Magnetic phase diagram of interfacially rough Fe/Cr multilayers

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Neutron-scattering measurements have revealed that the spin-density wave (SDW) inside the Cr spacer of Fe/Cr magnetic multilayers may be either commensurate (C) or incommensurate (I) depending on the temperature and Cr thickness N. We theoretically evaluate the magnetic phase diagram of Fe/Cr multilayers under the assumption that the nodes of the SDW lie at the Cr-Fe interface, as found by recent neutron-scattering measurements. While the C phase is never stable under this assumption, the paramagnetic to I transition temperature $T_N(N)$ takes on a seesaw pattern as the SDW wave vector switches between different allowed values. [S0163-1829(98)07717-0]

Fe/Cr multilayers have been the object of intense scrutiny since the discovery of giant magnetoresistance in 1988.[1] However, neutron-scattering techniques have only recently[2,3] been used to investigate their magnetic-phase diagram. These studies reveal that the spin-density wave[4] (SDW) within the Cr spacer may be either commensurate (C) or incommensurate (I) with the bcc lattice. The C phase is stabilized when the number of monolayers (ML) N inside the Cr spacer is less than 30 or when the temperature exceeds the Néel temperature 310 K of pure Cr. For $N \geqslant 30$ and $T < 310$ K, the I phase is stable. Although other measurements on multilayers[5] and wedges[6] suggest that the SDW is antiferromagnetically coupled with the neighboring Fe layers, the neutron-scattering measurements of Fullerton *et al.*[3] indicate that the nodes of the I SDW lie just inside the Cr-Fe interfaces. We find that a simple model based on the assumption that the SDW nodes lie at the Fe/Cr interfaces has some dramatic consequences. While the C phase is never stable, the paramagnetic (P) to I transition temperature $T_N(N)$ assumes a seesaw pattern as the SDW wave vector undergoes transitions between different allowed values.

Since the magnetic form factor of Cr is strongly peaked at the atomic sites,[4] the SDW within the Cr spacer may be approximated by the form

$$\mathbf{S}(z) = \hat{\mathbf{m}} \alpha_s g (-1)^{2z/a} \cos\left(\frac{2\pi}{a}\delta' z - \theta\right), \qquad (1)$$

where a is the bcc lattice constant, $\hat{\mathbf{m}}$ is the polarization direction, α_s is a constant, θ is an arbitrary phase, $g(T)$ is a temperature-dependent order parameter, and $\alpha_s g(0) = 0.6\mu_B$ for bulk Cr at zero temperature. Adjacent ML of Cr are separated by a distance of $a/2$. Because the hole Fermi surface of dilutely doped Cr alloys is slightly larger than the electron Fermi surface, the nesting wave vectors $Q_\pm = (2\pi/a)(1 \pm \delta)$ differ from $2\pi/a$. For pure Cr, the nesting mismatch δ is approximately[4] 0.05. The SDW ordering wave vectors $Q'_\pm = (2\pi/a)(1 \pm \delta')$ are obtained by minimizing the nesting free energy[7,8] $\Delta F(g,\delta')$ with respect to g and δ'. In terms of δ', the period of the SDW is given by a/δ'. When $\delta' = 0$, this period diverges and the SDW is C. For bulk Cr alloys, $0 \leqslant \delta' < \delta$ so that the SDW ordering wave vectors are always closer to commensuration than the nesting wave vectors. This paper employs the nesting free energy $\Delta F(g,\delta')$ evaluated[8] from a three-band model for the quasiparticle energies.

The material parameters of any Cr alloy enter the model free energy ΔF through the energy mismatch $z_0 = 4\pi\delta v_F/\sqrt{3}a$ (v_F is the Fermi velocity) between the electron and hole Fermi surfaces. Unlike the wave-vector parameter δ', which depends on temperature, both the nesting mismatch δ and the energy mismatch z_0 are constants. If T_N^* is the Néel temperature of a perfectly nested alloy with $\delta = 0$ and $z_0 = 0$, then the bulk free energy ΔF depends only on the ratio z_0/T_N^*. We use the value $z_0/T_N^* = 5$, which is appropriate for slightly strained Cr. At the bulk Néel temperature $T_{N,\mathrm{bulk}}$, this value for the energy mismatch corresponds to a SDW with the wave-vector parameter $\delta' = 0.043$ or with a period of $1/\delta' \approx 23$ lattice constants.

For a microscopically smooth interface, the Cr-Fe interaction is expected to be antiferromagnetic with the form $A\mathbf{S}_{\mathrm{Fe}} \cdot \mathbf{S}(z)$ at interfaces I ($z=1$) and II ($z=N$). Indeed, such an antiferromagnetic interaction was observed in some multilayers[5] and was obtained from first-principles calculations.[9] However, the recent neutron-scattering data by Fullerton, Bader, and Robertson[3] suggests that the SDW nodes actually lie 4–5 ML inside the Cr-Fe interfaces. This may be caused by surface roughness, which frustrates the antiferromagnetic interaction due to steps and interdiffusion at the interfaces. Because the SDW nodes lie near the interfaces, there is no long-range magnetic ordering of the Fe moments within the multilayer.

Assuming that the SDW nodes lie precisely at the interfaces, the wave-vector parameter δ' is restricted to the values $\delta'_n = n/(N-1)$, where $n-1 \geqslant 0$ is the number of nodes inside the spacer. We evaluate n by minimizing the nesting free energy $\Delta F(g,\delta'_n)$ with respect to both g and n. As confirmed experimentally by Fullerton, Bader, and Robertson,[3] this model assumes that the SDW is rigid so that the SDW amplitude and wave vector do not depend on the location z inside the spacer. Since the pair coherence length[10] of the I phase $\xi_0 \sim \hbar v_F/\pi g$ is about 10 Å, the SDW order parameters g and δ' are expected to be modified only within 5 or 6 ML from each interface.

The results of this calculation are provided in Figs. 1 and 2. Because the C SDW does not contain any nodes, the C phase is never stable. So the phase boundary in Fig. 1 separates the I and P phases. The Néel temperature T_N is normalized by the bulk Néel temperature $T_{N,\mathrm{bulk}}$, which is

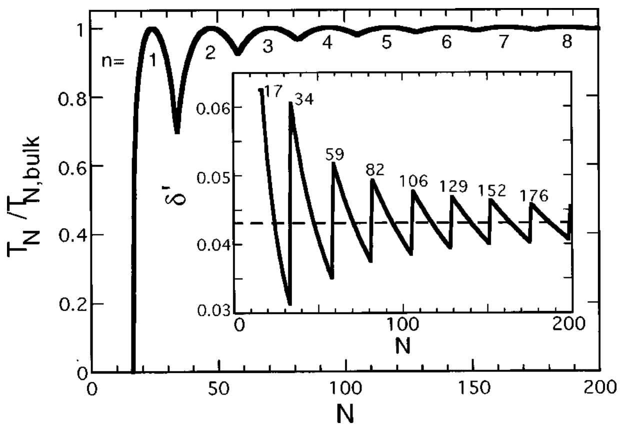

FIG. 1. The Néel temperature vs N with the number of SDW nodes given by $n+1$. The SDW wave-vector parameter δ' is plotted vs N in the inset with specific thicknesses denoted.

evaluated by allowing δ' to be a continuous parameter. For $N<17$ ML, a half-wavelength of the SDW cannot be squeezed into the Cr spacer so the Néel temperature drops to zero. As N increases, the SDW goes through cycles of expansions followed by sudden contractions with the addition of another node to the SDW. This appears as the seesaw pattern in both the Néel temperature and the wave-vector parameter δ'. In the plot of $T_N/T_{N,\mathrm{bulk}}$, we indicate the number $n+1$ of SDW nodes for each portion of the graph. The Néel temperature goes through maxima when δ' passes through its bulk value of 0.043. Notice that both T_N and δ' approach their bulk values as $N \rightarrow \infty$.

Near the discontinuous changes in the SDW wave vector with increasing N, two I SDW's with neighboring values of n have free energies that are almost equal. Just prior to the jump in n, the SDW may transform between different I states with increasing temperature. This behavior is shown in Fig. 2 for $N=106$ (at the top of a seesaw with $n=5$ at T_N) and $N=105$ and 104 (at the bottom of a seesaw with $n=4$ at T_N). The SDW envelopes for $n=4$ and 5 are sketched in the inset to this figure. If $N=105$ or 104, the SDW wave vector shifts from $n=5$ to $n=4$ with increasing temperature. Such

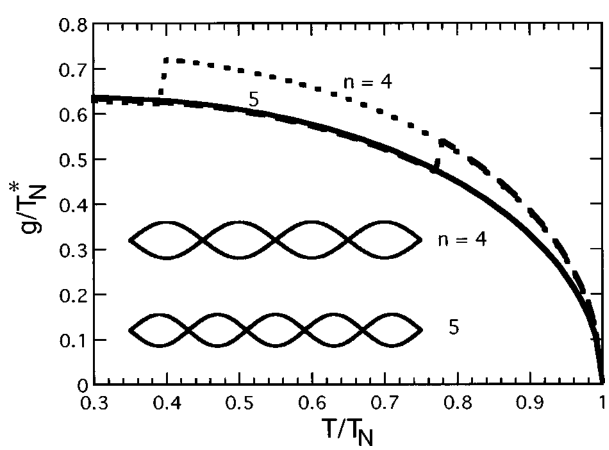

FIG. 2. The SDW order parameter g versus normalized temperature T/T_N for $N=106$ (solid), 105 (long dash), and 104 (short dash). The lower portions of the curves correspond to a wave vector with $n=5$ while the higher portions correspond to $n=4$. The corresponding envelopes of the SDW are sketched in the inset.

transitions do not occur for N smaller than 104 ML. They may be observed either directly through the change in the SDW wave vector or indirectly through the change in neutron-scattering intensity, which is proportional to the square of the SDW amplitude g. So far, no such transition has been observed in Fe/Cr multilayers.

Although the seesaw pattern of $T_N(N)$ is an inevitable consequence of forcing the SDW nodes to lie at the interfaces, the Néel temperature measured by Fullerton and co-workers[11,3] seems to be a smoothly increasing function of spacer thickness N. While their experimental resolution is probably inadequate to discern the predicted oscillations of the wave vector, the oscillation pattern of $T_N(N)$ should be readily observable. Another discrepancy is that the measured critical thickness of 30 ML below which the I phase becomes unstable is much larger than the predicted critical thickness of 17 ML separating the P and I phases.

One possible explanation for the latter discrepancy is that the multilayer interfaces are sufficiently rough to place the SDW nodes inside the multilayer spacer. Surface roughness may be expected to suppress the SDW ordering within a pair coherence length $\xi_0 \approx 6$ ML from the interfaces. As mentioned earlier, Fullerton, Bader, and Robertson[3] find that the SDW nodes lie to the inside of the Cr-Fe interfaces by 4–5 ML, which is suggestively close to the value of ξ_0. If the region within $\xi_0 \approx 6$ ML from the interface is paramagnetic, then the observed critical thickness of 30 ML would correspond to a ''true'' critical thickness of $30 - 12 = 18$ ML, very close to the predicted value of 17 ML. For thicknesses less than 30 ML or temperatures greater than 300 K, the residual antiferromagnetic coupling at the Cr-Fe interfaces may be sufficient to stabilize a C SDW in some regions of the Cr spacer, as found by Fullerton, Bader, and Robertson.[3]

Even if the first 6 ML from the Cr-Fe interface are paramagnetic, however, the Néel temperature would still be expected to show a deep minimum at $34 + 12 = 46$ ML or 66 Å. But our calculation of T_N has assumed that the first and last SDW nodes lie precisely N ML apart. If the SDW nodes can adjust their positions within ξ_0 from each Cr-Fe interface, then the sudden drop in the Néel temperature might be somewhat weakened.

Clearly, surface roughness plays a crucial role in constraining the SDW ordering within Fe/Cr multilayers. By contrast, the smoother interfaces and stronger antiferromagnetic interfacial coupling in Fe/Cr/Fe wedges allow the direct application of a model[12] with antiferromagnetic coupling at the Cr-Fe interfaces. In agreement with this model, the I-C transition temperature is elevated far above the bulk Néel temperature of pure Cr. Other consequences of this model are discussed elsewhere.[12]

To summarize, we have developed a model with the SDW nodes at the Cr-Fe interfaces. Whereas this model explains some features of Fe/Cr multilayers, a second model with SDW antinodes at the Cr-Fe interfaces may be more appropriate for Fe/Cr/Fe wedges.

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