Lattice and spin dynamics in bcc Fe, 10 at. % Be

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Body centered cubic $Fe_{1-x}Be_x$ alloys are known to display an enhanced tetragonal magnetostriction compared to Fe. In order to characterize the enhanced magnetoelasticity observed in this alloy system, we present detailed inelastic neutron scattering measurements of the phonon dispersion relations of a single crystal of bcc Fe, 10 at. % Be along the high symmetry directions [100], [110], and [111] at room temperature. We observe in particular that the frequency of transverse phonons propagating along the [110] direction with a $[1\bar{1}0]$ polarization at the zone boundary is reduced by 10% with respect to bcc Fe (the corresponding elastic shear constant $c' = \frac{1}{2}(c_{11} - c_{12})$ associated with this mode is approximately 70% that of pure Fe). The dispersion of spin waves has also been determined for energy transfers up to 40 meV and is found to follow the isotropic dispersion relation $E(q) = Dq^2$, with $D \sim 200$ meV/Å^2 [for Fe, $E(q) = Dq^2$, with $D = 280$ meV/Å^2]. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2150803]

INTRODUCTION

Recent investigations of the magnetoelastic properties of the alloy systems Fe–Ga,[1,2] Fe–Al,[3] and Fe–Be,[4] demonstrate a considerable enhancement of the tetragonal magnetostriction constant λ_{100}, with respect to α-Fe (body centered cubic structure). At room temperature, for example, an alloy of $Fe_{89}Be_{11}$ displays a sixfold increase in λ_{100} as compared to α-Fe.[4] Correspondingly, the elastic constants such as c_{11}, c_{12} and $c' = \frac{1}{2}(c_{11} - c_{12})$ are also observed to undergo significant variations. Such an extraordinary magnetoelastic behavior clearly highlights the potential technical applications of the aforementioned alloys. From the microscopic point of view, a complete characterization of the lattice and spin dynamics in these systems is highly desirable, as this allows for a realistic modeling of the atomic and magnetic interactions which may give rise to the magnetoelastic behavior. Reported here is an inelastic neutron scattering investigation of the phonon and magnon dispersion relations for a single crystal alloy of $Fe_{90}Be_{10}$ at room temperature. We observe a softening of the transverse $[\xi\xi 0]$ phonon mode with a $[1\bar{1}0]$ polarization and a reduction of approximately 25%–30% in the value of the spin wave stiffness constant D reported for pure iron.[5–7]

EXPERIMENT

A large cylindrical single crystal with a nominal composition of $Fe_{90}Be_{10}$ (approximately 1 cm in diameter and 3 cm in length) was prepared by Bridgman growth of an ingot of Fe (99.999% purity) and Be (99.9% purity). Details concerning the crystal growth of the Fe rich FeBe alloy system are outlined in Ref. 4. Room temperature inelastic neutron scattering measurements were performed on the thermal triple axis spectrometers BT2 and BT7 located at the NIST Center for Neutron Research, Gaithersburg, Maryland. A fixed final neutron energy of 14.7 meV was utilized for both spectrometers. For measurements of the phonon modes, the crystal was oriented in both the $[1\bar{1}0]$ and [010] scattering planes, giving access to all the longitudinal and transverse modes along the three high symmetry directions $[\xi 00]$, $[\xi\xi 0]$, and $[\xi\xi\xi]$ with ξ as the reduced wave vector in units of $2\pi/a$, where a is the cubic lattice constant. The neutron groups for the phonons were determined by constant-Q scans. The dispersion of the magnon modes for energy transfers of up to 40 meV was also measured along these three high symmetry directions using constant-E scans.

RESULTS AND DISCUSSION

The room temperature phonon dispersion relations for pure iron have been determined in numerous neutron scattering studies.[8–13] In this article, we compare our results for $Fe_{90}Be_{10}$ with the detailed and comprehensive data reported by Minkiewicz *et al.*[8] and Klotz and Braden.[13] The general trend in the dispersion behavior of both the longitudinal and acoustic modes is very similar to that observed for iron and, in addition, the velocities of sound waves obtained from the

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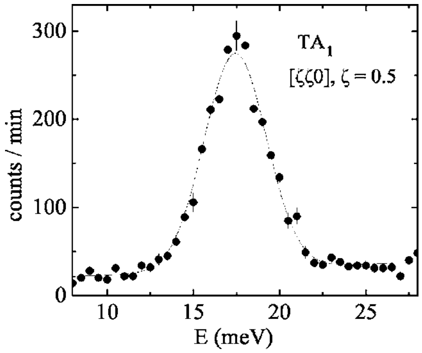

FIG. 1. Observed neutron group for the $[\xi\xi 0]$ TA_1 branch at the zone boundary (*N*-point) for $Fe_{90}Be_{10}$. ξ is the reduced wave vector in units of $2\pi/a$.

initial slopes of the phonon dispersion curves are in overall broad agreement with those calculated from the elastic constants as determined by ultrasonic techniques for $Fe_{88.7}Be_{11.3}$.[4] One notable difference is the energy of the transverse TA_1 mode with a propagation wave vector along $[110]$ and a $[1\bar{1}0]$ polarization, at the zone boundary (*N* point). The neutron group associated with this mode is displayed in Fig. 1. The observed energy of this mode, at 17.5 meV, is approximately 92% of that reported for pure iron (Minkiewicz *et al.*[8] report a value of 18.5 meV for this particular mode, while Klotz and Braden assign a value of just under 19 meV.[13]). A similar behavior for this particular mode has been recently observed in $Fe_{89.2}Ga_{10.8}$.[14] Furthermore, for the FeGa system, the TA_1 mode is observed to undergo an ever increasing and spectacular softening with increasing Ga composition. Similarly, the TA_2 mode, with an associated $[001]$ polarization, also appears to display a departure from that observed for iron, lying consistently at values greater than those for pure Fe as the zone boundary isapproached. The room temperature phonon dispersion curves for $Fe_{90}Be_{10}$ along the $[\xi\xi 0]$ direction are displayed in Fig. 2, together with the data for pure iron, taken from Refs. 8 and 13.

The composition dependence of the room temperature

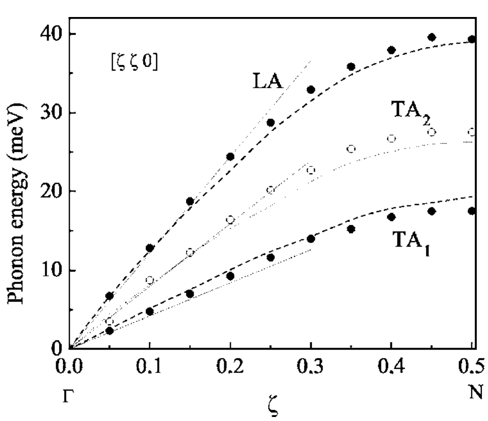

FIG. 2. The room temperature phonon dispersion curves for $Fe_{90}Be_{10}$ along the $[\xi\xi 0]$ direction. Dashed lines are those for iron taken from Refs. 8 and 13, whilst solid lines are the sound velocities calculated from the elastic constants for $Fe_{88.7}Be_{11.3}$ (see Ref. 4).

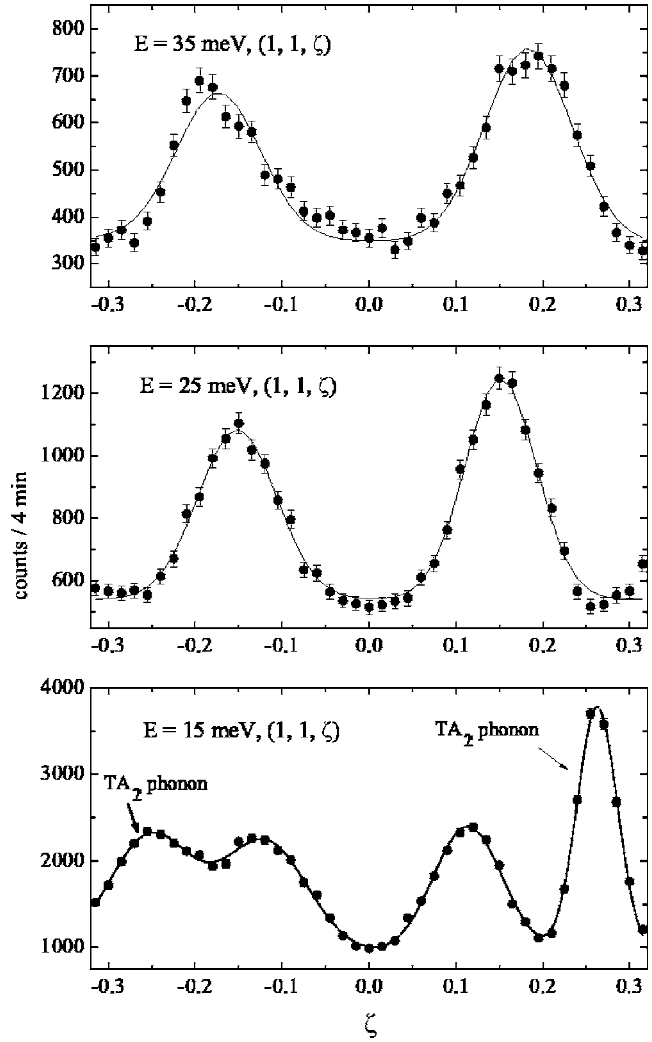

FIG. 3. Room temperature constant-*E* scans at 15, 25, and 35 meV for $Fe_{90}Be_{10}$ along the $[001]$ direction.

Fe magnetic moment, in Bohr magnetons, for dilute FeBe alloys is reported to obey the following relationship:[15]

$$\mu_{Fe} = 2.216 - 2.01 x_{Be}, \tag{1}$$

where x_{Be} is the fractional Be composition. For a composition of 10 at. % Be, the resulting magnetic moment per Fe atom is approximately 2 μ_B. It can thus be expected that the concomitant spin wave stiffness constant *D* (in units of meV Å^2) is also reduced for dilute FeBe alloys. The conventional isotropic magnon dispersion relation for ferromagnets at small values of q(Å^{-1}), is given by

$$E(q) = Dq^2. \tag{2}$$

The dispersion of spin waves for the FeBe alloy under investigation was tracked for energy transfers of up to 40 meV along the three high symmetry directions. The resulting dispersion relations were observed to be isotropic, as can be expected at relatively small values of the magnon wave vector *q*. Sample neutron groups of magnons observed at energy transfers of 15, 25, and 35 meV are displayed in Fig. 3 while the room temperature magnon spectrum up to 40 meV for $Fe_{90}Be_{10}$ determined from the presently available data is displayed in Fig. 4. With the assumption of an

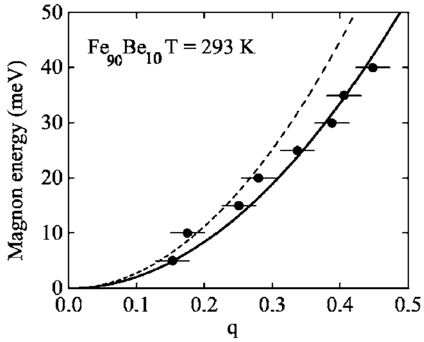

FIG. 4. Room temperature spin wave dispersion relation along [001] for $Fe_{90}Be_{10}$. The solid curve shows the relation $E=Dq^2$ for $D=210$ meV Å^2, while the dashed curve shows the dispersion relation observed at small values of q for pure Fe with $D=280$ meV Å^2. Units of q are in Å^{-1}.

isotropic magnon dispersion for small values of q, the available data were least squares fitted to Eq. (1) yielding a value of (210 ± 15) meV Å^2 for D. This value is a reduction of 25%–30% of the value of D determined for pure Fe.[5–7] This reduction in the spin wave stiffness constant is remarkably larger than that observed for corresponding concentrations of Fe–Si,[16] Fe–Ga,[17] and Fe–Al (Ref. 17) alloys.

Further measurements are presently underway in order to determine the temperature dependence of the spin wave stiffness constant for this particular alloy composition as well as measuring the magnon dispersion relationship to higher energies. Future work presently in progress will also aim to extend information on the phonon dispersion curves to alloys richer in beryllium and to correlate these with bulk elastic properties. The present results clearly show that a softening of the transverse $[\xi\xi 0]$ phonon mode with $[1\bar{1}0]$ polarization is also apparently present in the Fe–Be system, akin to that also observed for Fe–Ga alloys which also display similar and remarkable behavior in their magnetoelastic properties.

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