

Magnetic susceptibility of antiferromagnetic chromium containing nonmagnetic impurities

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The static spin susceptibility of antiferromagnetic chromium containing nonmagnetic impurities is calculated using a two-band model. Variation in the size of the electron and hole octahedron upon alloying is taken into account within the rigid-band approximation. The impurity phonon-scattering contributions to the susceptibility have been evaluated. The theory is compared with experimental results on binary chromium alloys containing dilute amounts of ruthenium and rhenium. Agreement is found to be quite good.

I. INTRODUCTION

In the spin-density-wave (SDW) state, chromium and its alloy exhibit interesting and, in many cases, poorly understood behavior. Because of the large amount of magnetic-susceptibility data now available on diverse binary chromium systems,¹⁻⁴ susceptibility calculations offer a very useful tool for enhancing our understanding of itinerant antiferromagnetism. Unfortunately, due to the complexity of the problem, approximations are unavoidable. Between these and the possible effects of other contributions to the susceptibility, one is unsure how much quantitative agreement is to be expected from a particular model.

Fedders and Martin⁵ examined the magnetic susceptibility of a two-band antiferromagnet just below the Néel temperature using a simple model in which the electron and hole octahedra were replaced by spheres of equal size. The dispersion relations for the electron band (band *a*) and hole band (band *b*) were taken to be linear. They found that just below the Néel temperature, the susceptibility decreased linearly with decreasing temperature, *T*. Crisan⁶ and Moyer *et al.*¹ extended Fedders and Martin's work to lower temperatures and found a *T*² dependence over a much greater range of *T*. Experimentally, this prediction appears to be born out for Cr-Ru alloys¹ but is less than accurate for Cr-Re alloys.² Moyer, Arajs, and Hedman⁷ generalized the model of Fedders and Martin to allow for more band-structure detail. Specifically, they included the curvature of the electron density of states at the Fermi surface. Treating the gap in the excitation spectrum as a parameter, they attempted to fit the susceptibility of pure chromium over the entire antiferromagnetic regime, with little success.

Our initial attempt at extending these results involved allowing for variation in the size of the electron and hole pockets, as well as including the varia-

tion of the Fermi energy with temperature due to the finiteness of the density of states of the remaining nonmagnetic bands (the reservoir). The approximation of spherical bands was retained. This is essentially the model first introduced by Rice.⁸ Our results were less than gratifying. Unlike the data on Cr-Ru and Cr-Re alloys, the theoretical susceptibility was very sensitive to alloy concentration. Also, the predicted gap at *T* = 0 was only half that which has been observed in optical-absorption studies.⁹

In what follows, we report our latest findings for the susceptibility of chromium alloys containing nonmagnetic impurities. The basic model is similar to that outlined in the preceding paragraph. Here, however, we allow for intraband scattering of the magnetic electrons by the impurity ions. This scattering introduces a finite lifetime for the electron-hole pairs. After the formalism has been developed in terms of a lifetime, intraband transitions due to electron-phonon scattering are readily added via a lifetime for such processes. Barker *et al.*¹⁰ have pointed out that this scattering is significant. The total scattering lifetime τ is then given as

$$\frac{1}{\tau} = \frac{1}{\tau_I} + \frac{1}{\tau_{ph}}, \quad (1)$$

where τ_I is the impurity-scattering lifetime and τ_{ph} is the phonon-scattering lifetime. τ_{ph} is calculated from the electron-phonon interaction using the Born approximation.

The theoretical development in the following section is based on the technique of the temperature Green's function. This follows closely previous work done on the excitonic state by Zittartz¹¹ and Maki and Sakurai.¹² For the susceptibility of itinerant antiferromagnets, the treatment is complicated by the presence of another variable *H* which measures the relative size of the electron and hole pockets in the chromium host.

II. GREEN'S FUNCTION AND GAP EQUATION

Our starting point is the following model Hamiltonian:

$$H = \sum_{\vec{k}\sigma} [E_a(\vec{k}) a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + E_b(\vec{k}) b_{\vec{k}\sigma}^\dagger b_{\vec{k}\sigma}] + \frac{1}{2} \bar{V} \sum_{\vec{q}\sigma} \rho_\sigma(\vec{q}) \rho_{-\sigma}(-\vec{q}) + \sum_{\mu\vec{q}\sigma} u_\mu(\vec{q}) \rho_\sigma(\vec{q}). \quad (2)$$

$a_{\vec{k}\sigma}^\dagger$ and $b_{\vec{k}\sigma}^\dagger$ are creation operators for electrons with wave vector \vec{k} and spin σ in band a and band b , respectively. \bar{V} is the transform of the (screened) electron-electron interaction potential which is taken as a constant. $u_\mu(\vec{q})$ is the transform of the impurity potential from an impurity at lattice site μ . The dispersion relations for the two bands are taken as (in units for which $\hbar=1$)

$$E_a(\vec{k}) = \frac{1}{2m^*} (\kappa^2 - \kappa_0^2), \quad (3)$$

$$E_b(\vec{k} + \vec{Q}) = \frac{1}{2m^*} (\kappa_0^2 - \kappa^2), \quad (4)$$

where m^* is the effective mass for electrons in both bands and \vec{Q} is the ordering wave vector of the SDW. The quantity

$$\rho_\sigma(\vec{q}) = \sum_{\vec{k}} a_{\vec{k}+\vec{q},\sigma}^\dagger a_{\vec{k}\sigma} + b_{\vec{k}+\vec{q},\sigma}^\dagger b_{\vec{k}\sigma} \quad (5)$$

is the partial charge-density operator.¹³

We introduce two auxiliary band functions

$$\epsilon(\vec{k}) = \frac{1}{2} [E_a(\vec{k}) - E_b(\vec{k} + \vec{Q})] \quad (6)$$

and

$$\omega(\vec{k}) = \frac{1}{2} [E_a(\vec{k}) + E_b(\vec{k} + \vec{Q})] - E_F. \quad (7)$$

E_F is the Fermi energy. $\omega(\vec{k})$ is actually independent of \vec{k} in our model and measures the size difference between the electron and hole spheres.

For mathematical conciseness, it is useful to introduce a four-component Nambu notation

$$\psi^\dagger(\vec{k}) = (a_{\vec{k}1}^\dagger, a_{\vec{k}1}^\dagger, b_{\vec{k}+\vec{Q}1}^\dagger, b_{\vec{k}+\vec{Q}1}^\dagger)$$

and

$$\psi(\vec{k}) = \begin{pmatrix} a_{\vec{k}1} \\ a_{\vec{k}1} \\ b_{\vec{k}+\vec{Q}1} \\ b_{\vec{k}+\vec{Q}1} \end{pmatrix}. \quad (8)$$

In addition, we introduce the matrices¹⁴ ρ_i and σ_i ($i=0, 1, 2, 3$). σ_0 and ρ_0 are the two- and four-dimensional identity matrices, respectively; the σ_i are the usual Pauli spin matrices. The remaining ρ_i are most easily defined through their multiplication rules with the σ_i

$$\rho_0 \sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \quad \rho_1 \sigma_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad (9)$$

$$\rho_2 \sigma_i = \begin{pmatrix} 0 & -i \sigma_i \\ i \sigma_i & 0 \end{pmatrix}, \quad \rho_3 \sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & -\sigma_i \end{pmatrix}.$$

We define a temperature Green's function by

$$G(\vec{k}, \vec{k}'; \tau) = -\langle T[\psi(\vec{k}, \tau) \bar{\psi}(\vec{k}', 0)] \rangle, \quad (10)$$

where T is the time-ordering operator and

$$\begin{cases} \psi(\vec{k}, \tau) \\ \bar{\psi}(\vec{k}, \tau) \end{cases} = e^{\beta \bar{H} \tau} \begin{cases} \psi(\vec{k}) \\ \psi^\dagger(\vec{k}) \end{cases} e^{-\beta \bar{H} \tau} \quad (11)$$

are the Heisenberg operators for the imaginary time $\beta\tau$. Also,

$$\bar{H} = H - \mu N, \quad (12)$$

where μ is the chemical potential and N is the electron number operator.

$G(\vec{k}, \vec{k}'; \tau)$ has the Fourier series expansion

$$G(\vec{k}, \vec{k}'; \tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} G(\vec{k}, \vec{k}'; i\omega_n) e^{-i\omega_n \beta \tau}, \quad (13)$$

$$\beta \omega_n = (2n + 1) \pi. \quad (14)$$

The correlations appropriate to the SDW state are⁵

$$\langle a_{\vec{k}\alpha}^\dagger(\tau) a_{\vec{k}'\beta}(0) \rangle = \delta_{\alpha\beta} \delta_{\vec{k}, \vec{k}'} \langle a_{\vec{k}1}^\dagger(\tau) a_{\vec{k}1}(0) \rangle, \quad (15)$$

$$\langle b_{\vec{k}\alpha}^\dagger(\tau) b_{\vec{k}'\beta}(0) \rangle = \delta_{\alpha\beta} \delta_{\vec{k}, \vec{k}'} \langle b_{\vec{k}1}^\dagger(\tau) b_{\vec{k}1}(0) \rangle, \quad (16)$$

$$\begin{aligned} \langle a_{\vec{k}\alpha}(\tau) b_{\vec{k}'\beta}^\dagger(0) \rangle &= \langle b_{\vec{k}'\beta}(\tau) a_{\vec{k}\alpha}^\dagger(0) \rangle^* \\ &= i \sigma_{\alpha\beta}^{(2)} \delta_{\vec{k}', \vec{k} + \vec{Q}} \langle a_{\vec{k}1}(\tau) b_{\vec{k}+\vec{Q}1}^\dagger(0) \rangle. \end{aligned} \quad (17)$$

These correlations describe a spin polarization in the y direction and reduce the number of independent, nonzero elements of $G(\vec{k}, \vec{k}'; i\omega_n)$ to 4. In matrix form they are

$$\tilde{G}(\vec{k}, \vec{k}'; i\omega_n) = \begin{pmatrix} G_{11}^{aa}(\vec{k}, \vec{k}'; i\omega_n) & G_{11}^{ab}(\vec{k}, \vec{k}'; i\omega_n) \\ G_{11}^{ba}(\vec{k} + \vec{Q}, \vec{k}'; i\omega_n) & G_{11}^{bb}(\vec{k} + \vec{Q}, \vec{k}'; i\omega_n) \end{pmatrix}. \quad (18)$$

This matrix is equivalent to the Green's function calculated by Zittartz for the singlet excitonic insulator. In the Hartree-Fock approximation we have [cf. Eq. (24) of Ref. 11]

$$\tilde{G}(\vec{k}; i\omega_n) = -\frac{1}{D} \begin{pmatrix} i\tilde{\Omega}_n + \epsilon & \tilde{\Delta}_n \\ \tilde{\Delta}_n & i\tilde{\Omega}_n - \epsilon \end{pmatrix}, \quad (19)$$

where

$$D = \epsilon^2 + \tilde{\Delta}_n^2 + \tilde{\Omega}_n^2, \quad (20)$$

$$\tilde{\Omega}_n = \tilde{\omega}_n + i\omega(\vec{k}) \equiv \tilde{\omega}_n + iH,$$

and $\tilde{\Delta}_n$ and $\tilde{\Omega}_n$ are solutions of the two coupled equations

$$\tilde{\Delta}_n = \Delta - \frac{1}{2\tau} \frac{\tilde{\Delta}_n}{(\tilde{\Omega}_n^2 + \tilde{\Delta}_n^2)^{1/2}}, \quad (21)$$

$$\tilde{\Omega}_n = \Omega_n + \frac{1}{2\tau} \frac{\tilde{\Omega}_n}{(\tilde{\Omega}_n^2 + \tilde{\Delta}_n^2)^{1/2}}.$$

τ is the lifetime (in the Born approximation) of the electrons at the Fermi surface due to intraband scattering by the impurities. The order parameter Δ in Eqs. (21) is a solution of

$$\Delta = -\frac{\bar{V}}{\beta} \sum_{\vec{k}, \omega_n} G_{\uparrow\uparrow}^{qp}(\vec{k}; i\omega_n). \quad (22)$$

Although Eq. (19) is identical in form to that given in Ref. 11, there is one significant difference. For electron and hole spheres of different size (finite H), $\tilde{\Delta}_n$ will be complex. The integrals leading to Eqs. (21) can be performed using the residue calculus, but care must be taken in locating the proper poles. The result is that the convention on the square root

$(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}$ requires that one take the root with positive real part.

If similar caution is observed when evaluating Eq. (22) for the gap, Zittartz's result is readily generalized to the more complicated equation

$$\begin{aligned} \ln \frac{T_{N,0}}{T} + \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta_{N,0} H_{N,0}}{2\pi} \right] - \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta H}{2\pi} \right] \\ = \frac{2\pi}{\beta} \text{Re} \sum_{n=0}^{\infty} \left(\frac{\omega_n}{\omega_n^2 + H^2} - \frac{\tilde{\Delta}_n/\Delta}{(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}} \right), \end{aligned} \quad (23)$$

where the subscript $N, 0$ means the subscripted quantity is evaluated at the Néel temperature in the absence of scattering. ψ is the digamma function and Re denotes "real part of." In the limit $T \rightarrow T_N$, $\Delta \rightarrow 0$, and Eq. (23) becomes

$$\begin{aligned} \ln \frac{T_{N0}}{T_N} = \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta_N H_N}{2\pi} + \frac{\beta_N}{2\pi\tau} \right] \\ - \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta_{N,0} H_{N,0}}{2\pi} \right]. \end{aligned} \quad (24)$$

Combining Eqs. (23) and (24), we obtain

$$\begin{aligned} \ln \frac{T_N}{T} + \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta_N H_N}{2\pi} + \frac{\beta_N}{2\pi\tau} \right] - \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta H}{2\pi} \right] \\ = \frac{2\pi}{\beta} \text{Re} \sum_{n=0}^{\infty} \left(\frac{\omega_n}{\omega_n^2 + H^2} - \frac{\tilde{\Delta}_n/\Delta}{(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}} \right). \end{aligned} \quad (25)$$

For numerical calculation, it is preferable to work with an equivalent form which makes the sum more rapidly convergent,

$$\ln \frac{T_N}{T} + \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta_N H_N}{2\pi} + \frac{\beta_N}{2\pi\tau_N} \right] - \text{Re}\psi \left[\frac{1}{2} + i \frac{\beta H}{2\pi} + \frac{\beta}{2\pi\tau} \right] = \frac{2\pi}{\beta} \sum_{n=0}^{\infty} \left(\frac{\omega_n + 1/\tau}{(\omega_n + 1/\tau)^2 + H^2} - \text{Re} \frac{\tilde{\Delta}_n/\Delta}{(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}} \right). \quad (26)$$

Here, we have subscripted τ in the first digamma function in anticipation of the electron-phonon interaction which will make the lifetime temperature dependent.

Until now, we have implicitly assumed that H is temperature dependent; henceforth, we take H to be constant. This is equivalent to assuming the reservoir has an infinite density of states. To take account of a finite reservoir, one would need to add an additional equation representing the conservation of the number of electrons.⁸

With H constant Eq. (26), together with Eqs. (21), allows one to calculate the gap as a function of temperature below T_N .

The total Green's function also can be obtained us-

ing Eq. (19) and the correlations Eqs. (15)–(17). In terms of the spin matrices introduced earlier,

$$G(\vec{k}; i\omega_n) = -\frac{1}{D} (i\tilde{\Omega}_n + \epsilon\rho_3 - \tilde{\Delta}_n\rho_2\sigma_2). \quad (27)$$

III. RENORMALIZED SPIN VERTEX AND SUSCEPTIBILITY

The components of the magnetic susceptibility tensor are¹²

$$\chi_{ij} = -\frac{\mu_B^2}{\beta} \sum_{\vec{k}, \omega_n} \frac{1}{4} \text{Tr}[\rho_0 \tilde{\sigma}_i G(\vec{k}; i\omega_n) \rho_0 \sigma_j G(\vec{k}; i\omega_n)], \quad (28)$$

where Tr denotes the trace operation, μ_B is the Bohr magneton, and $\tilde{\sigma}_i$ is the spin vertex renormalized by impurity scattering. The renormalized spin vertices are solutions of^{12,15}

$$\rho_0 \tilde{\sigma}_i = \rho_0 \sigma_i + n \int \frac{d^3 \kappa'}{(2\pi)^3} |u(\bar{\kappa} - \bar{\kappa}')|^2 G(\bar{\kappa}'; i\omega_n) \times \rho_0 \tilde{\sigma}_i G(\bar{\kappa}'; i\omega_n), \quad (29)$$

where n is the concentration of impurities. Inserting Eq. (27) for $G(\bar{\kappa}'; i\omega_n)$ and performing the integration in the same manner as for the Green's function, one obtains three independent algebraic equations for the $\tilde{\sigma}_i$,

$$\begin{aligned} \rho_0 \tilde{\sigma}_1 &= \rho_0 \sigma_1, \\ \rho_0 \tilde{\sigma}_2 &= A_{0,2} \rho_0 \sigma_2 + A_{2,0} \rho_2, \\ \rho_0 \tilde{\sigma}_3 &= \rho_0 \sigma_3, \end{aligned} \quad (30)$$

where $A_{0,2}$ and $A_{2,0}$ are given by

$$\begin{aligned} A_{0,2} &= 1 + \frac{A}{2\tau(1+u_n^2)(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}}, \\ A_{2,0} &= -\frac{i u_n A}{2\tau(1+u_n^2)(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}}, \end{aligned} \quad (31)$$

with

$$\begin{aligned} u_n &= \frac{\tilde{\Omega}_n}{\tilde{\Delta}_n}, \\ A &= \left[1 + \frac{1}{2\tau(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2}} \left(1 - \frac{2}{1+u_n^2} \right) \right]^{-1}. \end{aligned} \quad (32)$$

Using Eqs. (30)–(32), the diagonal components of the susceptibility tensor can be calculated by straightforward integration of Eq. (28). We obtain

$$\chi_{11} = \chi_{33} = \mu_B^2 N(0) \equiv \chi_0, \quad (33)$$

where $N(0)$ is the density of states at the Fermi surface. Thus in this model the spin susceptibility perpendicular to the SDW polarization is unaffected and remains the usual Pauli contribution. However, parallel to the SDW polarization we have

$$\begin{aligned} \chi_{22} &= \chi_0 \left[1 - \frac{2\pi}{\beta} \text{Re} \sum_{n=0}^{\infty} \left[(1+u_n^2)(\tilde{\Delta}_n^2 + \tilde{\Omega}_n^2)^{1/2} \right. \right. \\ &\quad \left. \left. \times \left[1 + \frac{\Delta - \tilde{\Delta}_n}{\tilde{\Delta}_n} \frac{u_n^2 - 1}{u_n^2 + 1} \right] \right]^{-1} \right]. \end{aligned} \quad (34)$$

For a polycrystalline sample, the measured susceptibility is

$$\chi_p = \frac{1}{3} \text{Tr} \bar{\chi}. \quad (35)$$

IV. PHONON-SCATTERING PROCESSES

The phonon-scattering contribution to the susceptibility is included by regarding the lifetime in the preceding development as a combination of an impurity and phonon-scattering lifetime according to Eq. (1). As observed previously, these are lifetimes for electrons at the Fermi surface. We treat the phonon lifetime in the Born approximation where it is given as

$$\frac{1}{\tau_{\text{ph}}} = \frac{2\pi}{\hbar} \sum_{\substack{n' \kappa' \sigma' \\ n_f}} |\langle n_f | \langle n' \kappa' \sigma' | H_{\text{int}} | n \kappa \sigma \rangle | n_i \rangle|^2 \delta(E_f - E_i) \quad (36)$$

Here $|n_i\rangle$ and $|n_f\rangle$ are the initial and final phonon states, respectively, whereas E_i and E_f are the initial and final energies of the entire system, electron and phonons. H_{int} is the electron-phonon interaction Hamiltonian in the harmonic approximation. Unlike the impurity lifetime, the phonon lifetime is temperature dependent. To include temperature effects, a thermal average must be performed over all initial phonon states.

To reduce Eq. (36) to manageable form, several approximations must be made:

- (i) Only intraband processes are considered.
- (ii) We ignore scattering involving optical phonons and consider only scattering by longitudinally-polarized acoustic phonons. Also, umklapp processes are ignored.
- (iii) The previous approximation is partly justified by the use of deformation potential theory to evaluate matrix elements of the interaction.¹⁶
- (iv) A linear dispersion relation is assumed to be valid for the phonon spectrum. Further, the spectrum is assumed to have a cutoff frequency, ω_D , given by

$$\omega_D = \frac{K_B \Theta_D}{\hbar}, \quad (37)$$

where Θ_D is the Debye temperature.

Applying these approximations to Eq. (36) and averaging over initial phonon states, we obtain, after a considerable amount of labor,

$$\frac{1}{\tau_{\text{ph}}} = \frac{1}{\tau_0} \left[1 + 6 \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} dx \frac{x^2}{e^x - 1} \right]. \quad (38)$$

τ_0 is a complicated constant which represents the scattering lifetime at $T=0$ due to virtual-phonon processes.

It is a fortunate consequence of this model that once the zero-temperature scattering lifetime and the Debye temperature are specified, the lifetime as a function of temperature is determined completely. A reasonably accurate estimate of the scattering lifetime τ_0 can be obtained from effective-mass studies of pure chromium. The lifetime has a temperature of

$T_{\text{ph}} \sim 320$ K (i.e., $\hbar/\tau_0 = K_B T_{\text{ph}}$).⁹ Also, the Debye temperature of chromium is known quite accurately¹⁷: $\Theta_D = 630$ K. We assume that alloying with dilute amounts of impurity does not alter these values significantly.

V. COMPARISON WITH EXPERIMENT

We first applied the theory developed above to pure chromium. With the Debye temperature and phonon lifetime τ_0 fixed at the previously specified values, the only variable parameters are H and χ_0 . χ_0 was chosen so that the theoretical and experimental results would agree at some specified temperature T_0 . H was then varied until the best fit was obtained. Table I lists the parameters used to construct the theoretical curve in Fig. 1. The table also gives the theoretically predicted gap Δ_0 at $T=0$. This gap is substantially larger than the experimental value⁹ (0.11 eV vs 0.075 eV). Some of the discrepancy probably results from assuming a commensurate structure for chromium. However, even for the alloys, for which a commensurate calculation is appropriate, the theoretical Δ_0 given in Table I are 10 to 20 percent higher than those found experimentally by Barker and Ditzemberger.⁹

As can be seen from Fig. 1, the agreement between theory and experiment for the susceptibility of pure chromium is quite good above ~ 120 K. Below this temperature, the experimental susceptibility drops off quickly to a minimum around 85 K. This minimum is one of the most intriguing aspects of the chromium susceptibility and is not explicable in terms of our model. Recently, Anghel and Crisan¹⁸ have made an attempt to explain this minimum by considering the possible coexistence of the SDW and itinerant electron ferromagnetism due to formation of a charge-density wave. Their model displays a minimum similar to that observed experimentally. However, their model also exhibits a divergence in the susceptibility at the ferromagnetic Curie temperature which is not observed experimentally. Whatever the origin of the minimum, the experimental points in Fig. 1 suggest that it is related to the spin-flip tran-

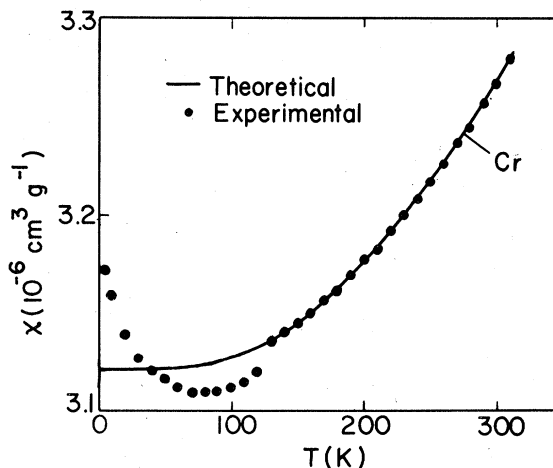


FIG. 1. χ_p vs T for pure chromium.

sition which takes place at 123 K. Below this temperature, the SDW switches from transverse to longitudinal polarization.

Alloying changes H and introduces an additional parameter, the impurity scattering lifetime, with its temperature equivalent, T_{sc} . However, in a rigid-band approximation in which H varies directly with concentration, we have

$$H = \left(1 - \frac{n}{n_p}\right) H_{\text{Cr}}, \quad (39)$$

where H_{Cr} is the value for pure chromium and n_p is the impurity concentration for perfect nesting. From our unpublished investigations of the Néel temperature of binary chromium alloys, we estimate $n_p = 3.8$ at. % for Cr-Ru alloys. If we assume that each Re atom donates half as many additional electrons to the bands as a Ru atom, we find $n_p = 7.6$ at. % for the Cr-Re alloys.

With Eq. (39), the alloy problem reduces to the determination of the two parameters χ_0 and T_{sc} . χ_0 was again chosen to give agreement between theory and experiment at some specified temperature, T_0 . For the largest impurity concentration of each type, T_{sc} was varied until the best fit was obtained. Since,

TABLE I. Parameters used to construct the theoretical curve in Fig. 1, and the predicted gap Δ_0 at $T=0$.

	T_{ph}	Θ_D	T_{sc}	T_0	H	Δ_0
Cr	320	630	0	140	0.021	0.11
Cr-Ru 2.1	320	630	140	320	0.009	0.16
Cr-Ru 3.0	320	630	200	320	0.004	0.18
Cr-Re 5.05	320	630	150	320	0.007	0.19
Cr-Re 6.52	320	630	220	320	0.003	0.19

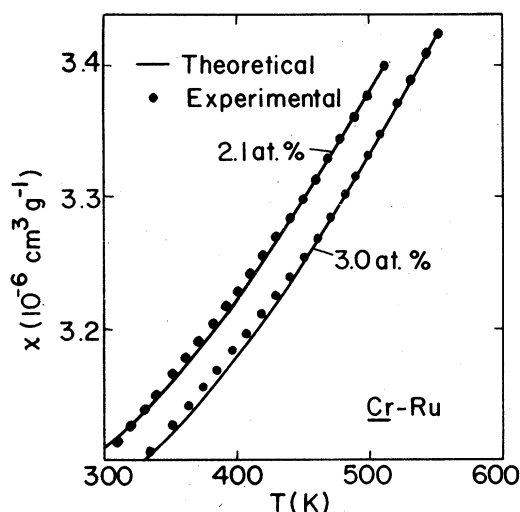


FIG. 2. χ_p vs T for chromium containing 2.1 and 3.0 at. % ruthenium.

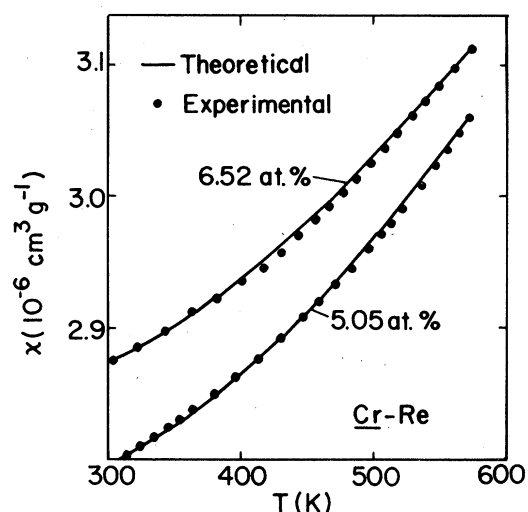


FIG. 3. χ_p vs T for chromium containing 5.05 and 6.52 at. % rhenium.

for low-impurity concentrations, the lifetime should be proportional to the concentration, a linear interpolation was used to obtain T_{sc} for the more dilute alloys.

Figures 2 and 3 show the results for Cr-Ru 2.1 and 3.0 at. % and Cr-Re 5.05 and 6.52 at. %, respectively. The theoretical curves were obtained with the parameters given in Table I. The experimental data which was used has been previously reported.^{1,2} (Unfortunately, no detailed studies have been carried out over the entire temperature region from 0 K to T_N .) For both alloy systems, the agreement is better for the lower concentration. This is expected since the theory is developed only to first order in the impurity concentration. Also, comparison of Figs. 2 and 3 shows that the agreement is slightly better for the Cr-Re alloys. This may indicate a breakdown in the Born approximation for the Cr-Ru alloys in which the

impurity ions possess a larger unshielded positive charge.

Overall, it appears that the model introduced here satisfactorily explains the behavior of the susceptibility of antiferromagnetic chromium when alloyed with dilute amounts of nonmagnetic impurities. It is worth emphasizing that the success of this model over the previous ones is primarily due to the inclusion of electron-phonon scattering.

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