straight line) in case of a strict Debye law. A deviation from the Debye behavior is clearly observed in Fig. 5. The low-energy peak (boson peak) is different for different concentrations and different alloys. The boson peak is more pronounced at lower Fe concentrations in both a-MgFe and a-ScFe alloy films.

In summary, we have observed access low-energy excitations (boson peak) in binary metallic a-MgFe and a-ScFe alloy thin films. The boson peak is found to be enhanced at lower Fe concentrations, similar to the case of a-RE_xFe_{1-x} alloy films (RE = Tb, Y) [1, 2]. Further investigations that will enlighten us about the origin of the boson peak anomaly are in progress.

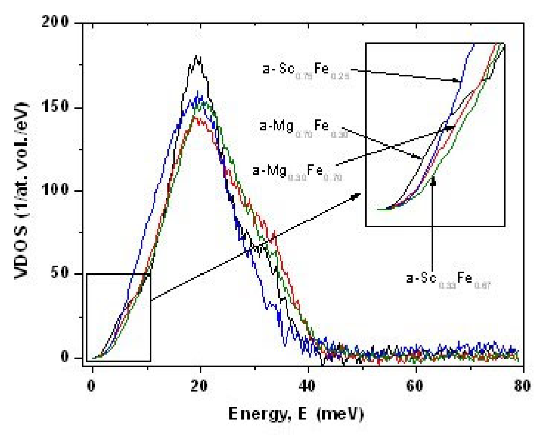

FIG. 4. [57]Fe projected partial VDOS [or g(E)] of a-MgFe and a-ScFe alloy thin films for different compositions.

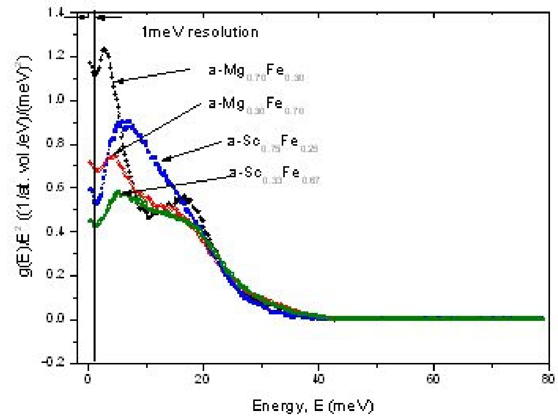

FIG. 5. $g(E)/E^2$ versus E for a-MgFe and a-ScFe alloy thin films.

Acknowledgments

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References

[1] T. Ruckert, W. Keune, B. Sahoo, W. Sturhahn, T.S. Toellner, E.E. Alp, and R. Röhlsberger, Hyperfine Interact. **144/145**, 65 (2002).

[2] W. Keune, T. Ruckert, B. Sahoo, W. Sturhahn, T.S. Toellner, E.E. Alp, and R. Röhlsberger, J. Phys.: Condens. Matter (in press, 2003).

[3] M. Seto, Y. Yoda, S. Kikuta, X.W. Zhang, and M. Ando, Phys. Rev. Lett. **74**, 3828 (1995).

[4] W. Sturhahn, T.S. Toellner, E.E. Alp, X.W. Zhang, X.W. Zhang, A. Ando, Y. Yoda, S. Kikuta, M. Seto, C.W. Kimball, and B. Dabrowski, Phys. Rev. Lett. **74**, 3832 (1995).

[5] A.I. Chumakov, R. Rüffer, H. Grünsteudel, G. Grübel, J. Metge, and H.A. Goodwin, Europhys. Lett. **30**, 427 (1995).