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Phase Diagram of CONF-9606136--3

Imperfect Ferromagnetic/Antiferromagnetic-Bilayers

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Abstract:

The phase diagram for ferromagnetic/antiferromagnetic bilayers with imperfect interfaces is calculated, using a Ising spin-1/2 model which is solved numerically in the mean field approximation for finite temperatures. We identify three stable phases: (i) domains in the ferromagnet, (ii) domains in the antiferromagnet and (iii) domain walls near the interfaces with homogeneous order within the layers. Phase transitions between these phases occur as a function of temperature, relative film thicknesses and step density.

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I. Introductions

Ever since antiferromagnetic interlayer coupling was first reported by Grünberg et al. for Fe/Cr/Fe-trilayers [1], this particular material combination has been extensively studied, both experimentally as well as theoretically [2]. But despite the rich literature on Fe/Cr-multilayers, only very few studies focus on the role of the intrinsic antiferromagnetic order in chromium for the magnetic properties of these structures. In general, chromium is regarded as an interlayer material able to mediate a strong exchange coupling and considered to be equivalent to a highly susceptible paramagnetic material [3]. Only recently, several experimental investigations have reported unusual magnetic properties in Fe/Cr-multilayers at low temperatures which have been attributed to the intrinsic antiferromagnetic order of Cr [4,5]. As discussed in these papers, the observed anomalies can be explained by a competition between the intrinsic ferromagnetic (FM) order in Fe and the intrinsic antiferromagnetic (AFM) order in Cr assuming interface imperfections. Recent theoretical investigations of the Fe/Cr-system by Vega et al. have shown that depending on the interface geometry various stable and metastable states can exist [6]. Furthermore, the strong temperature dependence of the experimentally observed anomalies indicates that the different ordering temperatures in Fe ($T_C = 1043$ K) and Cr ($T_N = 311$ K) play a crucial role. The goal of the present paper is to investigate how interface imperfections can modify the phase diagram of FM/AFM systems. This paper is restricted to the case of bilayers only; multilayers will be discussed in a forthcoming publication [7].

II. Model

To study the basic thermodynamic properties of interface coupled bilayer

structures, including the influence of interface defects, we have performed calculations using an Ising spin-1/2 model, which is solved in Mean Field Approximation (MFA). Figure 1a shows the geometric structure considered here: a bilayer with bcc(100) crystal orientation, ferromagnet on top, anti-ferromagnet on the bottom with an interface layer containing 2 atomic steps in between. We furthermore assume translational invariance perpendicular to the plane shown in fig. 1a (z-direction) as well as periodic boundary condition along the x-axis. In MFA, the local magnetization $m_i(T)$ of lattice site i is given by

$$m_i(T) = \tanh\left(\frac{H_i^{\text{eff}}(T)}{k_B T}\right) \quad (1)$$

with k_B and T being the Boltzmann constant and temperature respectively. The effective field $H_i^{\text{eff}}(T)$ at lattice site i is defined by

$$H_i^{\text{eff}}(T) = \frac{1}{4} \cdot \sum_j J_{ij} \cdot m_j(T). \quad (2)$$

As a consequence of the broken translational invariance, the exchange coupling constants J_{ij} are now dependent on the particular lattice site as shown in fig. 1b. We assume next neighbor exchange coupling only with three different exchange coupling constants: J_{AFM} between antiferromagnetic atoms, $J_{\text{FM}} (= -3.354 \cdot J_{\text{AFM}})$ between ferromagnetic atoms, and $J_{\text{I}} (= 1.831 \cdot J_{\text{AFM}})$ as the interface exchange coupling constant between ferro- and antiferromagnetic atoms [8]. The broken translational symmetry now requires that equation (1) and (2) are evaluated for each lattice site i separately. Thus, one has to solve the set of equation (1) and (2) self consistently and simultaneously for all lattice sites i to calculate the temperature dependent magnetic states of the bilayer system. In our numerical calculations, we found numerical self consistency to be sufficient when the induced change $\Delta m_i(T)$ between two

subsequent iteration steps was smaller than 10^{-6} for all i .

III. Results

For a multilayer system with perfect interfaces, the intrinsic FM and AFM order match in the bcc(100)-interface and therefore only one ordered phase exists [9]. In contrast, our calculations including imperfections show that there are 3 stable or metastable phases [10]. Pictures of these three phases are shown in fig. 2 with the gray scale corresponding to the local magnetization. In fig. 2a, we see homogeneous order in the AF material and a domain structure in the FM with the domain walls located at the interface steps (FM-domain state). The state shown in fig. 2b exhibits homogeneous order in the ferromagnetic material and domains in the antiferromagnet (AFM-domain state). In the third case (fig. 2c), we find intrinsic order in the ferromagnet as well as in the antiferromagnet, at least far away from the interface. But close to the interface, we see a domain wall structure which is essentially parallel to the interface and connects both interface steps (Interface domain wall structure). The domain wall is not located exactly at the interface because the exchange coupling in the interface is stronger than in the AFM-material ($|J_I| > |J_{AFM}|$). All three structures shown in fig. 2 are found to be at least metastable in almost the entire temperature range of interest ($0 < T < T_N$ with T_N being the Neel temperature of the AFM bulk system).

To achieve a proper thermodynamic description of the system, we have to compare the free energies of states (a) - (c) in fig. 2. These results are shown in fig. 3. As one can see from the curve on the left side of fig. 3, the FM-domain state has the lowest energy at low temperatures corresponding to a positive value of the free energy difference ΔF . At $T = 0.381 \cdot T_N$, ΔF becomes negative,

i. e. the energy of the interface domain wall state becomes lower than the corresponding FM-domain state energy and the system undergoes a phase transition. This behavior can easily be understood. At low temperatures, both materials have a strong tendency to be intrinsically ordered. Thus, the system accommodates the interfacial frustration by forming short domain walls in the thin FM-layer. With increasing temperature, the AFM shows a stronger reduction of the magnetic order than the FM ($T_C > T_N$) and formation of domain walls in the AFM becomes energetically favorable. Thus, the system exhibits an interface domain wall state for intermediate temperatures. For temperatures in the vicinity of T_N , the magnetic order in the antiferromagnet is dominated by the interface exchange coupling to the ferromagnet. Therefore, it is most favorable for the AFM-layer to exhibit a magnetic structure with coherent order across the interface, i. e. the AFM-domain state has an even lower energy than the interface domain wall state in this temperature range and a second phase transition at $T = 0.955 \cdot T_N$ occurs (see fig. 3).

Figure 4 shows the corresponding phase diagram for a bilayer system as a function of temperature and FM-layer thickness. The AFM-layer thickness and defect density are assumed constant. In agreement with the above discussion, the tendency to form domains in the ferromagnet is reduced with increased FM-layer thickness, because the domain wall energy is proportional to the wall area and therefore proportional to the FM-layer thickness. The phase transition between the interface domain wall state and the AFM-domain state is found to be independent from the FM-layer thickness. In both cases, the domain walls are located within the AFM and therefore, the FM-layer thickness does not play a role. In addition to the phase diagram shown in fig. 4, phase transitions have also been found as a function of AFM-layer thickness

as well as interface defect density.

In conclusion, we have examined the magnetic properties of FM/AFM-bilayers with interfacial defects. We find a complex magnetic phase diagram which depends on the layer thickness, defect density, exchange coupling strength, as well as temperature. Although originally motivated by experimental anomalies found in Fe/Cr-multilayers, our calculations should be applicable to FM/AFM-systems in general.

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and Cr in MFA. Furthermore, we assume $|J_I| > |J_{AFM}|$ in accordance with the results by Vega et al. [6]

- [9] R. W. Wang and D. L. Mills, Phys. Rev. B 46, 11681 (1992)
- [10] For certain starting conditions, our calculations produce additional self consistent solutions, but these states do not represent the free energy minimum at any temperature.

Figure captions:

- Figure 1: Bilayer structure with interface imperfections (bcc(100)-interface orientation): (a) entire unit cell, (b) interface step region; the different exchange coupling constants are indicated by different line types.

- Figure 2: Gray scale images of the possible magnetization states for the bilayer geometry ($T = 0.93 \cdot T_N$): (a) FM-domain state, (b) AFM-domain state, (c) Interface domain wall state. The gray scales correspond to the local magnetization m_i , except for the almost bulklike values ($m_i > 0.95$) in the FM-layer which are shown as open circles.

- Figure 3: Comparison of the free energy F for the magnetization states shown in fig. 2 as a function of temperature. The indices (a), (b), and (c) refer to the classification in fig. 2.

- Figure 4: Phase diagram for a bilayer structure given as a function of the temperature and ferromagnetic layer thickness

Figure 1a

Figure 1b

Figure 2

Figure 3

Figure 4