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Journal of Magnetism and Magnetic Materials 240 (2002) 267–269

journal of magnetism and magnetic materials

www.elsevier.com/locate/jmmm

Probing antiferromagnetic order with heat capacity in exchange-biased structures

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Abstract

We explore the magnetic heat capacity in exchange-biased ferromagnet/antiferromagnet bilayers theoretically. We show that changes in the antiferromagnetic structure due to the reversal of the ferromagnet layer can be detected by distinct features in the heat capacity. This offers a method for probing antiferromagnetic domains in exchange-biased systems. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Exchange biasing; Heat capacity; Thin films – bilayer

Exchange bias refers to the unidirectional anisotropy induced in a ferromagnet that is exchange coupled to an antiferromagnet [1,2]. The characteristic feature is termed the bias field which describes a shift of the hysteresis loop along the field axis. This shift can be accompanied by an enhanced coercivity, where the hysteresis loop of the coupled film is wider than that for a single ferromagnet film.

It is difficult to obtain quantitative predictions about the magnitude of exchange bias in any given system because it is strongly dependent on the details of the physical and chemical structure at the ferromagnet/antiferromagnet interface. However, it is certain that bias is not possible without a magnetically ordered antiferromagnet. Experiments have shown extensively that the bias fields disappear at the blocking temperature of the antiferromagnet. This is consistent with theoretical models, which predict that the formation of antiferromagnet domains or domain walls at the interface is required for bias [3–5]. Such magnetic structure cannot exist above the ordering temperature of the antiferromagnet.

A tantalizing prospect for probing antiferromagnet order was demonstrated recently by the direct measurement of heat capacities in antiferromagnetic superlattices [6]. The procedure is sufficiently sensitive to observe distinct peaks in the magnetic heat capacity as the ordering temperature of the superlattice is reached. The technique provides a direct means of measuring changes in the antiferromagnetic order, particularly at phase transitions, that is not possible with conventional magnetometry techniques. Theoretical calculations predict that similar heat capacity features should also appear at the surface spin–flop transition in very thin antiferromagnet films [7]. In this communication we show that such thermodynamic measurements can offer new ways to probe the antiferromagnet properties in exchange bias systems.

We study a ferromagnet/antiferromagnet bilayer with a three-dimensional atomistic spin model. The film consists of sheets of spins with a simple cubic crystal structure, oriented parallel to the surface of the bilayer. The antiferromagnet is assumed to have an easy-axis in the plane of the film, with an applied field oriented at 10° from the easy axis in the same plane to reduce computation time. Periodic boundary conditions are applied to the unit cell edges in the plane of the film, but the bilayer has a finite thickness. We only consider uncompensated interfaces here; results for compensated interfaces are presented elsewhere [8]. The equilibrium configuration is found by numerically integrating the time-dependent Landau–Lifshitz equation of motion for the coupled spins. The effective field, $\vec{H}_i^{\mathrm{eff}}$, experienced

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PII: S0304-8853(01)00819-8

by each spin, $\vec{S}_i$, has contributions from an external applied field $\vec{H}_0$, a nearest-neighbor exchange energy J_{ij}, and anisotropies, K_{AF} and K_0,

$$\vec{H}_i^{\mathrm{eff}} = \vec{H}_0 + g\mu_{\mathrm{B}} \times \left(\sum_j J_{ij}\vec{S}_j + K_{\mathrm{AF}}(\vec{S}_i \cdot \vec{z})\vec{z} - K_0(\vec{S}_i \cdot \vec{n})\vec{n} \right). \quad (1)$$

The uniaxial anisotropy, K_{AF}, is only non-zero in the antiferromagnet, and K_0 represents an easy-plane anisotropy that simulates magnetostatic fields generated by out-of-plane spin fluctuations. $\vec{n}$ is the unit vector perpendicular to the plane of the film and the AF easy axis is along the z direction. Temperature is included by using a local mean-field approach, where the thermally averaged magnetic moment, m, of each spin is calculated self-consistently using

$$\langle m \rangle = m_0\, B\left(\frac{\vec{m} \cdot \langle \vec{H}^{\mathrm{eff}} \rangle}{k_{\mathrm{B}}T} \right), \quad (2)$$

where B is the Brillouin function and $\langle \ldots \rangle$ denotes a thermal average. Thus, both the ground state and thermal averages are solved self-consistently within one calculation scheme. The ferromagnet and antiferromagnet have 20 monolayers each, with each layer represented by a 2×2 unit cell. The mean-field exchange constants are chosen to give ordering temperatures of $T_{\mathrm{C}} = 1043$ K for the ferromagnet and $T_{\mathrm{N}} = 79$ K for the antiferromagnet, which are appropriate for an Fe/FeF$_2$ system [9].

The heat capacity, C_{H}, is calculated once the equilibrium structure is found at a particular value of the external field, H. The average magnetic energy is evaluated at a given temperature and the derivative,

$$C_{\mathrm{H}} = \left(\frac{\partial U}{\partial T} \right)_{\mathrm{H}}, \quad (3)$$

is taken numerically by taking the difference of the energies at nearby temperatures. We use a four-point finite difference method to calculate the derivative, with a temperature interval of 0.0001 K.

From simple energy considerations for a perfect uncompensated interface [10], an expression for the bias field magnitude, H_{eb}, can be derived in terms of the antiferromagnet domain wall energy, σ_{w}, and the interlayer coupling, J_{I},

$$H_{\mathrm{eb}} = \frac{J_{\mathrm{I}}}{M_{\mathrm{F}}t_{\mathrm{F}}} \left[\left(\frac{2J_{\mathrm{I}}}{\sigma_{\mathrm{w}}} \right)^2 + 1 \right]^{-1/2}. \quad (4)$$

Here, M_{F} represents the saturation magnetization of the ferromagnet and t_{F} is the ferromagnet film thickness. For a perfectly flat interface, we may expect the interlayer coupling between the ferromagnet and antiferromagnet to be the same order of magnitude as the antiferromagnet exchange. In the Co/CoO system, for example, superexchange between Co^{2+} ions mediated by O^{2-} ions at the interface could give the same coupling as the bulk antiferromagnet exchange. Mauri et al. showed this large interlayer coupling can give observed bias field magnitudes if a partial wall in the antiferromagnet is formed at the interface. This is consistent with Eq. (4) in the limit $J_{\mathrm{I}} \gg \sigma_{\mathrm{w}}$, which predicts that the bias field is simply proportional to the antiferromagnet wall energy.

Numerical results are shown in Fig. 1 for $J_{\mathrm{I}} = J_{\mathrm{AF}}$. An examination of the calculated spin configurations shows that a partial wall is formed in the antiferromagnet as the ferromagnet reverses. This change in the antiferromagnet order is signalled by a large peak in the heat capacity at a field value corresponding to the bias field. The position of the peaks along the field axis moves with the zero-crossing of the magnetization curves (H_{eb}) shown in the inset, approaching zero field as the temperature is increased. The magnitude of the peaks is most pronounced at temperatures close to but below the Néel temperature. For example, at 60 K, a relative change in the heat capacity of 15% is observed and should be detectable in an experiment. An analysis of these heat capacity features is provided elsewhere [8].

For rough interfaces, there may exist certain regions at the interface where the average exchange coupling between the ferromagnet and the antiferromagnet is reduced significantly. In these regions the energy required to form a partial wall in the antiferromagnet

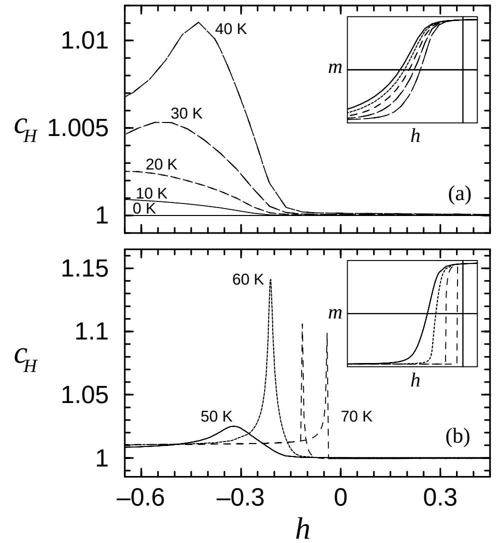

Fig. 1. Normalized magnetic heat capacity (c_{H}) as a function of normalized field $[h \equiv (HM_{\mathrm{F}}t_{\mathrm{F}})/\sigma_{\mathrm{w}}]$ during hysteresis loop sweeps for strong interlayer exchange, $J_{\mathrm{I}} = J_{\mathrm{AF}}$, at (a) low and (b) high temperatures. The heat capacity is normalized to the value at maximum positive field of the hysteresis loop. The magnetization curves are shown in the inset. Peaks in the heat capacity are due to the formation of a partial wall in the antiferromagnet.

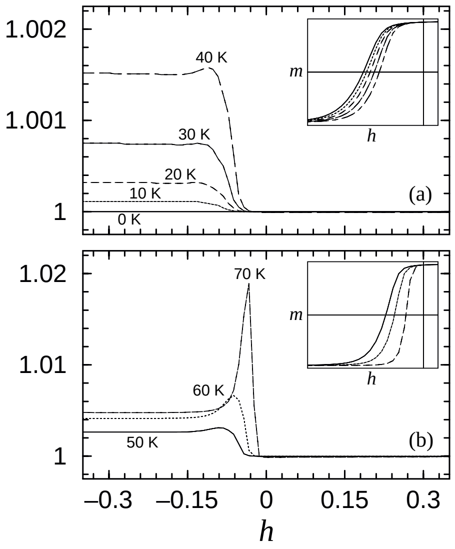

Fig. 2. Normalized magnetic heat capacity (c_H) as a function of normalized field (h) during hysteresis loop sweeps for weak interlayer exchange, $J_I = 0.1J_{AF}$, at (a) low and (b) high temperatures. The magnetization curves are shown in the inset. Features in the heat capacity arise from perturbations in the antiferromagnet spin orientations at the interface.

may be much greater than the interlayer coupling, i.e. $J_I/\sigma_w \ll 1$. It follows from Eq. (4) that domain wall formation is not energetically favorable and the bias field is proportional to the interlayer coupling J_I. This is consistent with the model proposed by Meiklejohn and Bean in which the antiferromagnet spins are assumed to be fixed along the anisotropy axis [1]. The effects of rigid antiferromagnet spins on the heat capacity is shown in Fig. 2, where the interlayer coupling is reduced by a factor of 10. The ferromagnet film was also reduced to 10 ML so that bias fields in a similar range to previous calculations are obtained. Similar peaks in the heat capacity are seen at the bias field but are smaller by an order of magnitude. This is not surprising because deviations in the equilibrium orientations of the antiferromagnet spins are observed to amount only to a few degrees (measured from the easy axis) during reversal.

We have examined the magnetic heat capacity for a ferromagnet exchange coupled to a single domain antiferromagnet. For more realistic structures, the effects of polycrystallinity and lateral domain structure at the interface must be considered. Nevertheless, these results give an indication of what might be observed in an experiment. It is clear that when significant changes to the antiferromagnetic order take place, such as the formation of a partial wall, the peaks in the heat capacity are quite distinct and are large enough to be measurable. For a distribution of antiferromagnet grains at the interface, the relative orientation of the anisotropy axes with the field direction will determine the extent of the partial walls formed. The macroscopic bias field observed then represents an average over the ensemble of partial walls [11], with similar weighted contributions to the heat capacity that may result in a broadened peak. Results for weak interlayer exchange show that contributions to the measured heat capacity from rigid antiferromagnet grains probably will not be measurable as relative changes are only on the order of a percent. For these measurements to be made in an experimental system, it may be necessary to study ferromagnet/antiferromagnet superlattices so that good signal-to-noise ratios for the heat capacity are obtained. We have not performed calculations for a superlattice structure explicitly, but we expect that similar behavior will be observed.

This work was supported by ARO Grant No. DAAG55-98-0294 and the Australian Research Council.

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