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We have modeled the magnetic properties of films of amorphous $Fe_{80}B_{15}Si_5$ from first principles. The model is based upon one premise and that is: the magnetic moment of iron in the amorphous matrix is the same as that of metallic iron. With no adjustable parameters and using measured parameters we calculate that $4\pi M_s$ = 1450 G, A = 1.26×10^{-6} ergs/cm, H_A = 30 Oe and ΔH = 14 Oe. The estimates are in reasonable agreement with measured values.

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"Influence of Pulsed Magnetic Fields on Uniaxial Stress of Films"

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Fifth Month Progress Report

Introduction

So far we have produced and magnetically characterized films of $Fe_{80}B_{15}Si_5$ under various annealing conditions, see previous monthly reports. In order to properly assess or estimate the effects of annealing upon the magnetic properties of the films it is essential to develop a realistic model which calculates the magnetic properties of the film from first principles in its "virgin" state (prior to annealing). The purpose of this monthly report is to establish the foundations of such a model and also to explicitly calculate magnetic parameters of the films.

Modeling of magnetic properties

We propose a simple model which assumes that the local atomic order originates from that of the crystalline equivalent phase(s) except that there is no coordination between sites separated by as much as 10 Å. In addition, the model assumes that although the local symmetry may be known, th occupation number may vary from site to site. Extend X-ray absorption fine structure (EXAFS) measurements[1] provide us with a measure of the average distance between magnetic ions and their respective coordination numbers. This type of information is sufficient to predict fundamental properties of the $Fe_{80}B_{15}Si_5$ system.

Saturation Magnetization

In calculating M_s we basically count the number of Fe magnetic ions inside a coordination shere having radius r as measured[1] by EXAFS. For example, in Table I we provide a measured value via EXAFS of $\approx$ 10 Fe ions

within a coordination sphere of radius 2.7 Å relative to a central Fe ion. Thus, the magnetization may be approximated by

$$M_s \approx M_{Fe} (n_o/n_{Fe})(r_{Fe}/r_o)^3, \quad (1)$$

where $M_{Fe} = 1740$ G,

$n_{Fe} = 14$,

$r_{Fe} = 2.866$ Å,

$n_o = 10$,

$r_o = 2.7$ Å.

In the above data M_{Fe}, n_{Fe}, and r_{Fe} are obtained from crystalline Fe data and values of n_o and r_o are measured by EXAFS on $Fe_{80}B_{15}Si_5$.[1] Substituting above values into Eq.(1) we estimate M_s to be ≈ 1490 Oe. This should be compared with a measured value of 1450 Oe for our samples of $Fe_{80}B_{15}Si_5$ at room temperature.

Exchange Stiffness Constant

In modeling the exchange stiffness constant we once again rely on the EXAFS measurements as presented in Table I to calculate A, the exchange stiffness constant, using the formula

$$A = 2J/r_o \langle s \rangle, \quad (2)$$

where $\langle s \rangle$ is given by

$$\langle s \rangle = s_{Fe}(n_o/n_{Fe}).$$

Here $s_{Fe} = 1.1$ for Fe (bcc Fe @ T = 25°C). Our estimate of A is 1.26×10^{-6} erg/cm. This is compared with a measured[1] value of 0.90×10^{-6} erg/cm.

Curie Temperature

From molecular field theory the expression for the Curie temperature (T_c) is

$$T_c = 2Jz\langle s\rangle(\langle s\rangle + 1)/3k_B, \quad (3)$$

where $z = 3.5 \pm 1$ is the first nearest neighbor number measured by EXAFS and $k_B = 1.38 \times 10^{-16}$ erg/^oK is the Boltzman's constant. We obtain an estimate of 515 K (±150K) for T_c. The measured value is 624 K.[1] The reader is reminded that the error associated with such calculations is significant due to the relative uncertainty associatied with the measurement[1] of z by EXAFS.

Anisotropy Field

There are three potential sources of uniaxial anisotropy field. The first source is due to the strain arising from a mismatch in thermal expansion coefficients between the substrate materials and the film. The uniaxial axis is typically normal to the film plane in these alloy films, since the stress or strain in the film plane is isotropic. The easy axis of magnetization is either in the film plane (all directions being equal) or normal to the film plane. This type of induced anisotropy field, $H_A^{\perp}$, manifests itself as a lowering or raising of the effective magnetization of the film ($4\pi M_s \pm H_A^{\perp}$).

The second source of uniaxial anisotropy is due to the incomplete occupancy of all sites by Fe ions. For example, if one were to assume the local symmetry is of a body-centered type where some ions are missing, it can be shown by simple application of the pair ion model[2] that this leads to a net contribution to the uniaxial anisotropy field. However, if the magnetic correlation between local sites is small and if the number of ions and the vacant sites are random from unit cell to unit cell this source of anisotropy field averages to zero over the entire film. One way of measuring such a local field would be to utilize a probe of sufficient sensitivity to

magnetic fluctuations over small regions (~ 20Å). We do not believe that EXAFS is sensitive to this type of local fluctuations in these materials.

Finally, it is well known that gas inclusions are incorporated in the film during processing. Typically, both working (argon) and residual (e.g. nitrogen, hydrogen, and oxygen, etc.) gases are entrapped in the film. The only assumption we make is that the entrapment of the gases establishes an anisotropic network of voids (or defects) in the film. The entrapment of these gases generate strain in the film plane. Relaxation occuring along the axis normal to the film plane is assumed to be negligible. Once a uniaxial stress or strain axis is established to be in the film plane there corresponds an anisotropy field, $H_A^{\parallel}$, of the following amplitude

$$H_A^{\parallel} = 3\lambda_s \epsilon \mu / 2M, \tag{4}$$

where

$\mu = 0.8 \times 10^{12}$ dyn/cm^2 (Lame's constant for polycrystalline Fe),

$\lambda_s = 32 \times 10^{-6}$ (R.C. O'Handley and M.O. Sullivan, J. Appl. Phys. 52, 184 (1981) and references therein),

$M = 1450$ G (measured by us),

$\epsilon = 0.001$ (lattice strain measured[1] by EXAFS).

Using these parameters our estimate of $H_A^{\parallel}$ is 30 Oe for $Fe_{80}B_{15}Si_5$ compared to a measured value of 13 to 15 Oe. We surmise that the effect of annealing is to drive out or annihilate trapped voids in the film during structural relaxation.

FMR Linewidth

The basic mechanism for magnetic relaxation is governed by the spin-lattice direct coupling as incorporated by Landau-Lifshitz damping formula:

$$\Delta H = 1.157 \times (\lambda/\gamma) \times (f/\gamma/M). \quad (5)$$

We have assumed a Lorentzian shaped absorption curve so that the derivative linewidth is given by the above expression where λ is the Landau-Lifshitz damping parameter (1.4×10^7 Hz), γ is defined as $1.4(g) \times 10^6$ Hz/Oe, g is measured to be 2.10 for $Fe_{80}B_{15}Si_5$, and f is the resonance frequency (9.5×19^9 Hz). We have assumed that λ is that of Fe. Thus, we imply that it is the spin moment of Fe that is relaxed to the lattice. We estimate a ΔH of 14 Oe. This compares with a measured value of ~ 30-40 Oe.

These films have shown evidence of inhomogeneous linewidth contributions due to variation of magnetization and/or anisotropy field near the film-substrate interface. For thin films of the order of 100 nm these variations are sufficiently important to effect the linwidth. For example, measured values of ΔH for films studied here are markedly higher ($\Delta H \approx$ 30-40 Oe) than the same alloys at 250 nm (ΔH = 20 Oe).

It is widely believed that amorphous materials contain defects on the order of 10-15 Å. In some sense one could argue for two magnon relaxation processes. However, efficient scattering of spin waves would occur only for short wavelengths comparable to the dimension of the defects. Since the scattering involves spin waves of the quasi-uniform procession mode with energetically degenerate spin wave modes, we can exclude the two magnon process. The wavelengths of degenerate magnons or spin waves are much longer than 10-15 Å.

Our intention in presenting these calculations is to alert the reader of the feasibility and value of applying EXAFS measured parameters for such

purposes. We acknowledge that more thorough and comprehensive studies have been undertaken in calculating these parameters.

Conclusions

Our basic premise is that the moment of Fe is the same as that of metallic Fe. Apparently, this point of view is valid in view of the remarkable comparisom between theory and experiment. Our estimates of the fundamental magnetic parameters were made by applying the measured[1] EXAFS parameters with no addional adjustable parameters!

We believe that this is the first study of its kind to apply EXAFS measurements to correlate changes in local atomic structure to changes in magnetic properties. Such studies are invaluable in determining the response of materials to practical processing techniques such as annealing and in gaining insight to the fundamental relationship between structure and magnetism.

Alloy	radial distance (Å)	coordination number	$\sigma^2_{300\ K}$ (Å²)	technique	reference
$Co_{74}Fe_6B_{15}Si_5$					
Co-Co	2.46	5.7	.0221	xafs*	[1]
Co-Co	2.69	8.2	.055*		
Co-B	2.11	2.6	.0113		
$Fe_{75}Ni_5B_{15}Si_5$					
Fe-Fe	2.48	3.7	.0181	xafs*	[1]
Fe-Fe	2.68	7.4	.0543		
Fe-B	2.11	2.3	.0180		
$Ni_{66}B_{33}$					
Ni-Ni	2.24	4.3	.0107	xafs	[3]
Ni-Ni	2.46	3.0	.0053		
Ni-Ni	2.63	3.9	.0204		
Ni-B	2.11	3.8	.0027		
$Fe_{83}B_{17}$					
Fe-Fe	2.56	10.5		x	[4]
Fe-B	2.27	2.4			
$Fe_{75}B_{25}$					
Fe-Fe	2.60	10.5		x	[5]
Fe-B	2.27	2.4			
$Co_{60}B_{40}$					
Co-Co	2.57	10.2		x	[6]
Co-B	2.03	3.9			
$Ni_{64}B_{36}$					
Ni-Ni	2.55	9.2		x,n	[7]
Ni-B	2.12	4.9			
$Co_{81}P_{19}$					
Co-Co	2.55	10.1		x,n	[8]
Co-P	2.32	2.10			
$Fe_{80}P_{20}$					
Fe-Fe	2.61	10.0		xafs	[9]
Fe-P	2.32	3.0			
$Fe_{67}Co_{18}B_{14}Si_1$					
Fe-Fe	2.51	7±2	.0224	xafs	[10]
Fe-Co	2.46	2.2±2	.0112		

$Fe_{75}B_{25}$				
Fe-Fe	2.62	12.2	DRP	[5]
Fe-B	2.07	2.07		
$Fe_{60}B_{40}$				
Fe-Fe	2.57	11.1	DRP	[5]
Fe-B	1.9	4.6		
$Fe_{76}B_{24}$				
Fe-Fe		10.97	DRP	[11]
Fe-B		1.94		
$Fe_{80}B_{20}$				
Fe-Fe		10.79	DRP	[10]
Fe-B		1.51		
$Fe_{85}B_{15}$				
Fe-Fe		11.25	DRP	[10]
Fe-B		1.06		

a	this parameter was fixed during fitting procedures
Möss	Mössbauer spectroscopy
x	x-ray diffraction analysis
n	neutron scattering
DRP	calculated using dense random packing models
xafs	extended x-ray absorption fine structure analysis, unless noted, data was acquired via transmission
xafs'	conversion-electron extended x-ray absorption fine structure analysis

Table I Summary of EXAFS data.[1]

$Fe_{80}B_{15}Si_5$	M_s(G)	A(10^{-6}erg/cm)	T_c(K)	H_A(Oe)	ΔH(Oe)
Estimated Values	1490	1.26	515±150	30	14
Measured Values	1450	0.90	624	13-15	30

Table II Comparison of estimated and measured magnetic parameters.

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