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To cite this version:

V. Harris, K. Kemner, B. Das, J. Woicik, P. Crespo, et al.. Mechanical-Alloying and Lattice Distortions in Ball-Milled CuFe. Journal de Physique IV Colloque, 1997, 7 (C2), pp.C2-1151-C2-1152. <10.1051/jp4:19972168>. <jpa-00255232>

HAL Id: jpa-00255232
https://hal.archives-ouvertes.fr/jpa-00255232
Submitted on 1 Jan 1997

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Mechanical-Alloying and Lattice Distortions in Ball-Milled CuFe


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Abstract. Extended X-ray absorption fine structure (EXAFS) measurements were used to obtain element-specific, structural and chemical information of the local environments around Cu and Fe atoms in high-energy ball-milled samples. Analysis of the EXAFS data shows both Fe and Cu atoms reside in face-centered-cubic sites with the first coordination sphere consisting of a mixture of Fe and Cu atoms reflecting the as-prepared stoichiometry. The calculated bond distances indicate a dilation in the bonds between unlike neighbors which accounts for the lattice expansion measured by X-ray diffraction.

The CuFe equilibrium phase diagram indicates little or no miscibility of either constituent into the other at room temperature, and only ~4 at. % of Fe dissolves into Cu and ~10 at. % Cu into Fe near their respective liquidus lines.[1] However, extended regions of metastable solubility can be attained via vapor-quenching techniques[2, 3]. Recently, an alternative path to vapor-quenching, high-energy ball-milling (HEBM), has been reported to form solid-solutions of elements having a positive heat of mixing.[4-6]

In this paper we report on extended X-ray absorption fine structure (EXAFS) measurements and analysis of HEBM Cu_{x}Fe_{1-x} samples. Using EXAFS, we illustrate that both the Fe and Cu atoms reside on close-packed face-centered-cubic (fcc) lattice sites, common to Cu, but not found in stable Fe phases. The calculated bond distances indicate a dilation in the bonds between unlike neighbors which accounts for the widely reported, but poorly understood, lattice expansion measured by X-ray diffraction. A complete description of the milling conditions used in processing these samples are presented elsewhere.[4, 6, 7]

X-ray absorption spectra encompassing the Fe and Cu K absorption edges were collected from the HEBM powders and Fe and Cu foil standards, using the X23B and X23A2 beamlines at the National Synchrotron Light Source. Both beamlines employ double-crystal, fixed-exit monochromators, with beamline X23B using a pair of Si (111) crystals, and X23A2 using a pair of Si (311) crystals. The EXAFS data were collected when the storage ring energy was 2.5 GeV with a ring current between 110 mA and 250 mA. The EXAFS analysis followed established procedures [8], which included the normalization of the extended fine structure to the absorption edge step height and energy, removal of a non-oscillatory background curvature, conversion to photoelectron wave vector (k) space, and Fourier transformation to radial (r) coordinates. Quantitative analysis of the near neighbor environment was accomplished by a non-linear least square parameterized theoretical EXAFS data generated via FEFF (vers. 3.11)[9]

X-ray diffraction measurements of both milled samples illustrate only one family of fcc diffraction peaks suggesting that the Fe and Cu coexists in a single fcc phase. Fig 1 (a) illustrates the Cu and Fe EXAFS from the Cu_{70}Fe_{30} milled sample, with Cu EXAFS data from the foil standard in k-space. The similarity between data sets, especially in phase and relative amplitude, indicate that indeed both Fe and Cu atoms reside on fcc lattice sites. Lattice parameters of 3.641 Å and 3.634 Å were measured for Cu_{50}Fe_{50} and Cu_{70}Fe_{30} samples, respectively. These values are significantly greater than that of fcc Cu, 3.615 Å, representing a 2.1% and 1.6% increase in unit cell volume, respectively, and are larger still compared with the values predicted by Vegard's law, i.e., 3.6025 Å for Cu_{50}Fe_{50} (a change of 3.24% in volume) and 3.6075 Å for Cu_{70}Fe_{30} (a change of 2.22% in volume).
Figure 2. Fourier-filtered, near-neighbor Cu (a) and Fe (b) EXAFS data (solid curves) for the Cu$_{87}$Fe$_{13}$ sample presented with the best fit data (dashed curve with symbols) obtained using parameterized EXAFS spectra.

Figure 3. Plot of lattice parameter versus Fe concentration in CuFe alloys.

Figure 2 is a plot of the Cu and Fe Fourier-filtered near neighbor EXAFS data with the best fits determined using simulated FEFF data. Best fits were obtained using two shells of atoms, one of Cu and the other of Fe, displaced from one another. These fits indicate that the nearest neighbor chemistry of the milled samples are very close to that of the nominal stoichiometry of the starting materials, indicating that atomic-level mixing has occurred and a supersaturated-solid-solution exists. From the fitting analysis, the nearest neighbor bond distances for like and unlike neighbors were calculated. Like neighbors have bond distances very close to that one would expect for elemental phases of fcc Cu and fcc Fe, i.e., Cu-Cu = 2.54 Å and Fe-Fe = 2.52 Å. However, the values for unlike pairs are calculated to be dilated to a distance of 2.625±0.01 Å. Lattice parameters calculated using these bond distances are presented in Fig. 3 and are found to be consistent with those measured via XRD. Specifically, values calculated from XRD measurements for the samples studied here are plotted with similar values from XRD measurements of vapor-quenched HEBM powders[10]. Values calculated using the atomic radii of Goldschmidt and Pauling, as well as those predicted from Vegard’s Law, are presented for comparison. These data illustrate that the bond dilations between unlike neighbor pairs are the source of the measured lattice expansion in HEBM samples.

Acknowledgments

This research was carried out, in part, at the National Synchrotron Light Source (Brookhaven National Laboratories, Upton, NY), which is sponsored by the U.S. Department of Energy.

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