

Susceptibility of dilutely doped CrFe alloys

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys.: Condens. Matter 10 6347

(<http://iopscience.iop.org/0953-8984/10/28/015>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.209

The article was downloaded on 14/05/2010 at 16:36

Please note that [terms and conditions apply](#).

Susceptibility of dilutely doped CrFe alloys

R S Fishman[†], V Yu Galkin^{‡§} and W A Ortiz[‡]

[†] Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6032, USA

[‡] Departamento de Física, Universidade Federal de São Carlos, Brazil

[§] I P Bardin Central Research Institute for Ferrous Metallurgy, 2 Baumanskaya 9/23, Moscow, 107055 Russia

Received 18 March 1998

Abstract. For low dopant concentrations, Fe is the only impurity atom which exhibits Pauli paramagnetism below the Néel temperature T_N of a Cr host. A series of measurements on $\text{Cr}_{1-x}\text{Fe}_x$ and $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys reveal that the magnetization M is sensitive to the amplitude of the spin-density wave (SDW) below T_N . The Fe moment also depends on the period of the SDW and is about 6% larger in the incommensurate than in the commensurate SDW state. Surprisingly, the differential susceptibility dM/dH peaks at the field H_p , which is about 5 kOe for low temperatures and small V concentrations. While H_p increases with the temperature, it decreases with the V and Fe concentrations. These observations may be explained by making the radical assumption that the rigidity of the Fe moment is broken by its interaction with the SDW. Whereas part of the Fe moment is bound to the SDW by the nesting free energy, the remainder experiences a weak effective field exerted by the surrounding SDW and by the ferromagnetically coupled, nearest-neighbour pairs of Fe atoms. The peak in dM/dH occurs when the external field H overcomes the antiferromagnetic field experienced by the single Fe atoms. This model explains the temperature and doping dependence of H_p , as well as the difference between the Fe moments in the commensurate and incommensurate SDW hosts.

1. Introduction

Due to the close relationship between their metallic and magnetic properties, transition-metal magnets continue to hold great interest for materials scientists. While Fe is often considered the prototypical transition-metal ferromagnet, Cr remains the prototypical transition-metal antiferromagnet. Although the magnetic moments of both Fe and Cr metals are generated by electron–hole pairs in the 3d band, their magnetic properties are otherwise quite different. One of the most intriguing and important problems in the field of itinerant magnetism is the effect on the Fe moment of its environment [1–4]. In this paper, we study the change in the Fe moment caused by the spin-density wave (SDW) of a Cr host. Remarkably, Fe is the only known impurity atom to exhibit Pauli paramagnetism [5] below the Néel temperature T_N of a dilutely doped Cr alloy [6, 7]. Depending on the dopant and impurity concentration, the SDW of Cr alloys may be either commensurate (C) or incommensurate (I) with the bcc lattice. Through a series of susceptibility measurements on two different classes of binary and ternary alloys, we study the effect of the SDW amplitude and phase on the Fe moment and susceptibility. We also present a simple phenomenological model which can explain those measurements.

The magnetic properties of Cr sensitively depend on the similar shape but slightly different size [8] of its electron ‘jack’ and hole ‘octahedron.’ These electron and hole

Fermi surfaces are imperfectly nested by the wavevectors $Q_{\pm} = (G/2)(1 \pm \delta)$, where G is a reciprocal-lattice vector with magnitude $4\pi/a$. To minimize the nesting free energy on both sides of the two Fermi surfaces [9], the actual wavevectors of the SDW at $Q'_{\pm} = (G/2)(1 \pm \delta')$ lie somewhat closer to $G/2$ with $0 \leq \delta' < \delta$. For pure Cr, $\delta' \approx 0.037$ [6] so the SDW is incommensurate with the bcc lattice and has a period of about $1/\delta' \approx 27$ lattice constants. Because the hole ‘octahedron’ is slightly larger than the electron ‘jack’, alloying Cr with impurities which donate electrons to the 3d band improves the nesting and decreases both δ and δ' . At some impurity concentration, $\delta' \rightarrow 0$ and the SDW becomes commensurate with the lattice. While both Fe and Mn act as electron donors and decrease δ' , V acts as an electron acceptor and increases δ' . For some ternary CrFeV and CrFeMn alloys [10, 11], the SDW undergoes an I-to-C or a C-to-I transition as a function of temperature. These alloys prove to be very useful for examining the effect of the SDW phase on the Fe moment.

Since the nesting wavevectors Q_{\pm} may lie along any of the three crystal axes, there are three sets of possible ordering wavevectors Q'_{\pm} . For pure Cr below its Néel temperature of 312 K but above 122 K, the ISDW is transversely polarized with spin polarization \hat{n} perpendicular to Q'_{\pm} . So two polarization domains correspond to each set of SDW wavevectors Q'_{\pm} . In the longitudinally polarized phase below 122 K, $\hat{n} \parallel Q'_{\pm}$ in three distinct domains. A single Q -state with Q'_{\pm} along the z -axis can be selected [14] by cooling through the Néel transition in a magnetic field $H = H\hat{z}$ with H greater than roughly 20 kOe or 2 T, depending on sample quality. So long as the field does not exceed 160 kOe, the SDW will remain in this Q -state below the spin-flip transition at 122 K. For a C alloy, the three Q -states are replaced [15] by three domains of the spin polarization \hat{n} .

Though both Mn and Fe act as electron donors in a Cr host, Mn impurities are much more effective at raising the chemical potential and lowering the incommensurability parameter δ' . While the triple point of $Cr_{1-x}Fe_x$ alloys lies at an Fe concentration of 2.4%, the triple point of $Cr_{1-x}Mn_x$ alloys lies at the much smaller Mn concentration of 0.3%. This is usually interpreted [7] to mean that Mn donates its extra electron to the conduction band whereas Fe retains most of its extra two electrons within a local moment.

A great deal of the previous work [16–21] on binary $Cr_{1-x}Fe_x$ alloys has concentrated on the behaviour of the nearest-neighbour pairs of Fe moments. If N Fe atoms are randomly distributed with concentration x , then the number of Fe atoms forming singles and pairs is given by [22]

$$\begin{aligned} N_1 &= N(1-x)^8 \\ N_2 &= 8Nx(1-x)^{14}. \end{aligned} \quad (1)$$

So for an Fe concentration of 2.7%, $N_1/N = 80.3\%$ of the Fe atoms are single, $N_2/N = 14.7\%$ are paired, and the rest form triplets and higher-order clusters. Susceptibility measurements [16–18] on heavily doped CrFe alloys ($x > 2.4\%$) indicate that the Fe atoms within each pair are strongly ferromagnetically coupled to each other. Consequently, the Fe pairs are only weakly affected by the SDW in the I phase [17] and not at all in the C phase. In contrast to the N_1 single Fe atoms, the $N_2/2$ Fe pairs are easily polarized by a magnetic field and behave like superparamagnetic entities [20].

The notion that the single Fe moment depends on the phase of the SDW was first introduced by Friedel and Hedman [17], who tried to explain the magnetic properties [16] of $(Cr-3\%Fe)_{1-x}V_x$ alloys. Friedel and Hedman proposed that the Fe moments are frozen in the C phase, resulting in a constant temperature-independent susceptibility and a vanishing Curie–Weiss (CW) constant. In the I phase, the Fe moments were expected to distort the SDW such that each Fe atom lies close to a maximum of the spin density. The single Fe

moments within the transversely polarized ISDW state were presumably free to rotate in the plane perpendicular to the SDW wavevectors Q'_{\pm} . Within the longitudinally polarized ISDW state, the spins were allowed to flip parallel to the wavevectors Q'_{\pm} . Consequently, the CW constants in the transversely and longitudinally polarized ISDW phases were predicted to be *higher* than in the paramagnetic (P) regime.

However, these ideas were motivated by measurements [16] which were not sensitive to whether the SDW was in its C or I phase. The more precise measurements described below indicate that the C and I values $\mu_A^{(C)}$ and $\mu_A^{(I)}$ of the Fe moment are only slightly different and that both are substantially smaller than the P value μ_P . Because doping with Fe quickly suppresses the longitudinally polarized phase, no experiments have yet distinguished the Fe moments in the transversely and longitudinally polarized ISDW states. Nevertheless, Friedel and Hedman were correct that the Fe moment depends on the SDW phase of the host.

Recently, Galkin *et al* [23] reported measurements on the class of $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys. For $x = 0$, the P Fe moment μ_P was found to be about $3.03 \mu_B$. Whereas the P moment $\mu_P(x)$ above T_N is a weak function of x [3, 4], the smaller moment $\mu_A(x)$ below T_N strongly depends on the V concentration. With increasing x , the Néel temperature and SDW amplitude are monotonically suppressed. About 2.5% V eliminates the SDW altogether. In binary Cr-2.7%Fe, μ_A is about half the size of μ_P . Doping with V diminishes the difference $\Delta\mu(x) = \mu_P(x) - \mu_A(x)$ between these two moments and $\Delta\mu(x)$ vanishes as x approaches 2.5%. Consequently, the reduction in the Fe moment below T_N must be attributed to its interaction with the SDW. Although $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys exhibit both C and I phases over wide ranges of x , Galkin *et al* did not consider the effect of the SDW phase on the Fe moment.

As first reported by us elsewhere [24], the Fe moment is about 6% larger in the I than in the C SDW phase. To exclude the effect of temperature on the SDW amplitude, we measured the Fe moment in two complementary alloys, $(\text{Cr}-2.7\%\text{Fe})_{99.71}\text{V}_{0.29}$ and $(\text{Cr}-1.5\%\text{Fe})_{99.79}\text{Mn}_{0.21}$, where the order of the C and I phases is reversed. Comparing the susceptibilities of these two alloys allowed us to unambiguously determine the effect of the SDW phase on the Fe moment.

In this paper, we report additional measurements on the $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloy system as well as new measurements on $\text{Cr}_{1-x}\text{Fe}_x$ alloys. Surprisingly [23], the differential susceptibility dM/dH peaks at a field H_p . For small temperatures and low V concentrations, H_p is about 5 kOe. The position of the peak increases with temperature and decreases with the V and Fe concentrations.

For the small Fe concentrations (<4%) used in this study, magnetic remanence does not occur [5] in binary CrFe alloys and so the observed non-linear behaviour cannot be explained by the formation of a spin-glass. However, the observed behaviour can be explained by making the radical assumption that the integrity of the Fe moment is broken by its interaction with the SDW. One part of the Fe moment is assumed to be strongly bound to the SDW with the same value as the missing Cr moment. The remainder experiences a weak effective field produced by the surrounding SDW and by the ferromagnetically coupled, nearest-neighbour Fe pairs. Only the second, unbound portion of the Fe moment responds to a small external field and contributes to the CW paramagnetism below T_N . To our knowledge, this is the first instance where the Fe moment does not behave as a single rigid entity.

Within this model, the peak in the differential susceptibility occurs when the external field $\mathbf{H} = H\hat{z}$ overcomes the weak antiferromagnetic field exerted by the SDW on the single Fe moments. Below H_p , the Fe moments on the \downarrow Cr sublattice experience a net effective field in the $-\hat{z}$ -direction. Above H_p , all of the Fe moments experience a net field

in the $+\hat{z}$ -direction. So the magnetization $M(T, H)$ increases rapidly in the vicinity of the peak field H_p . With higher V concentrations, the exchange field exerted by the SDW becomes weaker and H_p becomes smaller. The temperature dependence of H_p is caused by the ferromagnetic coupling between the single moments and the easily polarized pairs. As the temperature is raised, the Fe pairs become more difficult to polarize and H_p increases. As the Fe concentration grows, the effective field is strengthened by the nearest-neighbour pairs and H_p decreases. At least qualitatively, therefore, this model can explain the observed behaviour of the magnetic susceptibility in all of the Cr alloys studied.

This paper divides into four main sections. In section 2, we present the results of our susceptibility measurements. Section 3 describes our phenomenological model and its consequences. Finally, section 4 contains a discussion and a conclusion. We also propose an experiment to test the model developed in this paper.

2. Susceptibility measurements

Galkin and Fawcett [25] have previously described the preparation of the CrFe, CrFeV and CrFeMn samples. Each sample was then characterized by measuring the temperature dependence of its resistivity and thermal expansion. Magnetization measurements were performed with a SQUID magnetometer (MPMS-5S, Quantum Design) over the temperature range $2 \leq T \leq 400$ K in magnetic fields up to 50 kOe.

2.1. Low-field susceptibility

Fits to the low-field susceptibility $\chi = M(T, H)/H$ with $H = 10$ kOe were made using the expression

$$\chi = \chi_0 + \frac{C}{T - \Theta} \quad (2)$$

with parameters χ_0 , C and Θ . Here, χ_0 is the temperature-independent susceptibility of the Cr host, which is affected by doping through changes in the chemical potential. The Fe moment μ_A is extracted from the Curie constant $C = N\mu_A^2/3Vk_B$, where V is the volume of the alloy. In general, these expressions oversimplify the susceptibility, which contains distinct contributions from the single and paired Fe atoms. But for the relatively small Fe concentrations studied here, the single Fe moments dominate the susceptibility and equation (2) should be adequate.

To determine the difference between the C and I moments, we analysed the susceptibility of the alloys (Cr-2.7%Fe)_{99.71}V_{0.29} and (Cr-1.5%Fe)_{99.79}Mn_{0.21}. Thermal expansion and resistivity measurements [10, 11] were previously used to obtain the magnetic phase diagrams of these two alloys. While the CrFeV alloy [11] exhibits an I-to-C transition with decreasing temperature, the CrFeMn alloy [10] exhibits a C-to-I transition. For both alloys, the C and I phases extend over fairly wide temperature ranges, which facilitates the fits to equation (2).

The absence of anomalies in the magnetic susceptibilities indicates that the IC and CI phase transitions are either second order or weakly first order. Independent fits of $1/(\chi - \chi_0)$ versus temperature were performed in the C and I regimes of both alloys and presented in reference [24]. For both alloys, good results are obtained by assuming that χ_0 is the same in the C and I phases. The moments extracted from the fits are $\mu_A^{(C)} = 2.46\mu_B$ and $\mu_A^{(I)} = 2.62\mu_B$ for the CrFeV alloy and $\mu_A^{(C)} = 1.42\mu_B$ and $\mu_A^{(I)} = 1.51\mu_B$ for the CrFeMn alloy. In both cases, the Fe moment is about 6% larger in the ISDW host. For the CrFeV

sample, $\mu_A^{(C)}$ and $\mu_A^{(I)}$ are quite a bit larger than the moment $\mu_A = 2.1\mu_B$ obtained by fitting the susceptibility [23] over the whole range of temperatures from 50 to 200 K. However, the ratio $\mu_A^{(I)}/\mu_A^{(C)} \approx 1.06$ is more reliably given by these fits than the separate moments $\mu_A^{(C)}$ and $\mu_A^{(I)}$ of the C and I phases. A small decrease in χ_0 would lower both Curie constants while hardly changing the quality of the fits.

Antiferromagnetic interactions with negative Curie temperatures Θ were obtained for each alloy. In the C phase of both alloys, $\Theta \approx -8$ K. In their I phases, $\Theta \approx -26$ K. Such antiferromagnet interactions are consistently obtained [7] when equation (2) is used to fit the susceptibility of dilutely doped CrFe alloys.

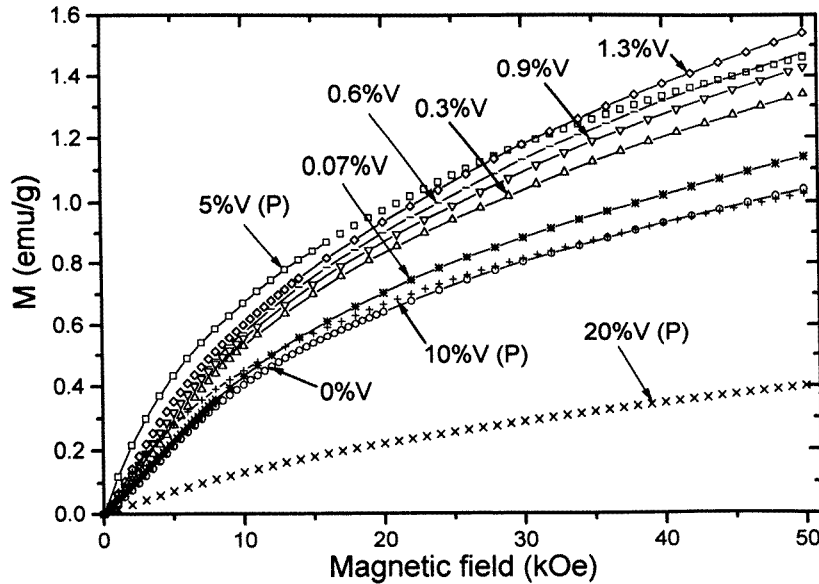


Figure 1. The magnetization M versus field H for $(\text{Cr}-2.7\% \text{Fe})_{1-x}\text{V}_x$ for several different values of x at $T = 2$ K. Paramagnetic alloys are denoted by P.

2.2. Nonlinear field dependence and the peak in dM/dH

Measurements on $(\text{Cr}-2.7\% \text{Fe})_{1-x}\text{V}_x$ alloys at $T = 2$ K are reported in figures 1 and 2. For a fixed magnetic field, the magnetization first increases with the V concentration within the SDW states ($x < 2.5\%$) and then decreases with x when the alloy is paramagnetic ($x > 2.5\%$). The paramagnetic behaviour is caused by the suppression of the free Fe moment [3, 4] as the number of V neighbours increases. At low temperatures, the magnetization of all $(\text{Cr}-2.7\% \text{Fe})_{1-x}\text{V}_x$ alloys plotted in figure 1 is a non-linear function of the magnetic field. As interpreted by Babic *et al* [20], the rapid rise in the magnetization at low fields is caused by the easily polarized pairs and clusters of Fe moments. The remainder of the magnetization for $x < 2.5\%$ increases almost linearly with the magnetic field through 50 kOe. Babic *et al* [20] observed the magnetization to saturate only at very high magnetic fields greater than 330 kOe. They attributed the linear increase in the magnetization and the slow saturation to the single Fe moments, which are tightly constrained by the SDW. In the next section, we provide a somewhat different interpretation of the field dependence of the magnetization.

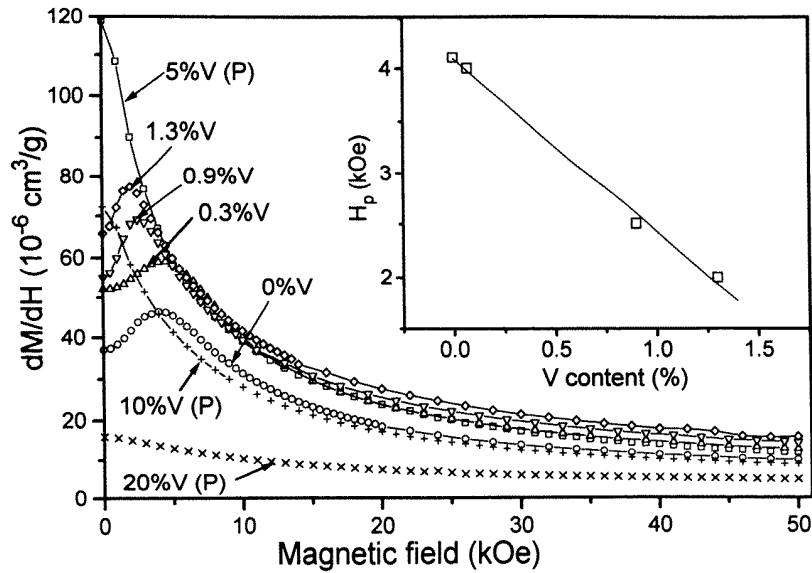


Figure 2. The derivative dM/dH versus H for the same alloys and temperature as in figure 1. The inset shows the peak field H_p versus x .

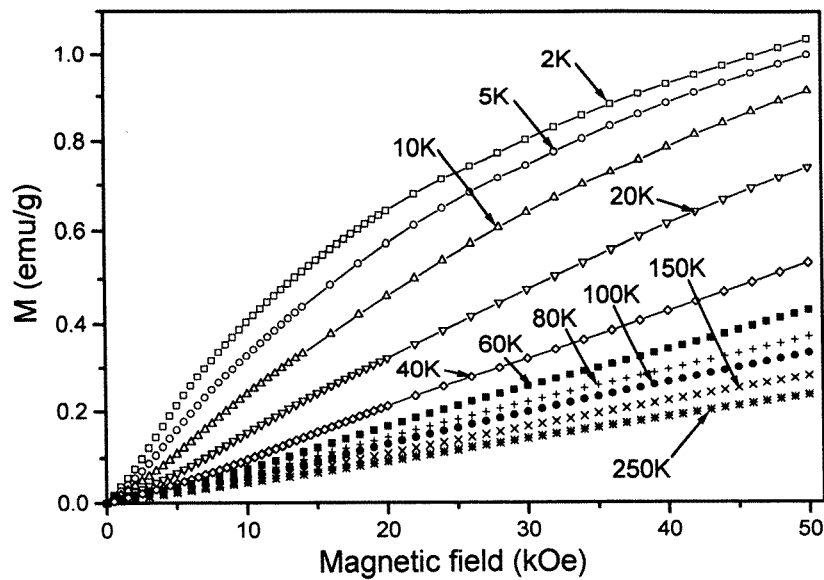


Figure 3. The magnetization M versus the field H for Cr-2.7%Fe for several different temperatures. Paramagnetic alloys are denoted by P.

Within the SDW state, the curves for the differential susceptibility plotted in figure 2 show a well-pronounced maximum that completely disappears upon eliminating the SDW by the addition of more than 2.5% V. The inset to figure 2 suggests that the peak field H_p decreases almost linearly with the V concentration.

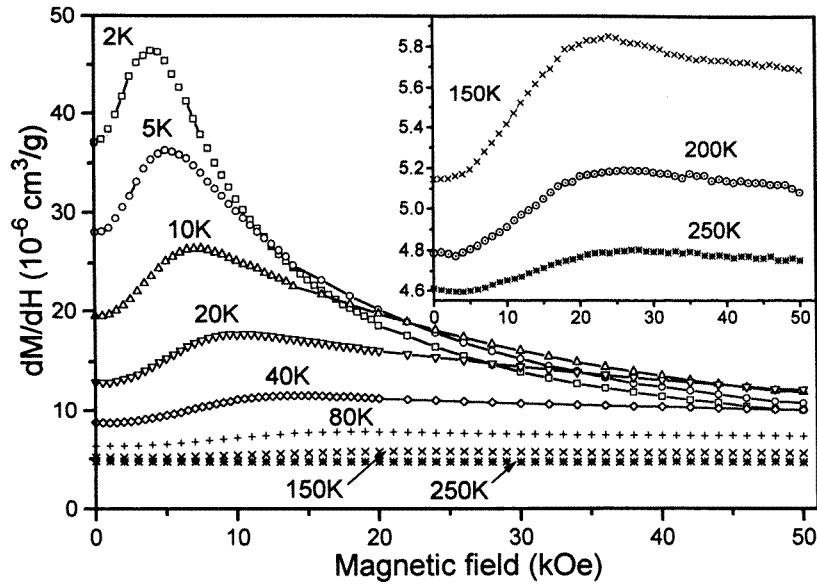


Figure 4. The differential susceptibility dM/dH versus H for Cr-2.7%Fe at $T = 2$ K.

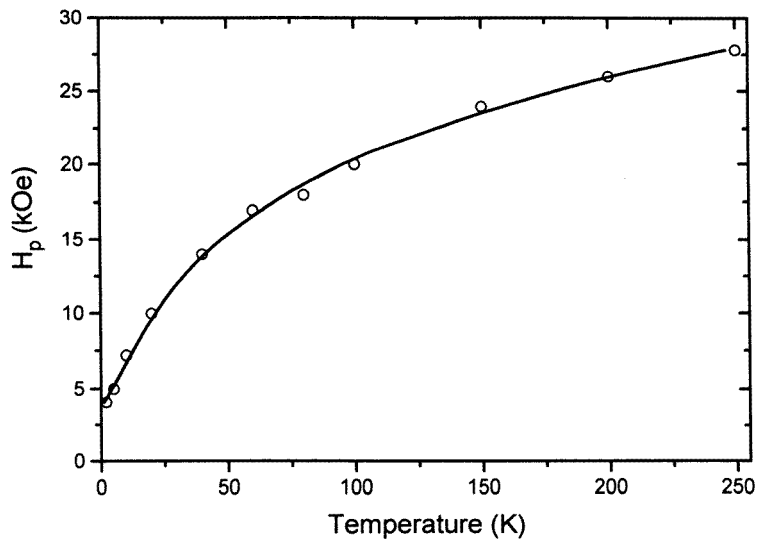


Figure 5. The peak field H_p versus T for Cr-2.7%Fe at $T = 2$ K.

As shown in figures 3 and 4 for binary Cr-2.7%Fe, the low-field magnetization and susceptibility become more highly non-linear at lower temperatures. Yet the inset to figure 4 and the peak field plotted in figure 5 indicate that this non-linear behaviour persists up to the Néel temperature of roughly 255 K. Since this alloy passes through a strongly first-order PC transition [7], the SDW amplitude does *not* vanish as the temperature approaches T_N . The peak field H_p is a monotonically increasing function of temperature with a maximum value of about 28 kOe near T_N . At low temperatures, H_p tends to a non-zero value of about

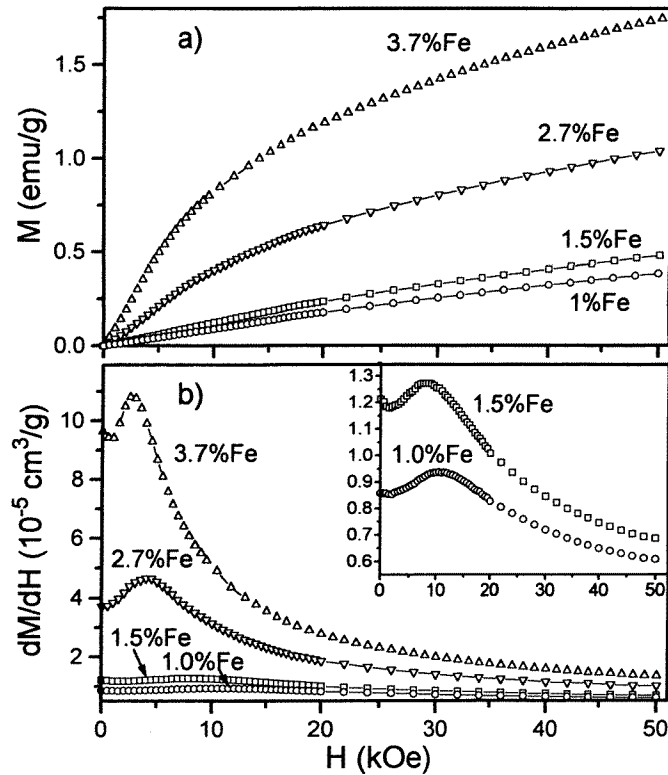


Figure 6. The (a) magnetization M and (b) derivative dM/dH versus H for $\text{Cr}_{1-x}\text{Fe}_x$ at 2 K.

3.5 kOe. We show in section 3.3 that this has important consequences for the magnetic interactions between the pair moments.

Measurements on the $\text{Cr}_{1-x}\text{Fe}_x$ alloy system at $T = 2$ K clearly show the effect of the Fe pairs on the magnetization plotted in figure 6(a). Our results for $M(H)$ are reminiscent of the magnetization curves plotted by Babic *et al* [20] for $x = 1$ to 14.2%. However, their measurements were not precise enough to distinguish the peak in dM/dH . For Fe concentrations of 1 and 1.5%, the deviation from linearity shown by $M(H)$ is very small. But as x increases, a larger fraction of the Fe moments are paired. The non-linear contribution of the easily polarized pairs is quite apparent in the alloys with Fe concentrations of 2.7 and 3.7%.

Each of these alloys shows a peak in the differential susceptibility dM/dH , which is plotted in figure 6(b). The peak shifts downwards as the Fe concentration increases. For Fe concentrations of 1 and 1.5%, the peak in dM/dH disappears above about 100 K, which is well below the Néel temperatures of those alloys. For Fe concentrations of 2.7 and 3.7%, however, the peak only disappears above T_N .

3. The model for the Fe moments and susceptibility

We now describe a simple model for the susceptibility of dilutely doped CrFe alloys. This model contains four basic ingredients: (a) the division of each single Fe moment into bound and unbound parts, (b) a weak, antiferromagnetic coupling between the unbound portion

of the single Fe moment and the surrounding SDW matrix, (c) a ferromagnetic interaction between the single Fe moments and the strongly coupled Fe pairs and (d) a magnetic interaction between the pair moments. The first and main ingredient of this recipe is needed to explain the difference between the Fe moments in the C and I SDW states. A rudimentary prescription for the susceptibility consisting of just the first two ingredients predicts both the peak H_p in dM/dH and its doping dependence but neither its temperature dependence nor its magnitude. Together, the first three ingredients explain the magnitude, temperature dependence and doping dependence of H_p . But the final ingredient is still required to understand the dependence of H_p/T on temperature. The fundamental assumption of this model is that the maximum value of the spin due to the combined bound and unbound portions of a single Fe moment is unchanged from above T_N .

Certainly, this model makes no claim to be complete. The direct magnetic interaction between the single Fe moments is ignored because it is not required to explain any of the observations discussed in the previous section. We also ignore the effect of the single moments on the pairs, since measurements [20] suggest that the pairs are coupled only to each other. Nonetheless, this model contains all the essential physics needed to understand the behaviour of dilutely doped CrFe alloys.

For zero field, related calculations have been performed by Hedgcock *et al* [26] and Kelly *et al* [18]. But neither theory predicts any difference between the C and I moments and neither treats the field dependence of dM/dH . In fact, reference [26] predicts that the Fe moment increases rather than decreases below T_N .

3.1. Effective moments in zero field

Taking the SDW wavevectors Q'_\pm to lie along the z -axis and replacing the strongly peaked Bloch wavefunctions by delta functions at every lattice site \mathbf{R} , the general form for the Cr spin at \mathbf{R} can be simply written as [27]

$$S_c(R_z) = (-1)^{2R_z/a} \hat{n} \alpha_s g(T) \cos\left(\frac{2\pi}{a} \delta' R_z + \frac{\theta}{2}\right) \quad (3)$$

where a is the lattice constant of the conventional bcc unit cell, \hat{n} is the spin polarization, α_s is a constant and $g(T)$ is the temperature-dependent order parameter. In the ISDW state, the phase θ is arbitrary but in the CSDW state with $\delta' = 0$, $\theta = \pi/2$. Hence, the amplitudes of the I and C SDWs are given by $\alpha_s g(T)$ and $\alpha_s g(T)/\sqrt{2}$, respectively. So across a second-order IC phase transition with the same order parameter g on both sides, the SDW amplitude drops by a factor of $1/\sqrt{2}$ but the rms magnetic moment is continuous. For the C phase at low temperatures [7], the magnetic moment of Cr is approximately $0.8\mu_B$ so the CSDW amplitude is given by $\alpha_s g(0)/\sqrt{2} \approx 0.4$. Infrared reflectivity measurements [6] in the C phase indicate that the energy gap $2\sqrt{2}g(0)$ induced by the formation of the SDW is about 380 meV.

The magnetic moments of both Fe and Cr metals consist of d-band electron-hole pairs. Above the Néel temperature, an Fe atom within a Cr-2.7%Fe alloy has an effective magnetic moment of $\mu_P = 2\mu_B \sqrt{s(s+1)} \approx 3.03\mu_B$. Ignoring the contributions of the Fe pairs, this corresponds to a spin s close to 1.095. Below the Néel temperature, some of the d-band electrons on the Fe atom join the electron-hole condensate of the SDW and generate a spin $S_c(R_z)$ equal to the missing Cr spin. Each such electron is bound to the SDW by the condensation energy of 380 meV. As suggested by the rather large Fe concentration at the triple point, the conduction-band electrons donated by the Fe impurities raise the chemical potential very little compared to its value in the absence of Fe doping. The remaining Fe

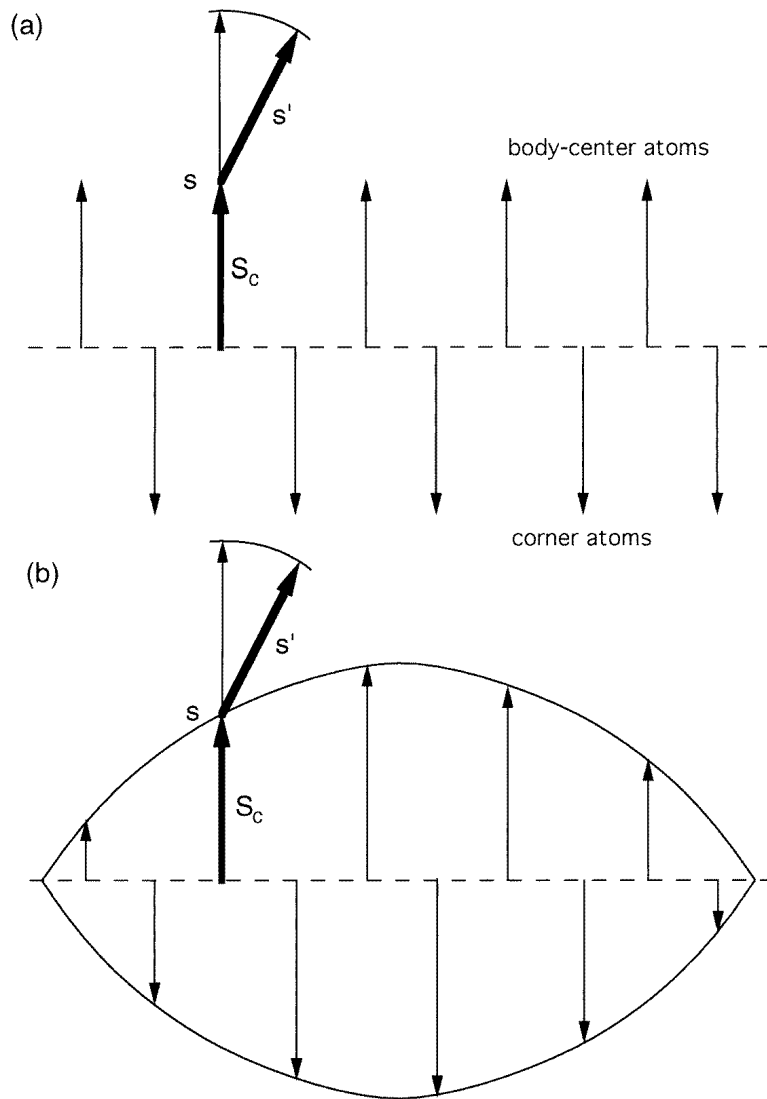


Figure 7. A schematic representation of the Fe moment within the (a) C or (b) I SDW states. Only s' contributes to the CW paramagnetic susceptibility.

d-band electrons remain localized at the Fe site to generate a local moment with spin s' , which is sketched in figure 7. Because this component is only weakly coupled to the SDW, it responds to an external field and is responsible for the CW paramagnetism of dilute alloys below T_N .

We now assume that the maximum number of electron-hole pairs on each Fe atom is the same as above T_N . For an itinerant antiferromagnet, the number of electron-hole pairs is proportional to the SDW amplitude. So averaged over z , the effective spin s' of the single Fe moment is given by $s' = s - s_c$, where $s_c \equiv \langle |S_c(R_z)| \rangle$. Hence, the maximum value of the spin at any Fe site due to the combined bound ($|S_c(R_z)|$) and unbound (s') portions of the Fe moment is assumed to be unchanged from its value s above T_N . With the definition

$s_c = \gamma \alpha_s g$, we find that

$$\gamma = \frac{\delta'}{a} \int_0^{a/\delta'} \left| \cos\left(\frac{2\pi}{a} \delta' z + \frac{\theta}{2}\right) \right| dz \quad (4)$$

equals $2/\pi$ for the I phase and $1/\sqrt{2}$ for the C phase. Since $2/\pi \approx 0.637 < 1/\sqrt{2}$, the effective moment $\mu_A = 2\mu_B \sqrt{s'(s'+1)}$ is slightly larger in the I phase than in the C phase. There is no predicted difference between the Fe moments within the transversely and longitudinally polarized ISDW phases.

Because the IC and CI phase transitions are second order or weakly first order, $\alpha_s g \approx 0.4\sqrt{2}$ is taken to be the same on both sides of each transition. Consequently, we find that $\mu_A^{(I)} = 2.26\mu_B$, $\mu_A^{(C)} = 2.17\mu_B$, and $\mu_A^{(I)}/\mu_A^{(C)} \approx 1.04$. Hence, the I moment is about 4% larger than the C moment. This ratio may be further enhanced by the gradual reduction in the I amplitude $\alpha_s g$ (see, for example, references [12, 13]) and the resulting growth in the I moment $\mu_A^{(I)}$ as the alloy passes deeper into the I phase. A 5% decrease of the SDW order parameter on the I side of the phase transition would explain the remaining 2% enhancement of $\mu_A^{(I)}/\mu_A^{(C)}$ observed in the experiments described in section 2.1.

Both $\mu_A^{(I)}$ and $\mu_A^{(C)}$ are smaller than the fitted values for the CrFeV alloy and larger than the fitted values for the CrFeMn alloy. Several factors can account for the observed differences in the Fe moments for those two alloys: impurity scattering, shifts in the chemical potential and variations in the local Fe environment. Within our simple model, s_c and s are the only free parameters and cannot accommodate all of these effects. In any case, the experimentally fitted moments are generally less dependable than the ratio $\mu_A^{(I)}/\mu_A^{(C)}$, which is close to the predicted value.

This model naturally explains the change in the effective moments $\mu_A^{(I)}$ and $\mu_A^{(C)}$ with doping. As the V concentration increases in the $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloy system [23], the order parameter g is suppressed and both $\mu_A^{(C)}$ and $\mu_A^{(I)}$ approach the P value μ_P . For temperatures below $0.9T_N$, $g(T)$ is relatively constant, so $\mu_A^{(C)}$ and $\mu_A^{(I)}$ are not sensitive functions of temperature.

Notice that the effective Fe moment in the I phase is larger than the C moment only if the Fe atoms are randomly distributed within the SDW. If the Fe atoms deform the SDW with the result that most lie at sites with a large spin density, as posited by Friedel and Hedman [17], then $\mu_A^{(I)}$ would be *less* than $\mu_A^{(C)}$. If, on the other hand, most of the Fe atoms lie close to the nodes of the SDW, then the ratio $\mu_A^{(I)}/\mu_A^{(C)}$ would be substantially greater than measured. So our results suggest that the Fe impurities are not very effective in distorting the SDW of the host. This conjecture is supported by neutron-scattering measurements [21], which indicate that Fe impurities do not perturb the moments of the surrounding Cr atoms in a C alloy.

3.2. Field dependence of the magnetization

To describe the field dependence of the magnetization, the unbound portion of the single Fe moment is coupled antiferromagnetically to the SDW matrix and ferromagnetically to the pair moments. For ease of exposition, we consider the case of a CSDW state with Cr spin s_c . This formalism can be easily adapted to the ISDW state by imposing the general relations $s' = s - s_c$ and $s_c \equiv \langle |\mathbf{S}_c(\mathbf{R}_z)| \rangle$.

As discussed in the introduction, the six domains of the transversely polarized ISDW correspond to the three possible orientations of the wavevectors \mathbf{Q}'_{\pm} and the two possible polarizations of the spin for each \mathbf{Q} -state. Several experimentalists [14, 28, 29] have investigated the effect of a magnetic field on the domain populations below T_N . As expected

for an antiferromagnet with $\chi_{\parallel} < \chi_{\perp}$, a magnetic field in the \hat{z} -direction flips the spins into one of the two crystal axes normal to (001). In the transversely polarized ISDW phase, the spins may lie along one of the two axes perpendicular to the wavevectors Q'_{\pm} . A magnetic field with $H \perp Q'_{\pm}$ reversibly switches the spins into the direction normal to both H and Q'_{\pm} . For the longitudinally polarized ISDW phase, the spins lie parallel to the SDW wavevectors. A strong magnetic field with $H \parallel Q'_{\pm}$ then irreversibly flips the SDW wavevectors and the spins to one of the crystal axes normal to H . Unfortunately, little is known [15] about the field dependence of the polarization domains in the CSDW phase because all three domains have the same magnetic peak at $G/2$.

In any SDW domain, the unbound portion of the single Fe moment experiences an exchange field H_{ex} in the direction of the missing Cr moment. This field has two origins. The first is the antiferromagnetic interaction of the unbound Fe moment with its eight Cr neighbours. The second is the local Hund's rule coupling at the Fe site, which favours the same z -component of the total spin as above T_N . Both mechanisms favour aligning the bound and unbound portions of the single Fe moment.

The effective field experienced by an Fe moment in the presence of an external magnetic field $H = H\hat{z}$ depends on the domain of the SDW. Consider first a polarization domain with spin parallel to \hat{z} . If the magnetic moment of the missing Cr atom at the Fe site is $\mu_c = 2\mu_B s_c$ and the average magnetic moment of each Fe pair is μ_2 , then the mean fields experienced by the Fe moments on the up and down sublattices are

$$\begin{aligned} H_{\text{eff}}^{\uparrow} &= H + J_0\mu_c + J_1\mu_2 \\ H_{\text{eff}}^{\downarrow} &= H - J_0\mu_c + J_1\mu_2 \end{aligned} \quad (5)$$

where J_0 and J_1 are coupling constants. In one of the two other polarization domains with spin perpendicular to \hat{z} , the Fe moments on the two sublattices experience effective fields with the same magnitude of

$$H_{\text{eff}}^{\perp} = \sqrt{(H + J_1\mu_2)^2 + (J_0\mu_c)^2} \quad (6)$$

and at angles of $\pm \tan^{-1}(J_0\mu_c/(H + J_1\mu_2))$ to the z -axis. For any spin polarization, the exchange field produced by the SDW at the Fe site is $H_{\text{ex}} = J_0\mu_c$.

Defining the normalized magnetization $m_2 = \mu_2/2\mu_B$ of the pair moments, the mean-field relations for the normalized magnetization $m_1 = \mu_1/2\mu_B$ of a single moment in parallel and perpendicular domains are given by

$$m_1^{\parallel} = \frac{1}{2}s' \left\{ B_{s'}(\beta's'(H' + s_c + \eta m_2)) + B_{s'}(\beta's'(H' - s_c + \eta m_2)) \right\} \quad (7)$$

$$m_1^{\perp} = s' \frac{H' + \eta m_2}{H_{\text{eff}}^{\perp}} B_{s'}(\beta's'H_{\text{eff}}^{\perp}) \quad (8)$$

where $B_s(x)$ is the Brillouin function. The above relations introduce the dimensionless variables $H' = H/2\mu_B J_0$, $H_{\text{eff}}^{\perp} = H_{\text{eff}}^{\perp}/2\mu_B J_0$, $T' = T/4\mu_B^2 J_0$ and $\eta = J_1/J_0$. When $m_2 = 0$ and the temperature is sufficiently large, equations (7) and (8) reduce to $2\mu_B m_1^{\parallel} = 2\mu_B m_1^{\perp} = (2\mu_B)^2 s'(s' + 1)H/3T$, as expected from the CW law.

Including the magnetic interaction between the pairs with coupling $J_{\text{pr}} = \kappa J_0$, the pair moments have magnetization

$$m_2 = s_2 B_{s_2}(\beta's_2(H' + \kappa m_2)) \quad (9)$$

where s_2 is the effective spin of an Fe pair. In the C phase, the pair moment is totally decoupled from the SDW and $s_2 = 2s$. A small interaction with the SDW persists in the I phase [17], so s_2 is slightly less than $2s$.

The differential susceptibilities of the single moments are given in dimensionless units by

$$\chi_1^{\parallel} = \frac{dm_1^{\parallel}}{dH'} = \frac{1}{2}\beta' s'^2 (1 + \eta\chi_2') \left\{ B_{s'}'(\beta' s'(H' + s_c + \eta m_2)) + B_{s'}'(\beta' s'(H' - s_c + \eta m_2)) \right\} \quad (10)$$

$$\chi_1^{\perp} = \frac{dm_1^{\perp}}{dH'} = s' (1 + \eta\chi_2') \left\{ \frac{s_c^2}{H_{\text{eff}}'^{\perp 3}} B_{s'}'(\beta' s' H_{\text{eff}}'^{\perp}) + \beta' s' \left(\frac{H' + \eta m_2}{H_{\text{eff}}'^{\perp}} \right)^2 B_{s'}'(\beta' s' H_{\text{eff}}'^{\perp}) \right\} \quad (11)$$

where $B_s'(x) = dB_s(x)/dx$. Finally, the susceptibility of the pairs is given by

$$\chi_2' = \frac{dm_2}{dH'} = \beta' s_2^2 \frac{B_{s_2}'(\beta' s_2(H' + \kappa m_2))}{1 - \beta' \kappa s_2^2 B_{s_2}'(\beta' s_2(H' + \kappa m_2))} \quad (12)$$

with a Curie temperature of $\Theta = (4/3)\mu_B^2 J_{\text{pr} s_2}(s_2 + 1)$ and an effective pair moment of $2\mu_B \sqrt{s_2(s_2 + 1)}$.

Clearly, both η and κ are functions of the Fe concentration x . As x increases, the fraction $N_2/N_1 \propto x$ of Fe moments in pairs grows, so the coupling $\eta > 0$ between the pairs and singles must also increase. Unlike $\eta(x)$, the coupling $\kappa(x)$ between the pair moments may not be a monotonic function of x . Depending on the magnetic interactions between the Fe pairs, κ can be either positive (F interactions) or negative (AF interactions).

3.3. The peak in dM/dH

Examination of equation (10) for χ_1^{\parallel} immediately reveals the origin of the peak in dM/dH . In low fields, the Fe moments on the \downarrow sublattice experience an effective field in the $-\hat{z}$ -direction. As the external field H' exceeds $s_c - \eta m_2$, the Fe moments on both sublattices experience an effective field in the $+\hat{z}$ -direction and the magnetization quickly increases. Consequently, the peak in dM/dH is generated solely by the SDW domains with $\hat{n} \parallel \mathbf{H}$. But as mentioned above, the relative population of the \parallel and \perp domains is expected to change as the field increases. A thermal-activation model was developed by Werner *et al* [14] to explain the field dependence of the domain populations in the ISDW phase of pure Cr. The energy E^{\parallel} or E^{\perp} of a domain with volume δV depends on whether the spin lies parallel or perpendicular to the external field. For pure Cr, the susceptibilities χ^{\parallel} and χ^{\perp} may be taken to be independent of the field and the domain energies are given by $E^{\parallel} = -\chi^{\parallel} H^2 \delta V/2$ and $E^{\perp} = -\chi^{\perp} H^2 \delta V/2$. Assuming that the thermal barrier between domains is sufficiently low, the domain populations may be considered to be in thermal equilibrium. Measurements [29] suggest that the average domain volume δV lies between 10^{-15} and 10^{-16} cm³. Despite its simplicity, the thermal-activation model has been remarkably successful at predicting a variety of physical properties.

For CrFe alloys, however, the field-dependent susceptibilities χ_1^{\parallel} and χ_1^{\perp} of the Fe moments are usually much larger than the susceptibilities of pure Cr. This can be verified from figure 6(b), where the susceptibility of $\text{Cr}_{1-x}\text{Fe}_x$ increases quite rapidly with the Fe concentration. Consequently, the thermal-activation model is much more difficult to implement for CrFe alloys than for pure Cr. In addition, the model has never been applied to the polarization domains of the CSDW phase, which is stabilized by Fe doping.

To avoid these difficulties, we shall assume that the three polarization domains of the CSDW phase are equally populated. Then the normalized magnetization and susceptibility

averaged over the single and pair Fe moments are

$$m = \frac{N_1}{3N} \left\{ m_1^{\parallel} + 2m_1^{\perp} \right\} + \frac{N_2}{2N} m_2 \quad (13)$$

$$\chi' \equiv \frac{dm}{dH'} = \frac{N_1}{3N} \left\{ \chi_1^{\parallel} + 2\chi_1^{\perp} \right\} + \frac{N_2}{2N} \chi_2'. \quad (14)$$

Hence, the magnetization and differential susceptibility per Fe atom are given by $M = 2\mu_B m$ and $dM/dH = \chi'/J_0$. Because we have only evaluated the contributions of the single and pair moments, these expressions do not include the magnetization and susceptibility of the Fe atoms in triplets and higher-order clusters. For an Fe concentration of 2.7%, $N - N_1 - N_2 \approx 0.05N$ of the Fe impurities belong to such clusters.

We define the peak field H'_p as the maximum in the \parallel susceptibility $\chi_1^{\parallel}(H')$. This peak may be slightly shifted or even hidden by the \perp and pair contributions to the total susceptibility. But the calculated H_p does not depend on the relative populations of the \parallel and \perp domains.

A ‘bare-bones’ model for χ' may be constructed by setting $\eta = 0$ and ignoring the interaction between the single and pair moments. For low temperatures, the \parallel susceptibility then peaks at $H'_p = s_c$. Doping with V suppresses the SDW amplitude s_c , so H_p decreases with the V concentration in $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys. As the temperature increases, the peak in $\chi_1^{\parallel}(H')$ eventually disappears. From equation (10), we find that the peak remains so long as $B_s''(\beta's's_c) > 0$ or $T' < 1.25s's_c$. Consequently, the peak disappears above the temperature $T_{\max} \approx 5\mu_B^2 J_0 s_c s'$. Since the observed peak in $\text{Cr}_{1-x}\text{Fe}_x$ alloys with $x \leq 1.5\%$ survives up to about 100 K, we estimate that $5\mu_B^2 J_0 s_c s' \approx 100$ K or 9 meV. Unfortunately, this implies that $H_p = 2\mu_B J_0 s_c \approx 660$ kOe (with $\alpha_s g = 0.6\mu_B$ [6] and $s_c = 0.19$), which is roughly 70 times too large at $T = 2$ K.

Once the single and pair moments are ferromagnetically coupled, the effective field experienced by the single Fe moments is greatly enhanced. For low fields, $m_2 \approx \chi_2' H'$. So in the limits $s's_c \gg T' \gg s_2 H'_p$, H'_p would be given exactly by

$$H'_p = \frac{s_c}{1 + \eta \chi_2'} \quad (15)$$

which may be quite a bit smaller than s_c . We first assume that the pair moments do not interact with one another so that $\kappa = 0$ and $\Theta = 0$. As $T' \rightarrow 0$, $\chi_2' \rightarrow s_2(s_2 + 1)/3T'$ and H'_p/T' approaches a constant. For Cr-2.7% Fe at 2 K, $H'_p/T' = 2\mu_B H_p/T$ is about 0.27. To approach this limit with $s_c = 0.4$ and $s_2 = 2.2$, we require that $\eta = 0.66$.

The results of this model with $s = 1.1$, $s_2 = 2.2$, $\eta = 0.66$, $\kappa = 0$ and an Fe concentration of 2.7% are presented in figures 8–11. In figure 8, we plot the magnetization $m(H')$ versus field H' for five different values of the SDW amplitude with $T' = 0.05$. The maximum value of $s_c \approx 0.4$ or $\mu_c \approx 0.8\mu_B$ is achieved in the C phase at low temperatures. For higher V concentrations or smaller values of s_c , the unbound portion of the Fe moment is more weakly constrained by the SDW and responds more readily to the external field. In contrast to Babic *et al* [20], who attributed the rapid rise of the magnetization at low fields to Fe pairs and clusters, we find that the magnetization below H_p is dominated by the contribution of Fe singles in \perp -spin domains. Above H_p , both \parallel - and \perp -spin domains make roughly the same contribution to the magnetization.

As suggested by equation (15) and plotted in the inset to figure 9, H'_p increases almost linearly with the SDW amplitude. But for $T' = 0.05$, this linear dependence breaks down below $s_c \approx 0.07$ and $H'_p \rightarrow 0$ as $s_c \rightarrow 0.04$. Although equation (15) still applies for $s_c = 0.1$, the small peak in χ_1^{\parallel} at H'_p is hidden by the other contributions to the total

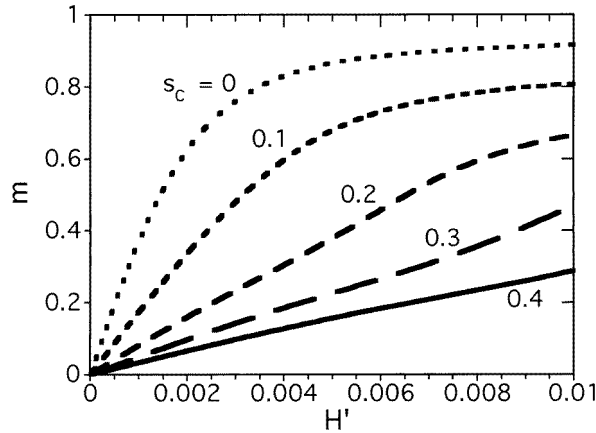


Figure 8. The average magnetization m per Fe atom versus H' for $T' = 0.05$, $\eta = 0.66$, $\kappa = 0$, $s = 1.1$, $s_2 = 2.2$, an Fe concentration of 2.7% and five different values of the SDW amplitude s_c .

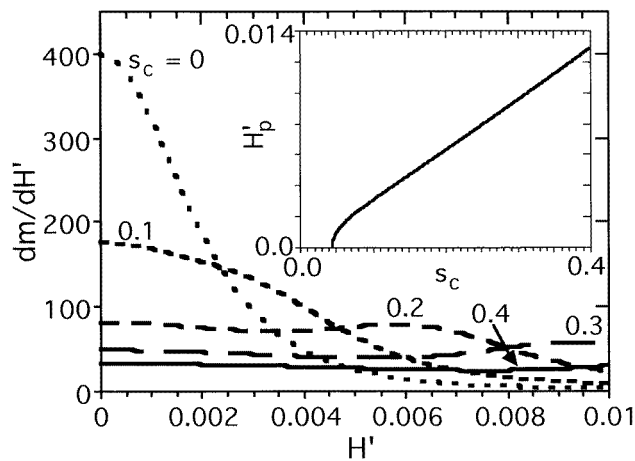


Figure 9. The differential susceptibility $\chi' = dm/dH'$ versus H' for the same parameters as in figure 8. The inset shows the peak field H'_p of $\chi'_1(H')$ versus the SDW amplitude s_c .

susceptibility χ' in figure 9. Recall that for $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys, H_p was observed to depend almost linearly on the SDW amplitude through the V concentration x in figure 2.

Fixing $s_c = 0.4$, we plot the magnetization and susceptibility versus the field for five values of the temperature in figures 10 and 11. When the field exceeds H_p , the Fe moments on the \downarrow sublattice experience an effective field in the $+\hat{z}$ -direction and the magnetization increases rapidly. At lower temperatures, the pairs of Fe moments are more easily polarized by the external field. So with decreasing temperature, the pair moments augment the effective field experienced by the single moments. Consequently, the magnetization becomes a steeper function of field, the peak in dm/dH' becomes more pronounced, and H_p becomes smaller, just as observed in figures 3, 4 and 5 for Cr-2.7%Fe.

Because $\eta(x)$ is a monotonically increasing function of the Fe concentration x , H_p grows as the Fe concentration is diminished. Along with the disappearance of the single Fe atoms,

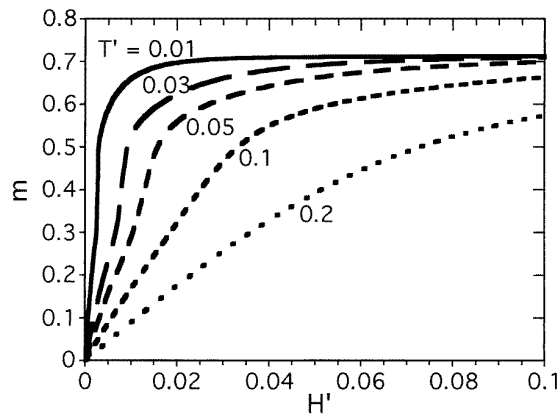


Figure 10. The average magnetization m per Fe atom versus H' for $s_c = 0.4$ and five different temperatures. The other parameters are the same as in figure 8.

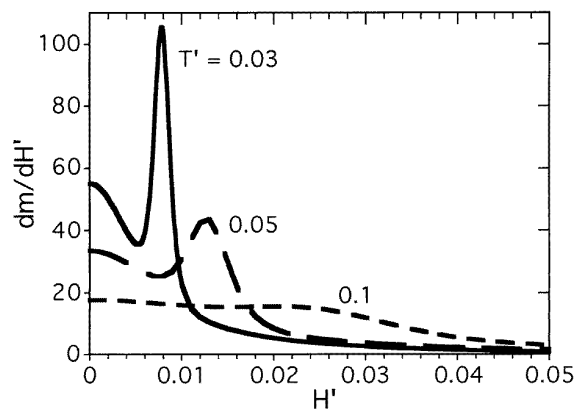


Figure 11. The differential susceptibility $\chi' = dm/dH'$ versus H' for the same parameters as in figure 10.

the magnetization vanishes and the susceptibility approaches the temperature-independent constant χ_0 . Since the ISDW amplitude $\alpha_s g \approx 0.6\mu_B$ is about half the size of the CSDW amplitude $\alpha_s g \approx 0.8\sqrt{2}\mu_B$ [7], T_{\max} is much smaller in I alloys with Fe concentrations of 1 and 1.5%. These results explain the behaviour of the magnetization and susceptibility plotted in figure 6 for $\text{Cr}_{1-x}\text{Fe}_x$ alloys.

In the absence of any direct interaction between the pair moments, χ'_2 is proportional to $1/T'$ at low temperatures. So as implied by equation (15) and plotted as the solid curve of figure 12, $H'_p \propto T'$ and H'_p/T' approaches a constant as $T' \rightarrow 0$. However, the measurements plotted in figure 5 for Cr-2.7%Fe indicate that H_p approaches a non-zero value of about 3.5 kOe as $T \rightarrow 0$. Consequently, the experimental values of $H'_p/T' = 2\mu_B H_p/T$ plotted in the inset to figure 12 increase quite rapidly at low temperatures.

This behaviour may be recovered by allowing the pair moments to interact. When the interactions between pairs are ferromagnetic with a positive Curie temperature $\Theta > 0$, H_p/T vanishes as $T \rightarrow \Theta^+$. But when the interactions are antiferromagnetic with a negative Curie

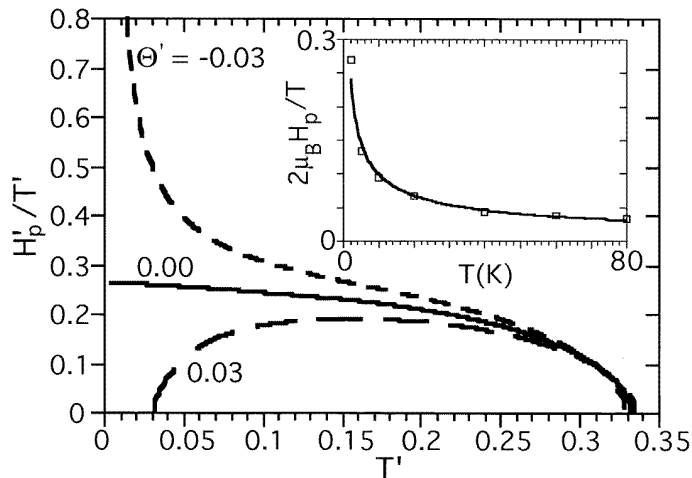


Figure 12. The function H'_p/T' versus T' for three values of Θ' with the other parameters the same as in figure 10. The inset shows the experimental values of $H'_p/T' = 2\mu_B H_p/T$ for the Cr-2.7%Fe alloy.

temperature $\Theta < 0$, H_p/T diverges as $T \rightarrow 0$. Strictly speaking, our expression for the pair susceptibility is only valid in the non-ordered regime above the antiferromagnetic ordering temperature of the Fe pairs. Nonetheless, figure 12 implies that the interaction among the pair moments must be antiferromagnetic in order to explain the observed temperature dependence of H_p/T .

Antiferromagnetic interactions with negative Curie temperatures were also obtained from the fits to the low-field susceptibilities of CrFeV and CrFeMn alloys in section 2.1. Our work suggests that these antiferromagnetic interactions are produced by the Fe pairs. The experiments summarized by Fawcett *et al* [7] reveal that the Curie temperature Θ increases with the Fe concentration and that the interactions become ferromagnetic for Fe concentrations above about 4%. So with increasing Fe concentration, the interactions between the Fe pairs and clusters become ferromagnetic.

Conspicuously absent from this model are the direct interactions between the single Fe moments. Although undoubtedly significant, such interactions are not required to explain the behaviour of the peak field H_p as a function of doping or temperature. In the absence of any coupling between the single and pair moments, direct interactions among the single moments cannot explain the observed temperature dependence of H_p . For example, if the single moments were coupled by the interaction $J_s = \lambda J_0$, then the susceptibility would peak at $H'_p = s_c - \lambda m_1$. But this peak closely coincides with the magnetization $m_1 \approx 0.5s'$, when the \uparrow sublattice is totally polarized and the \downarrow sublattice has an average magnetization close to 0. So if the single moments interacted only among themselves, $H'_p \approx s_c - \lambda s'/2$ would be roughly independent of temperature.

4. Discussion and conclusion

This paper has reported magnetization measurements on a series of $\text{Cr}_{1-x}\text{Fe}_x$ and $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ alloys. Peaks in the differential susceptibility dM/dH were found at low temperatures in the SDW state of every alloy studied. In all cases, the peak disappears

upon suppression of the SDW by V doping or by heating above the Néel temperature. Measurements suggest that the peak field H_p is an almost linear function of the V concentration. The position of the peak also decreases with the Fe concentration and increases with the temperature.

Crucial to the success of the model developed in section 3 is the coupling between the single and pair moments. For external fields less than H_p , the unbound portion of each single Fe moment is tightly constrained by the SDW. If the single and pair moments were decoupled, then H_p would be identical to the exchange field $H_{\text{ex}} = 2\mu_B J_0 s_c$. In the C phase with $s_c = 0.4$, the ‘unbound’ portion of the Fe moments would then be rigidly clamped by the SDW up to a field of about $H_{\text{ex}} \approx 1400$ kOe. Due to the coupling between the single and pair moments, an external field of less than 30 kOe can easily depin the unbound part of the single Fe moment.

The presence of superparamagnetic pairs may distinguish CrFe alloys from CrV, CrRu and CrCo alloys, which exhibit CW paramagnetism [7] above but not below T_N . Due to the absence of superparamagnetic pairs in those other alloys, the ‘unbound’ portion of the impurity moment may be tightly constrained by the SDW matrix up to very high external fields of order 1000 kOe. Consequently, the local moments do not appear in susceptibility measurements. Of course, our phenomenological model cannot reveal why superparamagnetic pairs form in CrFe alloys but not in those other systems. One possibility is that the nearest-neighbour coupling between impurity moments is antiferromagnetic in CrV, CrRu and CrCo alloys.

Clearly, the division of the impurity moment into bound and unbound parts in the relation $s = s'(\mathbf{R}) + |\mathbf{S}_c(\mathbf{R})|$ only makes sense when the impurity spin s is larger than $|\mathbf{S}_c(\mathbf{R})|$. When $s < |\mathbf{S}_c(\mathbf{R})|$, we expect the unbound part $s'(\mathbf{R})$ of the impurity moment to vanish. For the bound part of the impurity moment, there are two possibilities: either the bound moment will be suppressed compared to $|\mathbf{S}_c(\mathbf{R})|$ or the full moment $\mathbf{S}_c(\mathbf{R})$ will be preserved by the tunnelling of electron–hole pairs from the surrounding Cr atoms.

Not surprisingly, our model for CrFe alloys fails at high fields, when the bound portion of the Fe moment breaks free from the SDW matrix. Measurements [23] on $(\text{Cr}-2.7\%\text{Fe})_{1-x}\text{V}_x$ confirm that μ_A increases with field and approaches its P value for large fields above 50 kOe. In reference [23], the peak in dM/dH was attributed to the release of the bound Fe moment with field. However, the susceptibility measurements reported in section 2.1 indicate that the Curie constant of Cr–2.7%Fe does not change over the temperature range $50 \text{ K} < T < 250 \text{ K}$. This implies that the condensation energy gained by the bound Fe moment is at least twice the size of the energy $4\mu_B^2 J_0 s_c s' \approx 11$ meV constraining the unbound portion of the Fe moment in a C host. So it seems unlikely that the bound part of the Fe moment makes any significant contribution to the low-field susceptibility.

As seen in figure 10 for $T' = 0.01$ or $T \approx 4.7$ K, the magnetization is predicted to saturate at a field of about $H' = 0.02$ or $H \approx 70$ kOe. But measurements by Babic *et al* [20] reveal that the magnetization at $T = 4.2$ K has not yet saturated at a field of 330 kOe. This strongly suggests that the depinning of the bound Fe moments is responsible for the slow saturation of the magnetization.

Near the peak field H_p at low temperatures, the \parallel susceptibility is quite a bit larger than the \perp susceptibility, which raises an interesting possibility. Suppose that an I $\text{Cr}_{1-x}\text{Fe}_x$ alloy is zero-field cooled through the Néel transition into the superposition of three different, transversely polarized Q -states. As the field is raised through H_p at low temperatures, the neutron-scattering signal of the Q -state with $\mathbf{Q}'_{\pm} \parallel \mathbf{H}$ and $\hat{n} \perp \mathbf{H}$ should disappear. For Cr alloys that do not contain local moments below T_N , exactly the opposite is expected: the domains with $\mathbf{Q}'_{\pm} \perp \mathbf{H}$ should be suppressed [14] upon application of a

strong magnetic field.

This model makes no distinction between the effective Fe moments in the transversely and longitudinally polarized ISDW phases. Because Fe impurities quickly suppress the longitudinal ISDW phase [7], the difference between the transverse and longitudinal moments has not yet been tested experimentally. It would be interesting to perform such measurements on dilutely doped $\text{Cr}_{1-x}\text{Fe}_x$ alloys with $x < 1\%$.

Some discrepancies remain between theory and experiment. Mössbauer measurements [30] indicate that the exchange field H_{ex} exerted by the SDW on the Fe moments is about 225 kOe, independently of the Fe concentration and of the SDW phase! By contrast, the predicted exchange field $H_{\text{ex}} = 2\mu_{\text{B}} J_0 s_{\text{C}}$ sensitively depends on the SDW phase through the amplitude s_{C} . In the C phase, $H_{\text{ex}} \approx 1400$ kOe is substantially larger than the Mössbauer result. Additional Mössbauer measurements may be needed to resolve this disagreement.

It is important to bear in mind that Fe impurities may have other important effects on the Cr host. The RKKY interaction between the unbound portion of the Fe moment and the d-band electrons may enhance [27] the charge-density wave (CDW) observed in pure Cr [6] below T_{N} . Jiang and Fishman [27] argue that the strongly first-order PC transition [7] in $\text{Cr}_{1-x}\text{Fe}_x$ alloys with $x > 2.4\%$ is associated with the growth of the ICDW amplitude with Fe doping. As the ICDW amplitude increases, the C phase is favoured over the I phase and the triple point moves towards larger values of the nesting parameter δ . So even without donating electrons to the d band, Fe impurities would still act like electron donors by stabilizing the C phase at high concentrations.

Together, the experimental measurements and phenomenological model described in this paper present a radically new picture for the Fe moment in a Cr host. In contrast to previous authors [20], we have argued that the single moments are only partly constrained by the SDW matrix and play a crucial role in the magnetic susceptibility at low fields. Hopefully, this work will motivate other experimentalists and theorists to continue to explore the physics of this fascinating system.

Acknowledgments

One of us (RF) would like to acknowledge useful conversations with Dr Sam Liu. This research was partially supported by the Brazilian Agencies CNPq and FAPESP (VG and WO) and by Oak Ridge National Laboratory (RF) managed by Lockheed Martin Energy Research Corporation for the US Department of Energy under Contract No DE-AC05-96OR22464.

References

- [1] Berger A and Hopster H 1994 *Phys. Rev. Lett.* **73** 193
- [2] Davies A, Strosio J A, Pierce D T and Celotta R J 1996 *Phys. Rev. Lett.* **76** 4175
- [3] Mirbt S, Abrikosov I A, Johansson B and Skriver H L 1997 *Phys. Rev. B* **55** 67
- [4] Galkin V Yu, Ali N, Fawcett E and deCamargo P C 1998 *J. Phys.: Condens. Matter* **10** 4901
- [5] Ishikawa Y, Tournier R and Filippi J 1965 *J. Phys. Chem. Solids* **26** 1727
- [6] Fawcett E 1988 *Rev. Mod. Phys.* **60** 209
- [7] Fawcett E, Alberts H L, Galkin V Yu, Noakes D R and Yakhmi J V 1994 *Rev. Mod. Phys.* **66** 25
- [8] Fedders P A and Martin P C 1966 *Phys. Rev.* **143** 245
- [9] Fishman R S and Liu S H 1993 *Phys. Rev. B* **48** 3820
- [10] Fawcett E and Galkin V Yu 1992 *J. Magn. Magn. Mater.* **109** L139
- [11] Fawcett E and Galkin V Yu 1993 *J. Magn. Magn. Mater.* **119** 329
- [12] Hamaguchi Y, Wollan E O and Koehler W C 1965 *Phys. Rev.* **138** A737
- [13] Bacon G E and Cowlam N 1969 *J. Phys. C: Solid State Phys.* **2** 238

- [14] Werner S A, Arrott A and Kendrick H 1967 *Phys. Rev.* **155** 528
Werner S A, Arrott A and Atoji M 1968 *J. Appl. Phys.* **39** 671
Werner S A, Arrott A and Atoji M 1968 *J. Appl. Phys.* **40** 1447
- [15] Sternlieb B J, Lorenzo E, Shirane G, Werner S A and Fawcett E 1994 *Phys. Rev. B* **50** 16438
- [16] Hedman L E, Rao K V and Åström H U 1978 *J. Physique Coll.* **39** C6 788
- [17] Friedel J and Hedman L E 1978 *J. Physique* **39** 1225
- [18] Kelly J R, Moyer C A and Arajs S 1979 *J. Appl. Phys.* **50** 7516
- [19] Cywinski R and Hicks T J 1980 *J. Phys. F: Met. Phys.* **10** 693
- [20] Babic B, Kajzar F and Parette G 1980 *J. Phys. Chem. Solids* **41** 1303
Kajzar F, Parette G and Babic B 1981 *J. Phys. Chem. Solids* **42** 501
- [21] Moze O, Mitchell P W, Burke S K, Davis J R and Booth J G 1988 *J. Phys. F: Met. Phys.* **18** 527
- [22] Aidun R, Arajs S and Moyer C A 1985 *Phys. Status Solidi b* **128** 133
- [23] Galkin V Yu, Ortiz W A, Fawcett E, Ali N and deCamargo P C 1998 *J. Phys.: Condens. Matter* **10** 4911
- [24] Galkin V Yu, Ortiz W A and Fishman R S 1998 *J. Magn. Magn. Mater* at press
- [25] Galkin V Yu and Fawcett E 1993 *J. Magn. Magn. Mater.* **119** 321
- [26] Hedgcock F T, Strom-Olsen J O and Wilford D F 1977 *J. Phys. F: Met. Phys.* **7** 855
- [27] Jiang X W and Fishman R S 1997 *J. Phys.: Condens. Matter* **9** 3417
- [28] Street R, Munday B C, Window B and Williams I R 1968 *J. Appl. Phys.* **39** 1050
- [29] Steinitz M O, Kalejs J P, Perz J M and Fawcett E 1973 *J. Phys. F: Met. Phys.* **3** 617
Steinitz M O and Pink D A 1980 *J. Phys. F: Met. Phys.* **10** L247
- [30] Herbert I R, Clark P E and Wilson G V H 1972 *J. Phys. Chem. Solids* **33** 979