Materials Science

12C/2004G271

EXAFS study on local structure changes of MgNi alloys during mechanical alloying process

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Introduction

Mechanical alloying (MA) of elemental powder mixtures have been successfully employed and widely studied as a method for synthesizing amorphous alloys [1]. Mg-Ni system is one of the most attractive materials for hydrogen storage alloy. In this paper, we report structural change around Ni atom during solid state amorphization in a $Mg_{50}Ni_{50}$ alloy by x-ray absorption fine structure (XAFS) and x-ray diffraction measurements and discuss the mechanism of amorphization.

Experimental procedure

Mg-Ni alloys were prepared by mechanical alloying using a planetary ball-milling machine. Starting materials were pure Mg powder (99.8%, <325 mesh) and pure Ni powder (99.8%, 0.3-0.7nm).The x-ray diffraction patterns were measured using Cu K α radiation to observe phase change of $Mg_{50}Ni_{50}$ alloy.

The local structure around Ni atom was observed by x-ray absorption fine structure (XAFS). Ni K-edge (8339eV) XAFS measurements were carried out at the beam line BL12C in Photon Factory, KEK, Tsukuba, with Si(111) double crystal monochromator.

Results and discussion

The radial structure function, F(r), around Ni atom provided by the Fourier transform of Ni K-edge EXAFS spectra are shown in Fig.1. Although peak height decrease with milling time, F(r) for MA alloys up to 10h milling exhibit same pair correlation peaks as fcc-Ni up to 0.8nm. F(r) for 50h MA alloy is different from fcc-Ni; position of the first nearest peak at 2.2nm and long distance correlation peaks at around 0.4 to 0.5 nm are shift to shorter distance. In Fig.1, F(r) for $MgNi_2$ and Mg_2Ni intermetallic compounds obtained from EXAFS simulation using FEFF6 program are drawn. It is obvious that F(r) for MA50h alloy is similar to that of $MgNi_2$ intermetallic compound; i.e. the local structure around Ni atom change from fcc to $MgNi_2$-like structure between 10h to 50h of milling. The height of the peaks corresponding to the long range order of the crystalline phase are reduced with increasing milling time and almost vanish at 200h. Only the main peak near 0.23nm which corresponding to the short range order of the amorphous alloy remained.

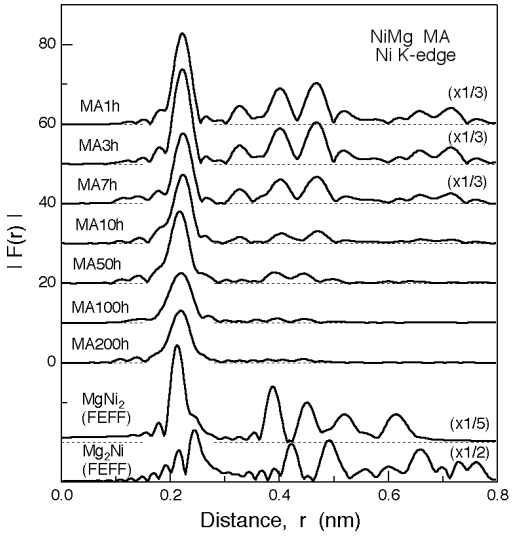

Fig. 1 Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), F(r), around Ni atom in the mechanically alloyed $Mg_{50}Ni_{50}$ as a function of milling time.

Summary

At early stage of milling (< 10h), a part of Ni atom diffuse into crystalline Mg and form highly disordered Mg-rich alloy. At the second stage of alloying (10h ~ 50h), Mg atoms diffuse into fcc-Ni, resulting in this Ni-rich Ni-Mg mixture forming $MgNi_2$-like short-range order, as seen in the EXAFS results. In the third stage (100h ~ 200h) amorphous phase appear, i.e. the long range order of crystalline phase disappear in the radial structure function, F(r) , obtained by XAFS measurements. Coordination numbers of Ni and Mg around Ni atoms in amorphous state are 4.3 and 7.7, and Ni-Ni and Ni-Mg atomic distances are 0.244 nm and 0.273 nm, respectively.

References

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