

## Nonlinear and nonlocal moment disturbance effects in Ni-Cr alloys\*

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We have made polarized-neutron diffuse-scattering measurements on Ni-rich Ni-Cr alloys to determine the magnetic moment distribution on an atomic scale. In contrast to previous unpolarized-neutron measurements, which contain all of the static moment fluctuations from the average, these measurements select out only those fluctuations at one site correlated with the presence of an impurity at another site. The polarized measurement is therefore intrinsically linear in the impurity site occupation. Comparison of the polarized and unpolarized results show that nonlinear effects are important for this system and therefore that both measurements are required to describe the spatial moment distribution away from the dilute impurity region. The total moment disturbance per impurity, obtained by fitting the polarized-neutron data to the local-environment model, decreases rapidly over the concentration region for which  $d\bar{\mu}/dc$  from magnetization data remains constant. We conclude that the impurity-induced moment disturbance has two components: a local-environment effect which we detect with neutrons and a nonlocal effect with range  $\geq 12.5 \text{ \AA}$  that remains undetected in the neutron experiment. We propose a charge-transfer model that contains both the nonlinear and nonlocal effects.

### INTRODUCTION

The spontaneous magnetization of Ni-based Ni-Cr alloys decreases linearly by  $5.2 \mu_B/\text{Cr}$  atom.<sup>1,2</sup> Neutron diffuse-scattering measurements<sup>3</sup> show that this remarkable effect is due largely to a decrease in the moments on the Ni atoms surrounding the impurity atoms. In the dilute region, the magnetic defect extends 5–6  $\text{\AA}$  from the impurity so there is considerable overlapping of the magnetic defects with increasing Cr content. The magnetic cross section per impurity was found to decrease with increasing Cr content and this was attributed to a breakdown of the linear superposition of effects in these overlapping regions. More recently, additional neutron measurements<sup>4</sup> were made near the critical-concentration region. It was noted that the cross sections became more sharply  $K$  dependent (longer-range effects) with increasing Cr content, and it was suggested that this was due to “magnetic polarization clouds” of increasing range on approaching the critical region. The decreasing cross section per impurity was then attributed to a decreasing concentration of these clouds. Both of these neutron studies were made using unpolarized neutrons, for which the analysis requires the assumption of a linear superposition of effects in the overlapping regions. We have made measurements on the Ni-Cr system using polarized neutrons, for which this assumption is not required. By comparison of the two data sets, we find that nonlinear effects are important and therefore that both polarized- and unpolarized-neutron data are required to understand the magnetic moment behavior on an atomic scale.

### THEORY

The moment-defect and the polarization-cloud concepts are different physical descriptions of the same effect, i.e., that the magnetic moment on an atom depends on the local environment of that atom. The theory of magnetic disorder scattering of unpolarized neutrons from such a system has been given by Marshall<sup>5</sup> for the linear-superposition case and extended by Balcar and Marshall<sup>6</sup> to the nonlinear case. We will make use of the nonlinear model, for which the moment on a host atom at site  $n$  is

$$\mu_n(n) = \bar{\mu}_n + \sum_R g(R)(p_{n+R} - c) + \sum_{R,T} a(\vec{R}, \vec{T})(p_{n+R} - c)(p_{n+T} - c). \quad (1)$$

Here,  $\bar{\mu}_n$  is the average host moment,  $c$  is the fractional impurity content, and  $p_{n+R}$  is a site-occupation operator that has a value of unity if there is an impurity at  $\vec{n} + \vec{R}$  and is zero otherwise. The linear moment disturbance produced on a host atom at  $\vec{n}$  by an impurity atom at  $\vec{n} + \vec{R}$  is  $g(R)$ , while  $a(\vec{R}, \vec{T})$  is the additional nonlinear response to impurity atoms at both  $\vec{n} + \vec{R}$  and  $\vec{n} + \vec{T}$ .  $a(\vec{R}, \vec{T})$  is symmetric and vanishes if  $\vec{R} = \vec{T}$ . Balcar and Marshall write a similar function for the moment on an impurity atom as a function of environment, but we will neglect impurity moment fluctuations because we find that the average Cr moment is small, probably zero, in this system. For a random alloy, the magnetic disorder cross section for unpolarized neutrons is given by<sup>6</sup>

$$\frac{d\sigma}{d\Omega}(K) = 0.0484c(1-c)[f(K)]^2 T(K), \quad (2)$$

in which  $f(K)$  is an appropriate form factor and  $T(K)$  has the form

$$T(K) = [M(K)]^2 + c(1-c)[Q(K) + Q(0)] + 2c(1-c)^2[(1-c)L(K) - 2N(K)]. \quad (3)$$

The Fourier transforms are

$$M(K) = \mu_i - \bar{\mu}_h + (1-c) \sum_{\mathbf{R}} g(\mathbf{R}) e^{i\mathbf{R}\cdot\mathbf{K}}, \quad (4)$$

$$Q(K) = \sum_{\mathbf{R}} [g(\mathbf{R})]^2 e^{i\mathbf{R}\cdot\mathbf{K}}, \quad (5)$$

$$L(K) = \sum_{\mathbf{R}, \mathbf{T}, n} a(\mathbf{R}, \mathbf{T}) \alpha(\mathbf{R} - \mathbf{n}, \mathbf{T} - \mathbf{n}) e^{i\mathbf{R}\cdot\mathbf{K}}, \quad (6)$$

$$N(K) = \sum_{\mathbf{R}, \mathbf{T}} a(\mathbf{R}, \mathbf{T}) g(\mathbf{R} - \mathbf{T}) e^{i\mathbf{R}\cdot\mathbf{K}}. \quad (7)$$

In the analysis of unpolarized-neutron cross sections, it has generally been assumed that the  $c$ -dependent terms in Eq. (3) are negligible so that  $T(K) = [M(K)]^2$ . This assumption is certainly justified for dilute alloys, but may not be valid for more concentrated alloys, especially if the impurity-induced moment disturbances are large. Fortunately, it is possible to check for the importance of the nonlinear terms by polarized-neutron diffuse-scattering methods. In contrast to the unpolarized cross section, which contains all of the static-moment fluctuations from the average, the polarized cross section selects out only those fluctuations at  $\mathbf{n}$  that are correlated with an impurity at  $\mathbf{n} + \mathbf{R}$ . The polarized cross section then assumes the simple form

$$\Delta \frac{d\sigma}{d\Omega}(K) = 1.08c(1-c)(b_i - b_h)f(K)M(K), \quad (8)$$

in which  $b_i$  and  $b_h$  are the impurity and host nuclear amplitudes and  $\Delta d\sigma/d\Omega$  refers to the difference between the cross section with incident neutrons polarized parallel and antiparallel to the sample magnetization and perpendicular to the scattering plane. (See Appendix.)

### EXPERIMENTAL RESULTS

Polarized-neutron diffuse-scattering measurements were made on Ni-Cr alloys containing 1-, 5-, and 10-at.% Cr. The samples were 2-mm-thick polycrystalline plates that had been annealed at 1000 °C for 24 h and then quenched to room temperature. These were found to be macroscopically homogeneous and single-phase fcc by electron probe and x-ray analysis. The samples were mounted in symmetrical transmission geometry

and maintained at 4.2K in a 57.3-kOe field during the course of the measurements. The diffuse intensity inside of the first Bragg reflection was measured, corrected for instrumental background, incomplete incident polarization, and sample depolarization, and finally converted to absolute cross sections by calibration with a V standard. These were corrected for multiple Bragg scattering by the usual method,<sup>7</sup> using the observed spin-dependent transmissions, and then converted<sup>8</sup> to  $M(K)$  values by use of Eq. (8). These are shown as the open data points in Fig. 1, where a comparison is made with the  $[T(K)]^{1/2}$  values from the unpolarized data. These agree at the 1-at.% level but are quite different at the higher Cr levels. We attribute this to the nonlinear terms which appear in Eq. (3) with a multiplicative factor of  $c$ . For the more concentrated alloys,  $[T(K)]^{1/2}$  is not a useful function except for illustrative purposes as in Fig. 1. We will therefore consider  $M(K)$  from the polarized data and  $T(K) - [M(K)]^2$  from the combined data. These are shown in Figs. 1 and 2, respectively. The  $M(K)$  data exhibit a strong  $K$  dependence, indicating that the  $g(\mathbf{R})$ 's extend to large distances. In that event, the least-squares fitting

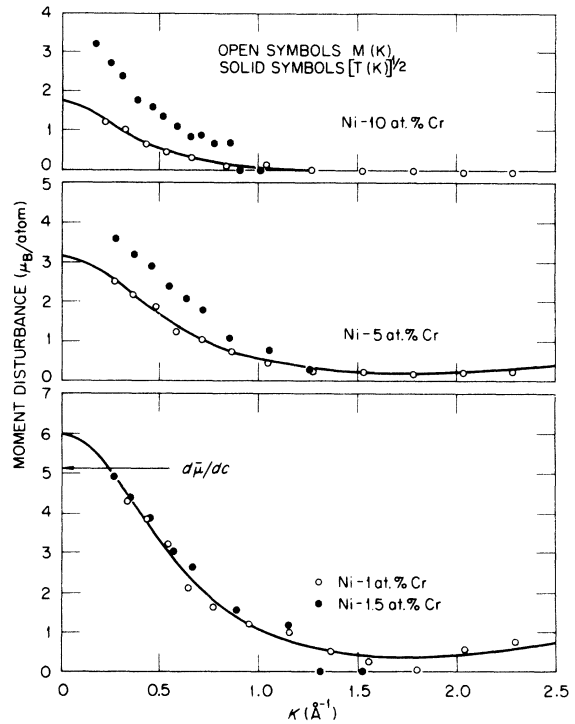


FIG. 1.  $K$ -dependent moment disturbance data for Ni-Cr alloys. The open symbols are polarized-neutron  $M(K)$  data while the closed symbols are unpolarized-neutron  $[T(K)]^{1/2}$  data from Ref. 3 (1.5-at.% Cr), Ref. 4 (10-at.% Cr), and the present work (5-at.% Cr).

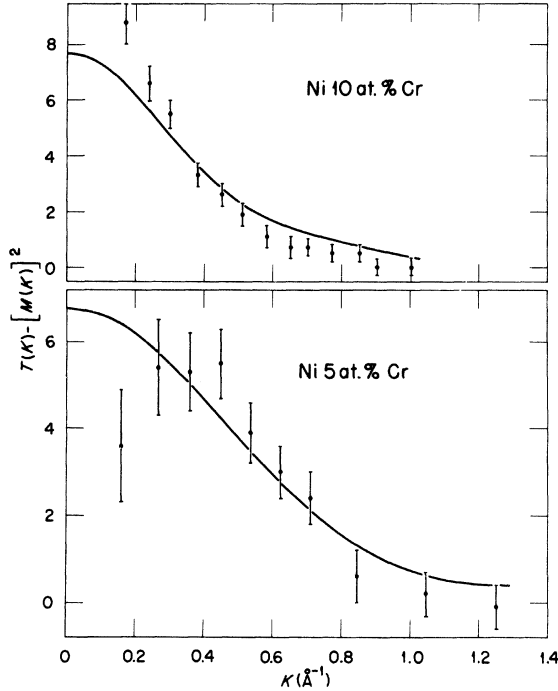


FIG. 2.  $K$ -dependent nonlinear moment disturbance data for 5- and 10-at.% Cr in Ni alloys. The solid curves are fitted to Eq. (3) with the simplifying assumptions described in the text.

of Eq. (4) to the limited data sets of Fig. 1 leads to convergence problems. We avoid these problems by constraining the outer  $g(R)$ 's to a Yukawa-type  $R$  dependence while leaving the inner  $g(R)$ 's as free parameters. There is little difference in the fits or in the parameters, with free  $g(R)$ 's extending to first, second, or third shells. For simplicity, then, we take the fit with free  $g(R)$ 's in the first shell so that

$$g(R) = g(R_1)R_1/Re^{-\kappa(R-R_1)}. \quad (9)$$

The fitted parameters are given in Table I and the corresponding  $M(K)$  functions are shown as the solid curves in Fig. 1. The errors listed in Table I include the statistical and fitting errors as well as the estimated uncertainties in the multiple-Bragg-scattering corrections. The latter domi-

nates in all three cases.

With the  $M(K)$  parameters established, it is now possible to partially characterize the nonlinear terms. First of all, we note that the  $Q(K) + Q(0)$  contribution is readily calculable from the parameters of Table I, and is small. The remaining sums,  $L(K)$  and  $N(K)$ , require some simplifying assumptions for parameterization of the data. Our assumptions are (i) that nonlinear effects occur only if one of the impurity atoms is a first neighbor of the host atom and (ii) that the nonlinear effect decreases exponentially with distance from the host atom, i.e., if  $|T| = R_1$  and  $\vec{R} \neq \vec{T}$ , then

$$a(\vec{T}, \vec{R}) = a(\vec{R}, \vec{T}) = a(R_1, T_1)e^{-B(R-R_1)}. \quad (10)$$

The  $T(K) - [M(K)]^2$  data can then be fitted with the two parameters,  $a(R_1, T_1)$  and  $B$ . The fitted curves are shown in Fig. 2 and the corresponding parameters are given in Table I. The fitted curves describe the data reasonably well for the 5-at.%-Cr alloy, but are not sufficiently long ranged to adequately describe the data at the 10-at.%-Cr level. This suggests a breakdown of our assumption that nonlinear effects occur only if one of the impurities is a nearest neighbor of the host atom. Nevertheless, these parameters indicate the type of nonlinear effects occurring in this system. Although equally good fits were obtained with positive and negative solutions for  $a(R_1, T_1)$ , only the positive solutions are tabulated because of the observed concentration dependence of  $M(0)$ . Balcar and Marshall<sup>6</sup> show that

$$\frac{d\bar{\mu}}{dc} = M(0) \quad (11)$$

and

$$\frac{1}{2} \frac{dM(0)}{dc} = (1-c) \sum_{\vec{R}, \vec{T}} a(\vec{R}, \vec{T}) - \sum_{\vec{R}} g(R) \quad (12)$$

for those systems in which the moment fluctuations depend only on the site occupations. Actually,  $M(0)$  becomes less negative with increasing Cr content while  $d\bar{\mu}/dc$  remains constant. Equation (11) is therefore not valid for this system. Nevertheless, the positive  $dM(0)/dc$  behavior is indicative of positive values for  $a(\vec{R}, \vec{T})$ .

TABLE I. Moment disturbance parameters for Ni-Cr and Ni-V alloys.

Alloy	$\mu_i - \bar{\mu}_h$	$M(0)$	$g(R_1)$	$\kappa$	$a(R_1, T_1)$	$B$
Ni-1-at.%-Cr	$-0.8 \pm 0.6$	$-6.0 \pm 0.6$	-0.20	0.60	...	...
Ni-5-at.%-Cr	$-0.39 \pm 0.13$	$-3.2 \pm 0.2$	-0.11	0.60	0.182	0.79
Ni-10-at.%-Cr	$-0.05 \pm 0.07$	$-1.7 \pm 0.1$	-0.04	0.38	0.026	0.11
Ni-5-at.%-V	$-0.41 \pm 0.05$	$-3.0 \pm 0.1$	-0.12 $\pm 0.01$	0.63 $\pm 0.06$	0.145	0.80

This data analysis was made with the assumption of no positional short-range order (SRO) for these alloys. Since SRO would effect the moment distributions, an independent measurement of the nuclear disorder cross sections was made by using unpolarized neutrons and an applied saturating field. This cross section has the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{nucl}} = c(1-c)(b_i - b_h)^2 \sum_R \alpha(R) e^{i\mathbf{R}\cdot\mathbf{R}}, \quad (13)$$

in which the  $\alpha(R)$ 's are the usual SRO parameters. No significant  $K$  dependence could be detected for the 5-at.%-Cr alloy but, at 10-at.% Cr, there was a slight  $K$  dependence corresponding to  $\alpha(R_1) = -0.019 \pm 0.017$  if attributed completely to first-neighbor correlations. In order to obtain a more significant result, we prepared an alloy containing 25-at.% Cr. The cross-section data for this alloy yield  $\alpha(R_1) = -0.046 \pm 0.014$  for the nearest-neighbor model. This can be used to estimate the SRO effects for the more dilute alloys by assuming that  $\alpha(R_1)$  is proportional to  $c(1-c)$ . This seems to be a reasonable assumption since, at the 10-at.%-Cr level, it yields  $\alpha(R_1) = -0.022$ , which agrees both with our own value ( $-0.019$ ) and with that quoted by Rainford, Aldred, and Low<sup>4</sup> (consistent with  $-0.02$ ). Thus, it appears that there is some SRO in Ni-Cr alloys but this is quite small and will not significantly alter the moment distributions obtained by the random-alloy assumption.

#### DISCUSSION

The moment disturbance parameters in Table I describe the moment distribution in Ni-Cr alloys within the framework of the local-environment model. The only one of these parameters that is independent of the model is  $\mu_i - \bar{\mu}_h$  if  $\mu_i$  is taken as the average impurity moment. This difference in average moments is then the most direct result of the neutron data and can be combined with the bulk magnetization,  $\bar{\mu} = c\bar{\mu}_{\text{Cr}} + (1-c)\bar{\mu}_{\text{Ni}}$ , to obtain the average moment of the Cr and Ni atoms in the alloy. Magnetizations and individual moments are given in Table II. The Ni moments are well determined but there are large errors associated with the Cr moments because of the low Cr content. However, the Cr moment is not significantly different from zero for any of the alloys. To better understand the role of the  $g(R)$  and  $a(R, T)$  parameters, it is instructive to consider the moment on a host atom as a function of concentration and of the number of impurity neighbors. Consider a model in which nearest-neighbor effects are taken into account explicitly while more-distant-neighbor effects enter as an averaged-concentration effect. Equation (1) can then be written as the

TABLE II. Moment values for Ni-Cr and Ni-V alloys.

Alloy	$\bar{\mu}^a$	$\bar{\mu}_{\text{Ni}}$	$\mu_{\text{Cr}}$
Ni-1-at.%-Cr	0.562	0.570	$-0.2 \pm 0.06$
Ni-5-at.%-Cr	0.355	0.375	$-0.02 \pm 0.12$
Ni-10-at.%-Cr	0.095	0.100	$0.05 \pm 0.06$
Ni-5-at.%-V	0.325	0.346	$-0.065 \pm 0.048$
		$\pm 0.008$	

<sup>a</sup> Magnetization data from Refs. 1, 2, and 12.

moment on a host atom as a function of the site-occupation operators summed over the  $\rho$  nearest-neighbor sites:

$$\begin{aligned} \mu_h(\phi_\rho, c) = & \bar{\mu}_h - 12cg(R_1) + 132c^2a(R_1, T_1) \\ & + [g(R_1) - 22ca(R_1, T_1)] \sum_\rho \phi_\rho \\ & + a(R_1, T_1) \sum_{\rho, \rho'}' \phi_\rho \phi_{\rho'}, \end{aligned} \quad (14)$$

where the prime on the double sum indicates that  $\rho \neq \rho'$ . Thus, the actual moment disturbance produced by a nearest-neighbor impurity atom is  $g(R_1) - 22ca(R_1, T_1)$  rather than simply  $g(R_1)$ , as in the linear model. Since  $g(R_1)$  is negative and  $a(R_1, T_1)$  is positive, the net effect is large and negative for this system. For example, at 5-at.%Cr the disturbance is  $-0.310\mu_B$  per nearest-neighbor impurity. Thus, two impurities would tend to drive the host moment negative. The positive last term, however, prevents this from happening.

This occurrence of comparable linear and nonlinear effects is an unusual and interesting feature of the Ni-Cr data, but even more interesting is the concentration dependence of  $M(0)$ . As noted previously,  $d\bar{\mu}/dc = M(0)$  if the moment fluctuations are due to site occupation. A comparison of the fitted values of  $M(0)$  and  $d\bar{\mu}/dc$  from magnetization data is given in Fig. 3. Here, the lower data points are for random alloys and the upper data points are corrected for SRO. Clearly, the  $M(0)$  values for the local-environment model do not correspond to  $d\bar{\mu}/dc$ . We conclude that there are two effects contributing to the moment decrease as Cr is added to Ni. There is a local-environment effect,  $M(0)$ , which dominates in the dilute region but which becomes less important with increasing Cr content. In addition there is a nonlocal effect of sufficiently long range that it is not detected by this neutron method.

Clearly, the Ni-Cr system is a special case as it exhibits both nonlocal and nonlinear moment disturbance effects which have not been detected for other Ni-based alloys. We suggest two factors

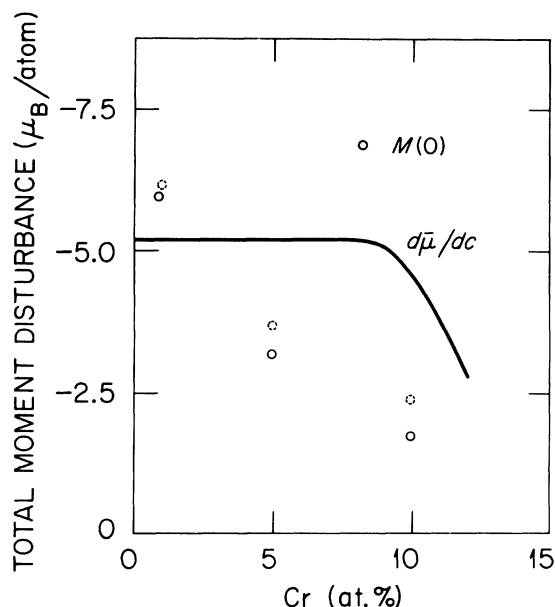


FIG. 3. Comparison of the neutron and magnetization values of the total moment disturbance per impurity atom. The solid curve is from the data of Refs. 1 and 2. The two data points at each concentration correspond to  $M(0)$  values with (higher) and without (lower) correction for SRO.

that contribute to this: (i) the large charge contrast in the Ni-Cr case and (ii) the presence of both chemical and magnetic environment effects. We consider the chemical effect due largely to charge transfer, which shifts the energy levels and local state densities of those Ni atoms near Cr atoms. The magnetic effect arises from electron-electron interactions but can be treated as a molecular-field effect. Thus, the absence of a moment at the impurity site decreases the effective field experienced by nearest-neighbor Ni moments, which therefore have smaller moments than in pure Ni. This moment decrease is passed along as a decrease of effective fields and moments in successive shells surrounding the impurity. The charge-transfer effect is expected to be short ranged, mostly nearest neighbor, but this is transmitted to more distant neighbors via the molecular field, so that a separate determination of the two effects for a given system is not possible. However, by comparison of the total environmental effect caused by impurities of different charge contrast, inferences can be drawn regarding their relative magnitudes. For example, consider the moment disturbance produced on an Ni atom by nearest-neighbor Cr and Cu atoms. Since neither of these impurities have moments in Ni, their magnetic effects should be comparable. The ob-

served total effects are, however, quite different,  $-0.20\mu_B/\text{Cr}$  and  $-0.038\mu_B/\text{Cu}$ ,<sup>9,10</sup> and this suggests an appreciable chemical effect for Cr impurities. The magnitude of this chemical effect depends on the functional dependence of the host moment on effective field and on the Ni-Cu chemical effect, neither of which is known. However, if the moment disturbance in Ni-Cu is attributed to magnetic effects only, then the Ni moments in the successive shells surrounding a Cu atom define the functional dependence over a limited region of  $\mu_h$  vs  $\mu_{\text{eff}}$  within the nearest-neighbor molecular-field model. In this approximation, about half of the total environmental effect in Ni-Cr should be attributed to a chemical effect.

Since the magnetic effect depends on site occupation and is limited to a few neighbor distances, it seems necessary to associate the nonlocal effect in Ni-Cr with the chemical, or charge-transfer, effect. We propose a simple model of this type based on the mismatch of  $d$ -electron energy levels of Ni and Cr as indicated, for example, by the band-structure calculations of Hasegawa and Kanamori,<sup>11</sup> which show separate energy bands for Ni and Cr in the alloy. In a more localized sense, we assume that there are also  $d$ -electron energies and wave functions associated with finite chains of near-neighbor Cr atoms. We then assume charge transfer from the Cr atoms in these chains to the neighboring Ni atoms and that addition or removal of a Cr atom at any point along the chain will alter the charge transfer at every point along the chain. This is, then, a mechanism for moment reduction at Ni sites caused by Cr atoms at large distances. It is important to note that this mechanism requires both charge transfer and mismatched  $d$  levels. This may explain why the nonlocal effect is not observed for Ni-Fe, Ni-Co, and Ni-Cu, which have less charge contrast than Ni-Cr. With increasing Cr content, the probability of finding long Cr chains increases so there would be an increase in the long-range and a decrease in the short-range charge-transfer effects "seen" by the neutron method. This would produce the other unusual feature of the Ni-Cr data, i.e., a nonlinear response to site occupation. This is easily seen since the long-range effect depends on both the probability of site occupation and the probability that the site is connected to a chain of impurity atoms. This suggests that the nonlocal and nonlinear effects observed for Ni-Cr should also appear for other systems with high charge contrast. We find that this is indeed the case for a Ni-5-at.-%-V alloy for which we measured both the polarized and unpolarized diffuse cross sections. The  $M(K)$  and  $[T(K)]^{1/2}$  data are shown in Fig. 4 and the fitted parameters and moment values ap-

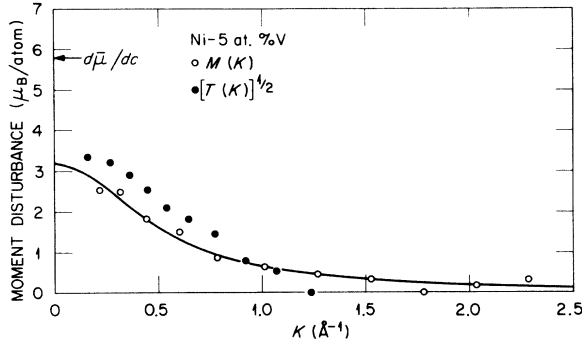


FIG. 4.  $M(K)$  and  $[T(K)]^{1/2}$  data for a Ni-5-at.%-V alloy.

pear in Tables I and II. The behavior is nearly the same as for the Ni-Cr alloy of the same impurity content.

This model has the features necessary to explain the data but is difficult to treat quantitatively. The experiment indicates a nonlocal moment disturbance with a range  $\geq \pi/K_{\min} \approx 12.5 \text{ \AA}$  and with a magnitude of  $d\bar{\mu}/dc - M(0)$ , i.e., about  $2\mu_B/\text{Cr}$  at  $c = 0.05$  and  $3\mu_B/\text{Cr}$  at  $c = 0.10$ . This range corresponds to approximately five first-neighbor distances, which can be related to impurity-atom chain length by considering a self-avoiding random walk of  $n$  steps for which  $\langle R^2 \rangle = n^{1.2}$ . Thus, a chain of impurities interacting to first-neighbor distances and with an rms length of  $12.5 \text{ \AA}$  would require 15 steps. Unfortunately, the probability distribution of  $n$ -step chains in a fcc lattice has not yet been treated, while the pseudolattice calculations that can be made seriously overestimate the probabilities in the concentration region of interest. However, calculations for a Cayley tree with coordination number 12 indicate that a 15-step chain has too low a probability to account for  $d\bar{\mu}/dc - M(0)$  at  $c = 0.05$ . A shorter chain with both first- and second-neighbor interactions is indicated.

#### APPENDIX

In this appendix, we derive the cross section for diffuse scattering of polarized neutrons from a binary alloy. With the incident-neutron polarization parallel or antiparallel to the sample magnetization and perpendicular to the scattering plane, the scattering amplitude at site  $\vec{n}$  is  $b_n \pm 0.27 \times \mu_n f_n(K)$ , in which  $b$  is the nuclear amplitude,  $\mu$  is the moment,  $f(K)$  is the form factor, and the  $\pm$  signs refer to the neutron spin state. The diffuse cross section measures the fluctuations from the average and has the form

$$\frac{d\sigma}{d\Omega}(K)^{\pm} = \frac{1}{N} \left( \sum_n e^{i\vec{R}\cdot\vec{n}} \{b_n - \langle b \rangle \pm 0.27[\mu_n f_n(K) - \langle \mu f(K) \rangle]\} \right)^2. \quad (\text{A1})$$

Only the nuclear-magnetic cross terms are retained in the difference between the "+" and "-" cross sections, i.e.,

$$\begin{aligned} \Delta \frac{d\sigma}{d\Omega}(K) &\equiv \frac{d\sigma}{d\Omega}(K)^+ - \frac{d\sigma}{d\Omega}(K)^- \\ &= \frac{1.08}{N} \sum_{n,m} e^{i\vec{R}\cdot(\vec{n}-\vec{m})} (b_n - \langle b \rangle) \\ &\quad \times [\mu_n f_n(K) - \langle \mu f(K) \rangle]. \end{aligned} \quad (\text{A2})$$

By summing over one index and introducing a configurational average, denoted by  $\langle \dots \rangle$ , this becomes

$$\begin{aligned} \Delta \frac{d\sigma}{d\Omega}(K) &= 1.08 \sum_R e^{i\vec{R}\cdot\vec{R}} \langle (b_{n+\vec{R}} - \langle b \rangle) \\ &\quad \times [\mu_n f_n(K) - \langle \mu f(K) \rangle] \rangle. \end{aligned} \quad (\text{A3})$$

We then introduce a site-occupation operator  $p_n$  which is unity if there is an impurity atom at  $\vec{n}$  and zero otherwise. The nuclear amplitude at  $\vec{n} + \vec{R}$  is then

$$b_{n+\vec{R}} = p_{n+\vec{R}} b_i + (1 - p_{n+\vec{R}}) b_h, \quad (\text{A4})$$

where  $b_i$  and  $b_h$  are the impurity and host amplitudes. The average nuclear amplitude is  $c b_i + (1 - c) b_h$ , so that

$$b_{n+\vec{R}} - \langle b \rangle = (p_{n+\vec{R}} - c)(b_i - b_h) \quad (\text{A5})$$

and the difference cross section becomes

$$\Delta \frac{d\sigma}{d\Omega}(K) = 1.08 (b_i - b_h) \sum_R e^{i\vec{R}\cdot\vec{R}} \langle (p_{n+\vec{R}} - c) \mu_n f_n(K) \rangle. \quad (\text{A6})$$

For the local-environment model, we simplify by assuming no impurity moment fluctuations and that  $f(K)$  is the same for all atoms. The moment at site  $\vec{n}$  is then

$$\mu_n = p_n \mu_i + (1 - p_n) \mu_h(n), \quad (\text{A7})$$

where  $\mu_h(n)$  is taken from Balcar and Marshall's model,<sup>6</sup>

$$\begin{aligned} \mu_h(n) &= \bar{\mu}_h + \sum_R g(R) (p_{n+\vec{R}} - c) \\ &\quad + \sum_{R,T} a(\vec{R}, \vec{T}) (p_{n+\vec{R}} - c) (p_{n+\vec{T}} - c). \end{aligned} \quad (\text{A8})$$

In taking the configurational average for Eq. (A6), it is convenient to rewrite Eq. (A7) in the form

$$\mu_n = (p_n - c)[\mu_i - \mu_h(n)] + c\mu_i + (1 - c)\mu_h(n), \quad (\text{A9})$$

which gives

$$\begin{aligned} \langle (p_{n+R} - c)\mu_n \rangle &= \langle (p_{n+R} - c)(p_n - c)[\mu_i - \mu_h(n)] \rangle \\ &+ (1 - c)\langle (p_{n+R} - c)\mu_h(n) \rangle. \quad (\text{A10}) \end{aligned}$$

Most of these terms vanish for a random alloy, for which the averages are

$$\begin{aligned} \langle (p_{n+R} - c)(p_n - c)[\mu_i - \mu_h(n)] \rangle &= c(1 - c)(\mu_i - \bar{\mu}_h)\delta_R \\ (\text{A11}) \end{aligned}$$

and

$$\langle (p_{n+R} - c)\mu_h(n) \rangle = c(1 - c)g(R). \quad (\text{A12})$$

The difference cross section therefore becomes

$$\Delta \frac{d\sigma}{d\Omega}(K) = 1.08c(1 - c)(b_i - b_h)f(K)M(K), \quad (\text{A13})$$

in which

$$M(K) = \mu_i - \bar{\mu}_h + (1 - c) \sum_R g(R)e^{i\mathbf{K} \cdot \mathbf{R}}. \quad (\text{A14})$$

These are Eqs. (8) and (4), respectively.

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