ORNL/CP-99130

CONF-981101--

MMM '98, November 9-12, 1998, Miami, FL

HELICAL SPIN-DENSITY WAVE IN FE/CR TRILAYERS WITH PERFECT INTERFACES

R. S. Fishman

SOLID STATE DIVISION
OAK RIDGE NATIONAL LABORATORY
Managed by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
Under
Contract No. DE-AC05-96OR22464
With the
U. S. DEPARTMENT OF ENERGY
OAK RIDGE, TENNESSEE

July 1998

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Helical Spin-Density Waves in Fe/Cr Trilayers with Perfect Interfaces

R.S. Fishman

Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6032

Abstract

Despite the presence of only collinear, commensurate (C) and incommensurate (I) spin-density waves (SDW's) in bulk Cr, the interfacial steps in Fe/Cr multilayers are now believed to stabilize a helical (H) SDW within the Cr spacer. Yet H SDW's were first predicted in an Fe/Cr trilayer with perfect interfaces when the orientation of the Fe moments does not favor C ordering: if the number of Cr monolayers is even (odd) and the Fe moments are pointing in the same (opposite) direction, then a C SDW does not gain any coupling energy. Under these circumstances, a simple model verifies that H ordering is indeed favored over I ordering provided that the Fermi surface mismatch is sufficiently small or the temperature sufficiently high.

PACS numbers: 75.30.Fv, 75.30.Ds, 75.70.Cn

Recent neutron-scattering measurements [1] have led to the surprising result that helical (H) spin-density waves (SDW's) are present in Fe/Cr multilayers. It has been well-established for many years [2] that H SDW's are not stable in bulk Cr alloys, where only collinear, commensurate (C) and incommensurate (I) SDW's appear. For example, pure Cr enters an I SDW state below its Néel temperature of 310 K while CrMn with a Mn concentration above 0.3% enters a C SDW state. Prior to the recent neutron-scattering measurements, Slonczeski [3] predicted that steps at the interfaces of Fe/Cr multilayers would stabilize a H SDW. But even before Slonczewski's work, Stoeffler and Gautier [4] argued that under the right conditions, a H SDW would be stable in an Fe/Cr/Fe trilayer with perfect interfaces. In this paper, we use a simple model to verify that a H SDW is indeed stable in a perfect Fe/Cr trilayer for the right Fe orientations, temperature, and material parameters.

Measurements on Fe/Cr wedges [5] and first-principles calculations [6] have found that Fe and Cr moments are antiparallel at a perfect Fe-Cr interface. Take the coupling energy at each such interface to be $A\mathbf{S}_{\rm Fe} \cdot \mathbf{S}(z)$, where $A > 0$ is the antiferromagnetic coupling constant, $\mathbf{S}_{\rm Fe}$ is the Fe moment, and $\mathbf{S}(z)$ is the Cr moment in a trilayer with interfaces normal to the z axis. Then for an even (odd) number N of Cr monolayers, coupling energy would be gained by a C SDW when the Fe moments are antiparallel (parallel). Indeed, the properties of Fe/Cr wedges, where the top Fe moments are unconstrained, may be predicted from a simple model [7] which adds the coupling energy $E_{\rm coup}$ at the two interfaces to the bulk free energy of the Cr spacer. As predicted by this model and implied by the NIST measurements [5], a C SDW obtains a lower free energy than an I SDW for small N or high temperatures - precisely the conditions for the interfacial coupling energy to dominate over the bulk free energy of the Cr spacer.

But if the top and bottom Fe moments are constrained by an external field to be parallel (antiparallel) for even (odd) N, then the coupling energy gained by a C SDW at one interface would be lost at the other. Under these circumstances, a H SDW may be more stable than either a C or I SDW. All three possible spin configurations [8] are sketched in Fig.1 for $N = 10$ and parallel Fe moments. Stoeffler and Gautier [4] conjectured that, in order for

the SDW to avoid forming nodes, a H SDW may be favored over an I SDW under these circumstances. However, pure Cr naturally enters an I state with 27 ML's between nodes. So more work is needed to find the appropriate conditions for the formation of a H SDW.

All possible SDW states of Cr alloys are produced by the nearly perfect nesting [9,10] of electron and hole Fermi surfaces which are roughly octahedral in shape. The hole Fermi surface is slightly larger than the electron Fermi surface. Consequently, the nesting wavevectors $Q_\pm = (G/2)(1 \pm \delta)$ differ from $G/2$, where $G = 4\pi/a$ is the smallest reciprocal lattice vector for a bcc lattice with constant a. But to acheive the lowest overall free energy [11], the ordering wavevectors of the SDW $Q'_\pm = (G/2)(1 \pm \delta')$ lie slightly closer to $G/2$ than the nesting wavevectors with $0 \leq \delta' < \delta$.

If the Bloch wavefunctions are approximated by delta functions at every lattice site and $\mathbf{Q}'$ is taken along the z axis, then I and H SDW's may be written as

$$\mathbf{S}_{\rm I}(z) = \hat{m}\alpha_s g(-1)^{2z/a}\cos\Big(\frac{2\pi}{a}\delta' z - \theta\Big), \tag{1}$$

$$\mathbf{S}_{\rm H}(z) = \alpha_s g(-1)^{2z/a}\Big\{\hat{x}\cos\Big(\frac{2\pi}{a}\delta' z - \theta\Big) + \hat{y}\sin\Big(\frac{2\pi}{a}\delta' z - \theta\Big)\Big\}, \tag{2}$$

where α_s is a constant, $\hat{m}$ is the polarization of the I SDW, θ is an arbitrary phase, and $g(T)$ is the order parameter. At low temperatures in bulk Cr [2], $\alpha_s g(0) \approx 0.6\mu_{\rm B}$. For an I SDW, the distance between nodes is $1/\delta'$ ML's. For a H SDW, this is the distance for a π twist. Keep in mind that a H SDW can be smoothy generated from a C SDW by simply twisting one end. But an I SDW cannot be smoothly transformed into a C SDW.

By doping pure Cr with Mn or Fe, both δ and δ' are diminished. Above some critical impurity concentration, which depends on temperature, $\delta' \to 0$ and the SDW becomes commensurate. In this limit, Eqs.(1) and (2) reduce to C SDW's with the same amplitude [12].

The energy mismatch between the electron and hole Fermi surfaces is given by $z_0 = 4\pi\delta v_F/\sqrt{3}a$, where v_F is the Fermi velocity. We also introduce the Néel temperature $T_{\rm N}^* \approx 80$ meV of a perfectly nested alloy with $\delta = 0$ and $z_0 = 0$. For pure Cr, $z_0 \approx 5T_{\rm N}^*$. If the Fermi

surfaces are modeled as octagons, then the change in the bulk SDW free energies below T_N may be evaluated within the random-phase approximation [11,13] and are denoted by $\Delta F_I(g, \delta', T, z_0)$ and $\Delta F_H(g, \delta', T, z_0)$. When $\delta' = 0$ both free energies reduce to the free energy of a C SDW.

Adding the coupling energy at the two interfaces to the free energy of a Cr spacer with thickness $L = (N-1)a/2$, we obtain the free energy of an Fe/Cr trilayer per cross sectional area a^2:

$$E_{I,H} = A\Big(\mathbf{S}^I_{Fe} \cdot \mathbf{S}_{I,H}(0) + \mathbf{S}^{II}_{Fe} \cdot \mathbf{S}_{I,H}(L)\Big) + \Delta F_{I,H} a^2 L. \tag{3}$$

This assumes the SDW to be rigid, with the same amplitude and wavevector throughout the spacer. To determine the lowest-energy configuration, we minimize this free energy with respect to g, δ', and θ for both the I and H phases. It is straightforward to show that the energies E_I and E_H only depend on the single dimensionless coupling constant $\gamma = A\alpha_s S_{Fe}/(V/N)\rho_{eh}/T_N^*$, where ρ_{eh} is the density-of-states of the nested Fermi surfaces. Since the interfacial coupling is linear in the SDW amplitude, it always induces some SDW ordering within the spacer and the paramagnetic phase is never stable.

For any nonzero γ, the interfacial coupling applies a torque which transforms a C SDW into a H SDW. In the H phase, the angle between neighboring Fe and Cr moments approaches 180 degrees for large γ or high temperatures, when the interfacial coupling dominates over the spacer's free energy. As $\gamma \to 0$, the H SDW evolves into a C SDW with moments rotated 90 degrees away from the Fe moments.

Since the C SDW is unstable for $\gamma > 0$, the phase boundary plotted in Fig.2 for $N \to \infty$ separates the H and I SDW phases. The dashed curve in Fig.2 denotes the paramagnetic phase boundary of bulk Cr while the solid dot denotes the bulk triple point. To the right of this point, a bulk Cr alloy enters the I phase; to the left, it enters the C phase. Recall that z_0 can be controlled by doping: it is increased by doping with V and decreased by doping with Mn or Fe.

When $z_0/T_N^* > 3.35$, the IH phase boundary for large N lies above the bulk Néel tempera-

ture. Under this condition and for fixed Fe moments that frustrate C ordering, $T_{\rm IH}(N \to \infty)$ is implicitly given by the relation

$$\sum_{n=0}^{\infty} \mathrm{Re}\left\{ \frac{1}{(n + 1/2 + i z_0/8\pi T_{\rm IH})^m} \right\} = 0, \qquad (4)$$

with $m = 5$. By contrast, the IC phase transition temperature $T_{\rm IC}(N \to \infty)$ for perfect interfaces and free Fe moments that can choose the lowest-energy orientation is given by the same condition with $m = 3$ [7]. For a fixed z_0, $T_{\rm IH}$ is always larger than $T_{\rm IC}$. Below the bulk Néel temperature, the IH phase boundary is solved by expanding the energies $E_{\rm I}$ and $E_{\rm H}$ in powers of δ'. Along the IH phase boundary for large N, both the I and H SDW's have a half-period of $1/\delta' = (N-1)$ ML's. Therefore, the I SDW contains only a single node while the H SDW undergoes a single π twist between $z = 0$ and $z = L$. In the limit of large N, these phase boundaries are independent of the coupling constant γ. As indicated by Fig.2, the H phase is re-entrant in a narrow range of $z_0/T_{\rm N}^*$ between 3.19 and 3.35. When $z_0/T_{\rm N}^* < 3.19$, the I phase is never stable and the trilayer with parallel (even N) or antiparallel (odd N) moments always supports the H phase.

With decreasing thickness or increasing γ, the interfacial coupling grows and the IH phase boundary shifts to favor the H phase. For example, when $\gamma = 2$ and $z_0/T_{\rm N}^* = 5$, $T_{\rm IH}/T_{\rm N}^*$ shrinks from 3.17 to 1.89 as N decreases from ∞ to 10.

So we have verified the conjecture of Stoeffler and Gautier [4] that the H SDW phase may be stabilized for perfect interfaces, provided that the Fe moments frustrate C ordering. But in contrast to those authors, we find that the H phase is stable only over a restricted range of temperatures and thicknesses. As the mismatch z_0 between the Fermi surfaces increases, the bulk free energy of an I SDW becomes progressively lower than that of the C and H SDW's. Consequently, the range of stability of the H phase is more restricted for large z_0. When z_0 is sufficiently small (below $3.19 T_{\rm N}^*$), the H phase is stable for any temperature, thickness, and interfacial coupling $\gamma > 0$.

The stability of a H SDW may be tested in an Fe/CrMn trilayer with nearly atomically flat Fe whiskers. When the Fe moments frustrate C ordering, the out-of-plane Cr moments

produced by a H SDW may be measured either electromagnetically or through the magnetic response of an Fe film wrapped around the trilayer.

The author would like to thank Drs. Sam Liu, Lee Robertson, Andreas Schreyer, and Zhupei Shi for helpful discussions. This research was supported by Oak Ridge National Laboratory managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under Contract No. DE-AC05-96OR22464.

REFERENCES

[1] A. Schreyer, J.F. Ankner, Th. Zeidler, H. Zabel, C.F. Majkrzak, M. Schäfer, and P. Grünberg, Euro. Phys. Lett. **32**, 595 (1995); A. Schreyer, C.F. Majkrzak, Th. Zeidler, T. Schmitte, P. Bödeker, K. Theis-Bröhl, A. Abromeit, J.A. Dura, and T. Watanabe, Phys. Rev. Lett. **79**, 4914 (1997).

[2] E. Fawcett, Rev. Mod. Phys. **60**, 209 (1988); E. Fawcett, H.L. Alberts, V. Yu. Galkin, D.R. Noakes, and J.V. Yakhmi, Rev. Mod. Phys. **66**, 25 (1994).

[3] J.C. Slonczewski, J. Magn. Mang. Matt. **150**, 13 (1995).

[4] D. Stoeffler and F. Gautier, J. Magn. Magn. Matt. **121**, 259 (1993).

[5] J. Unguris, R.J. Celotta, and D.T. Pierce, Phys. Rev. Lett. **67**, 140 (1991); **69**, 1125 (1992).

[6] S. Mirbt, A.M.N. Niklasson, Bi. Johannson, and H.L. Skriver, Phys. Rev. B **54**, 6382 (1996).

[7] Z.P. Shi and R.S. Fishman, Phys. Rev. Lett. **78**, 1351 (1997); R.S. Fishman and Z.P. Shi, J. Phys. C **10**, L277 (1998).

[8] The I SDW sketched in Fig.1 is transverse with moments perpindicular to the ordering wavevector. A longitudinal I SDW with moments in the z direction is also possible and appears in pure Cr below 120 K.

[9] W.M. Lomer, Proc. Phys. Soc. London **80**, 489 (1962).

[10] P.A. Fedders and P.C. Martin, Phys. Rev. **143**, 8245 (1966).

[11] R.S. Fishman and S.H. Liu, Phys. Rev. B **48**, 3820 (1993).

[12] In bulk Cr, the phase θ of the C SDW is constrained so that the *rms* moments of the I and C SDW's are the same for the same order parameter g. But the energy of the trilayer is minimized with respect to the phase θ so that the *amplitudes* of the C, H,

and I SDW's are now identical. This requires a charge modulation of the trilayer with some electrons transferring from the Fe layers to the Cr spacer.

[13] R.S. Fishman, (unpublished).

Figure Captions

Fig. 1 A sketch of C, H, and I SDW's coupling parallel Fe moments for $N = 10$.

Fig. 2 The IH phase boundary (solid) for an Fe/Cr trilayer with energy mismatch z_0 and $N \to \infty$. For bulk Cr, the Néel temperature is given by the dashed curve, with the triple point labeled by a solid circle.

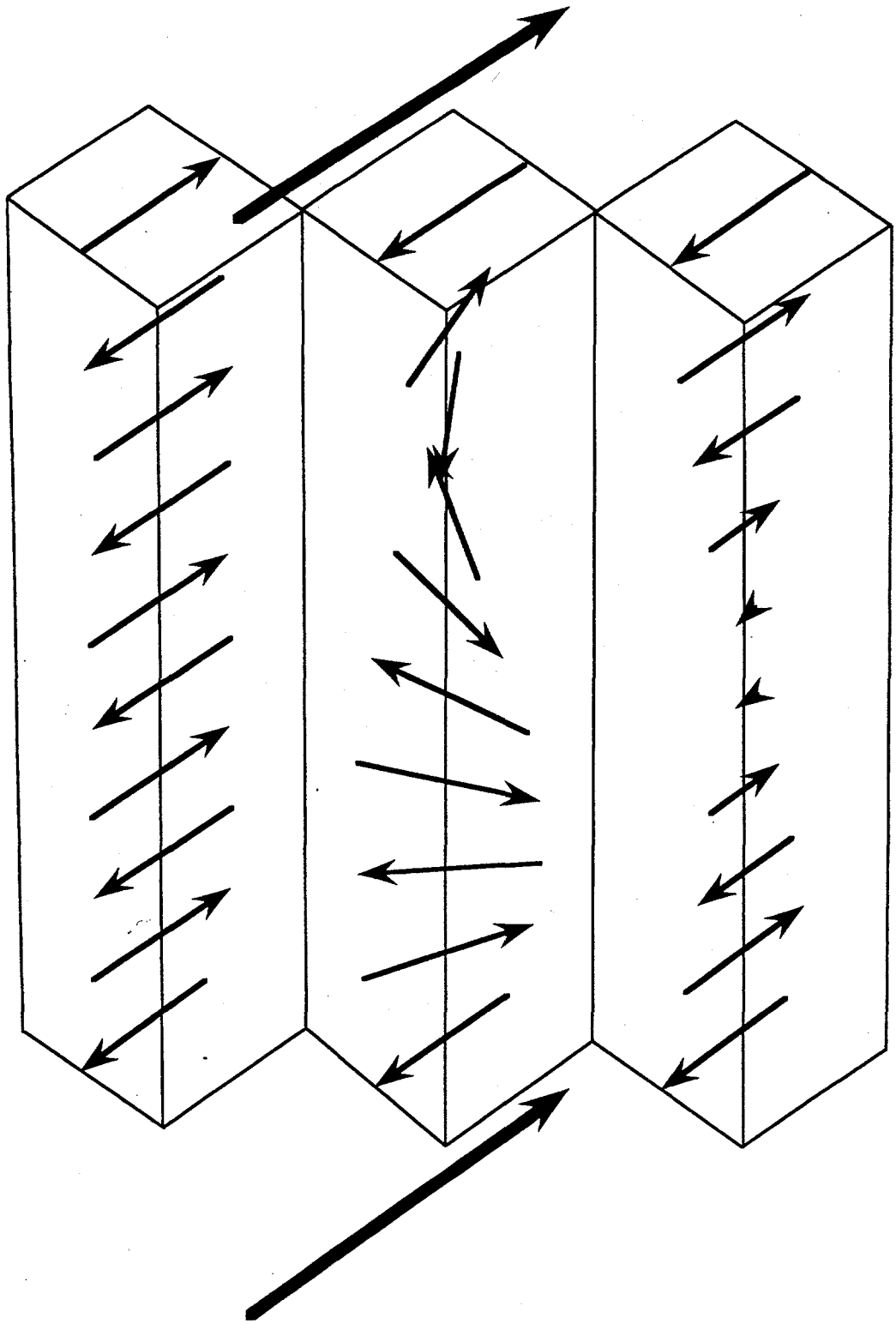

Fig. 1

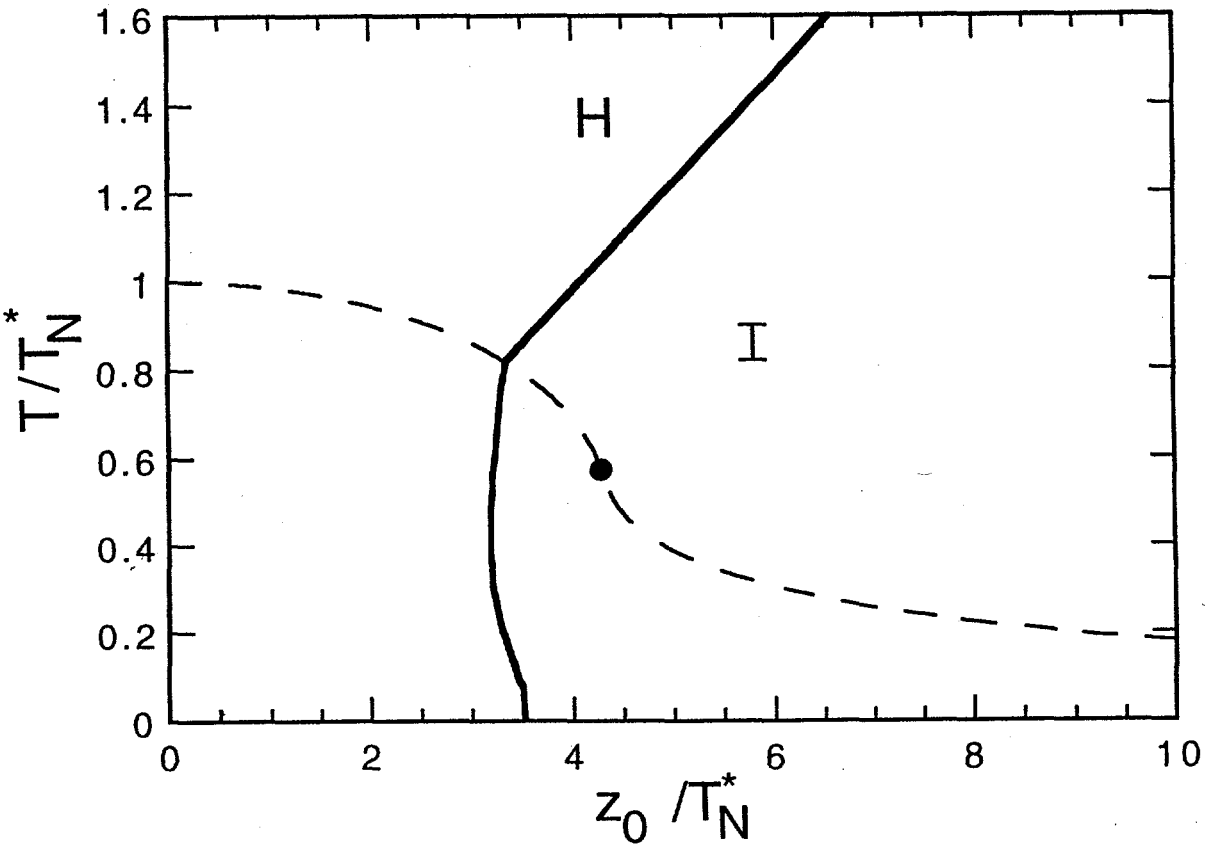

Fig. 2