

states proposed by RG.

⁸In the range $650 < T < 1210$ K, the configurations of Co_I and Co_{II} sublattices would be $\text{Co}_a^{III} \text{Co}_b^{II} \text{Co}_c^{III} \text{Co}_d^{4+}$ and $\text{Co}_a^{3+} \text{Co}_b^{4+} \text{Co}_c^{III} \text{Co}_d^{II}$, respectively. At 650 K, $d \approx 0$. The preferential excursions of La^{3+} ions towards Co_I found by RG in the $650 < T < 925$ -K range in $b > d$; the Co_I -O and Co_{II} -O separations are similar in this temperature range. Further, in this temperature range, it is likely that $a \approx b + c + d$, so that the e_g electrons spend equal time at all Co ions, a behavior which is reasonable near the LI transition. As $T \rightarrow 1210$ K, $b \approx d \approx 0$, and the La^{3+} ions are midway between the Co_I and Co_{II} subarrays. When $T > 925$ K, $a < c$ and the

Co_I -O separation should be smaller than the Co_{II} -O separation, as observed by RG (Ref. 1). At $T \geq 1210$ K, the configurations of the two cobalt sites are likely to be $(t_2^6 \sigma^{*5})_a (t_2^5 \sigma^{*1})_{1/2-a}$ and $(t_2^4 \sigma^{*2-5})_a (t_2^5 \sigma^{*1})_{1/2-a}$.

⁹This is consistent with our Mössbauer results, except that we find that ordering occurs after the transfer of σ -bonding d electrons from Co^{3+} to Co^{III} ions.

¹⁰ GdCoO_3 shows transitions around 500 and 980 K, the latter corresponding to the LI transition. Our results on GdCoO_3 significantly differ from those of A. Casalot, P. Dougier, and P. Hagenmuller [J. Phys. Chem. Solids **32**, 407 (1971)], who failed to see the first-order transition at 980°K.

Effect of Pressure and Alloying on the Itinerant Antiferromagnetic Ordering in Cr-Fe Alloys

Rajaram Nityananda and A. S. Reshamwala

Materials Science Division, National Aeronautical Laboratory, Bangalore-17, India

and

A. Jayaraman

Bell Telephone Laboratories, Murray Hill, New Jersey 07974, and Materials Science Division, National Aeronautical Laboratory, Bangalore-17, India

(Received 8 March 1972)

We have investigated the effect of hydrostatic pressure on chromium-rich iron alloys with Ru and Mn additions. The results show that addition of Fe to Cr rotates the commensurate-incommensurate phase boundary and causes the reversal in the ordering sequence of the magnetic transitions observed in Cr-Fe alloys. Many other anomalous characteristics of Cr-Fe alloys are explained.

The itinerant antiferromagnetic transitions in chromium-rich alloys containing a wide variety of transition metals have been studied extensively at atmospheric pressure¹⁻⁹ and also at high pressure.¹⁰⁻¹² Of these, the behavior of Cr-Fe alloys^{3-5, 10, 12} is unique and also poorly understood. The anomalous situation with regard to Cr-Fe alloys^{4, 5} is the following: (1) the lowering of T_N when Fe is added; (2) the appearance of only the incommensurate (I) phase at low Fe concentration ($< 2\%$); (3) the appearance of the commensurate (C) phase at higher concentration of Fe, but at a lower temperature than the I phase; (4) the sharp and large resistivity rise ($\Delta\rho/\rho \approx 40\%$) at the I-C transition; and (5) the presence of local magnetic moment on Fe, which is only weakly coupled to the antiferromagnetic (AF) state of Cr. In this study we have investigated, under pressure, Cr-Fe alloys with Ru or Mn additions. The important finding is that a triple point between paramagnetic (P), I, and C phases exists in Cr-Fe alloys as in Cr-Mn or Cr-Ru alloys,¹¹ but the addition of Fe to Cr twists

the I-C phase boundary and reverses the magnetic ordering sequence P-C-I observed in the latter alloys.¹¹ It is suggested that the sharp resistance anomaly at the I-C transition and the progressive loss of sharpness^{10, 12} with pressure may be due to the closeness of the latter to the P-I transition at low pressure, and their separation at higher pressure.

Hydrostatic pressure was generated as described earlier.¹³ The resistivity anomaly was used to follow the transitions. Figure 1 shows the resistivity as a function of temperature at various pressures, for Cr-3% Fe-0.5% Ru. In the inset the resistivity-temperature data for Cr-3% Fe is shown.¹² The addition of 0.5% Ru has raised the T_N by 125°, and has broadened the sharp resistivity anomaly seen in Cr-3% Fe alloy. We believe this transition to be the P-C transition. When pressure is applied, T_N falls at a rate of about 15°/kbar. In the range 9-11 kbar the resistance anomaly becomes almost as steep as that seen for the I-C transition in Cr-3% Fe alloy and has a clearly identifiable inflection point, which we be-

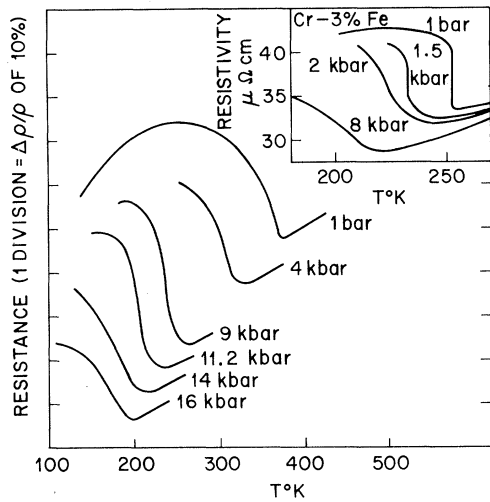


FIG. 1. Resistivity anomaly of Cr-3% Fe-0.5% Ru alloy at various pressures. The curves have been given arbitrary displacements for clarity. Inset illustrates the resistivity-temperature behavior of Cr-3% Fe alloy.

lieve is associated with the occurrence of the I-C transition. At high pressure this steepness is lost, as in Cr-3% Fe alloy. Similar results are obtained for Cr-3% Fe-1% Mn. We identify the inflection point of the steep resistivity anomaly (see Fig. 1) as the I-C transition temperature and the minimum as the T_N of the P-I transition. The minimum observed at lower pressures (below 8 kbar) is taken to be the T_N of the P-C transition. In Fig. 2 the pressure-temperature data are plotted. The resulting phase diagram shows the stability regions of the P, I, and C phases and the triple point. The sharp peak in slope at about 8 kbar and the values of dT_N/dP are consistent with the identification of the phase boundary up to 8 kbar as the P-C transition and the boundary between 8 and 18 kbar as that of the P-I transition. The slope of the I-C boundary could not be determined as well, because of the disappearance of the steep resistivity anomaly and the associated inflection point, rapidly with increasing pressure. The dashed line is therefore only approximate. However, it is a thermodynamic necessity that the slope of the I-C boundary should be greater than that of the P-C boundary.

In the inset (a) to Fig. 2 we present the phase diagram of Cr-3% Fe alloy.¹² If the phase boundaries P-I and I-C are extrapolated, as shown by the dashed lines in the diagram, they meet at a triple point in the negative pressure region near -1.5 kbar. Earlier experiments on Cr alloys

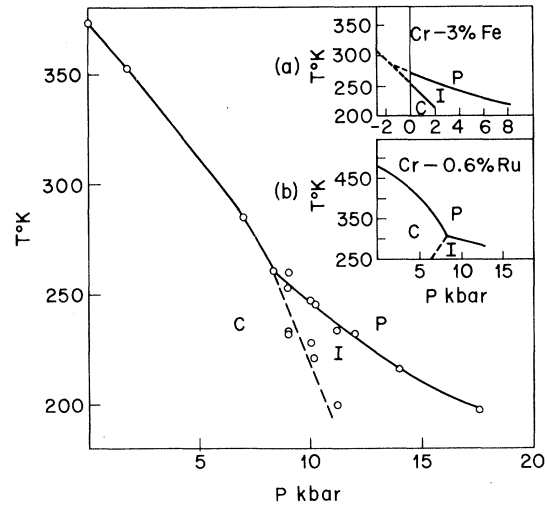


FIG. 2. P - T diagram of Cr-3% Fe-0.5% Ru alloy. The insets show phase diagrams of Cr-3% Fe and Cr-0.6% Ru alloys.

have established that adding a nonmagnetic transition metal, which increases the number of electrons per atom (e/a), is equivalent to applying negative pressure.¹² On this basis, addition of 0.5% Ru is equivalent to about 10 kbar negative pressure, which then brings the triple point within the positive pressure region (see Fig. 2).

Pressure studies on Cr with Ru and Mn additions¹¹ have shown that a triple-point between P, C, and I phases exists in the negative-pressure region for pure chromium. In the inset (b) to Fig. 2 the phase diagram for Cr-0.6% Ru is shown. A comparison of the I-C boundary of this Cr-Ru alloy with that of the Cr-Fe-Ru alloys shows that the addition of Fe to Cr rotates the I-C phase boundary and changes the slope from positive to negative. It is this effect which is responsible for the ordering sequence P-I-C observed (when temperature is reduced) in Cr alloys containing more than 2% Fe. The above ordering sequence is different from the one observed in Cr with Ru or Mn additions. We can now qualitatively explain the behavior of alloys with lower concentrations of Fe (<2% Fe). With the addition of Fe, the main effect is the rotation of the I-C phase boundary towards the P-I boundary. The I-C transition will appear at atmospheric pressure only when the I-C boundary enters the positive pressure region. This would account for the existence of a critical concentration (about 2% Fe) for observing the P-I transition.

Thermodynamically the change of slope of the I-C line means that the addition of Fe has in-

creased the entropy of the I phase relative to the C phase. Syono and Ishikawa suggested¹⁰ that the entropy of electronic origin in the C phase would decrease relative to the I phase, since the Fermi surface truncated by an energy gap of magnetic origin increases discontinuously at the I-C transition. However, this argument for the lower entropy of the C phase runs into difficulty in Cr-Mn and Cr-Ru alloys where the C phase has a larger entropy, although the antiferromagnetic energy gap is strikingly larger for the C phase.¹⁴ It is well known that Fe forms a local moment of $1.4\mu_B$ in Cr.¹⁵ The presence of local moments would cause strong scattering, and this may be expected to have a profound influence on the AF state of Cr. Since the incommensurate phase is more sensitive to scattering this would tend to reduce the stability field of the I phase rather drastically. This can be realized by rotating the I-C phase boundary as discussed, thus contributing to the reversal of the entropy. There can also be another mechanism that can increase the entropy of the I phase relative to the C phase. If we assume some coupling of the Fe local moment to the AF state of chromium (the susceptibility and Mössbauer data¹⁶ suggest only very weak coupling), a weak orienting effect on the Fe local moments follows and this may be expected to be stronger in the C phase than in the I phase where the moments at the nodes of the sinusoidal modulation of spin density would be comparatively free. This will increase the entropy of the I phase relative to the C phase.

The Fe atoms are believed to contribute 0.5 electrons to the d band of chromium.⁴ This should increase the e/a ratio which in turn should increase T_N . *Per contra* a decrease of T_N is observed with the addition of Fe to chromium. However, strong scattering by the Fe local moment and the consequent depairing effect may be responsible for the lowering of T_N , instead of the expected increase. Ishikawa, Hoshino, and Endoh⁴ have reported from neutron diffraction studies that Cr alloys containing more than 4 at. % Fe show only the commensurate transition. This, in fact, is to be expected. If the added Fe contributes some fraction of its electron to the d band of Cr, the e/a ratio would increase, which in turn would shift the system to the negative pressure region. Above a certain concentration of Fe the e/a ratio increase would have moved the system past the triple point [see Fig. 2, inset (a)] and then, only the P-C transition would take place on cooling.

The resistance anomaly associated with the I-C transition in Cr-Fe alloy is an abrupt increase in resistivity of about 40%. The origin of this anomaly is somewhat difficult to understand simply on the basis that I-C transition involves a truncation of additional parts of the Fermi surface. For, in Cr-Mn alloys hardly any resistivity anomaly shows up in the I-C transition despite the fact that the antiferromagnetic energy gap is larger for the commensurate phase.¹⁴ This in itself is puzzling. Further, in Cr-3% Fe alloys application of hydrostatic pressure of only 2.5 kbar wipes out the sharp resistivity anomaly^{10, 12} (this of course is perfectly reversible) associated with the I-C transition. For the abrupt resistivity anomaly and its disappearance we suggest the following: The resistivity of Cr-3% Fe alloy, for instance, would have followed the solid line shown in Fig. 3 if the P-I transition were the only transition occurring. However, in Cr alloys containing more than 2% Fe the I-C transition occurs abruptly accompanied by a sudden lattice expansion (as suggested by Ishikawa, Hoshino, and Endoh⁴) and the resistance also jumps at this point, following the dashed line shown in inset (b). When pressure is applied, the P-I transition and the I-C transition diverge from one another because of the large pressure effect (a factor of 5 larger) on the latter. Now the resistivity would follow the solid line over a larger temperature range and then rise abruptly at the I-C transition, as shown in the dashed line marked 2 in Fig. 3. Soon a pressure would be reached where the two transitions are so far apart they do not overlap. Although the I-C transition may be taking place as abruptly as at lower pressures, the absence

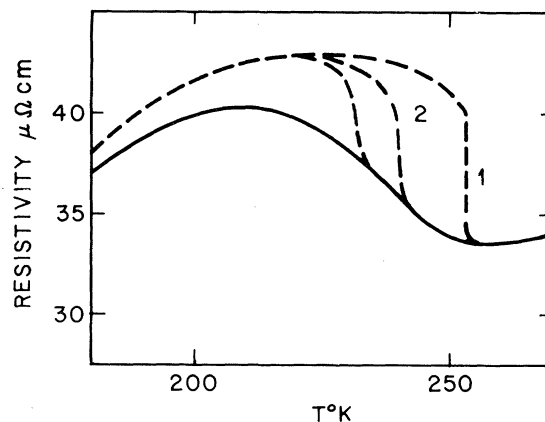


FIG. 3. Resistivity anomaly associated with P-I transition (solid curve) and that of superposed I-C transition in Cr-Fe alloy (dashed curves).

of any marked resistivity anomaly at the transition would make it invisible. This may account for the initial abruptness and progressive loss of this character of the resistivity anomaly.

In Cr-Co alloys Co has a local moment, but unlike Fe it is strongly coupled to the AF state of chromium.¹⁷ We have also investigated a number of these alloys under pressure and find that the behavior is quite different. These results will be published in detail elsewhere.

We would like to thank Dr. T. M. Rice for many illuminating discussions and E. Corenzwit for Cr alloys. One of us (A.J.) would like to thank the John Simon Guggenheim Foundation for the award of a Fellowship at the time the experimental part of this work was done.

¹W. C. Koehler, R. M. Moon, A. L. Tregò, and A. R. Mackintosh, Phys. Rev. **151**, 405 (1966).

²A. L. Tregò and A. R. Mackintosh, Phys. Rev. **166**, 495 (1968).

³S. Arajs and G. R. Dunmyre, J. Appl. Phys. **37**, 1017 (1966).

⁴Y. Ishikawa, S. Hoshino, and Y. Endoh, J. Phys. Soc. Jap. **22**, 1221 (1967).

⁵A. Arrott, S. A. Werner, and H. Kendrick, Phys. Rev. **153**, 624 (1967).

⁶S. Arajs, J. Less-Common Metals **22**, 519 (1970).

⁷S. Arajs, Phys. Status Solidi (a) **1**, 499 (1970).

⁸S. Arajs, T. F. DeYoung, and E. E. Anderson, J. Appl. Phys. **41**, 1426 (1970).

⁹S. Arajs, Can. J. Phys. **47**, 1005 (1969).

¹⁰Y. Syono and Y. Ishikawa, Phys. Rev. Lett. **19**, 747 (1967).

¹¹A. Jayaraman, T. M. Rice, and E. Bucher, J. Appl. Phys., **41**, 969 (1970).

¹²T. M. Rice, A. Jayaraman, and D. B. McWhan, J. Phys. (Paris), Colloq. **32**, C1-39 (1971).

¹³R. G. Maines, Rev. Sci. Instrum. **41**, 1415 (1970).

¹⁴A. S. Barker, Jr., and J. A. Ditzenberger, Phys. Rev. B **1**, 4378 (1970).

¹⁵Y. Ishikawa, R. Tournier, and J. Filippi, J. Phys. Chem. Solids **26**, 1727 (1965).

¹⁶G. K. Wertheim, J. Appl. Phys. **32**, 110 (1961).

¹⁷Y. Endoh, Y. Ishikawa, and H. Ohno, J. Phys. Soc. Jap. **24**, 263 (1968).

Determination of Deformation Parameters of ²⁰Ne and ²²Ne by Inelastic Scattering of Polarized Protons*

R. de Swinarski,† A. D. Bacher,‡ F. G. Resmini,§ G. R. Plattner,|| and D. L. Hendrie
Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720

and

J. Raynal

Service de Physique Théorique, Centre d'Etudes Nucléaires de Saclay, Gif-sur-Yvette, France
(Received 2 August 1971)

Measurements of cross sections and analyzing powers have been made for the inelastic scattering of 24.5-MeV polarized protons leading to the lowest 0^+ , 2^+ , and 4^+ states in ²⁰Ne and ²²Ne. The results for both ²⁰Ne and ²²Ne are best reproduced when the full Thomas form of the deformed, spin-dependent optical potential is employed in a coupled-channel calculation. In contrast to ²⁰Ne, the results for ²²Ne indicate that only a small hexadecapole deformation is needed to reproduce both the cross sections and the analyzing powers for the ²²Ne ground-state rotational band.

It has long been believed on theoretical grounds that many nuclei in the s - d shell have a permanent deformation. Recent experiments and more elaborate theoretical calculations have confirmed this hypothesis. In addition, measurements of the inelastic scattering of protons¹ and α particles² from ²⁰Ne, analyzed in the coupled-channel formalism, have shown that a large hexadecapole (Y_4) deformation was needed to reproduce both the shape and magnitude of the cross sections leading to the lowest 2^+ , 4^+ , and 6^+ states in

²⁰Ne. A similar analysis¹ of other inelastic scattering data in the s - d shell has shown that both the Y_2 and Y_4 moments vary considerably throughout this region. These conclusions are in qualitative agreement with the results of Hartree-Fock-Bogoliubov-type calculations.³ With this in mind, we have measured the analyzing powers of the reactions ²⁰Ne(p, p')²⁰Ne* and ²²Ne(p, p')²²Ne* using polarized protons, leading to the lowest-lying 0^+ , 2^+ , and 4^+ states.⁴ Such measurements are of interest to further test the spin-dependent part of