Local magnetic moments and g' in Fe-Ni alloys

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This paper presents a local-model calculation of the composition dependence of g', the effective magnetomechanical ratio, for Fe-Ni alloys. The model incorporates magnetic moments from scattering experiments as well as Einstein-de Haas measurements of g' for pure Fe and pure Ni. Excellent agreement is obtained with Scott's room-temperature g' values on slow-cooled alloy samples. This good agreement supports the assumption that the local atomic g' value does *not* change upon alloying, while the local magnetic moment does. Estimates of the first short-range order parameter are obtained. These are all found to be zero or negative, and to be small in absolute magnitude.

I. INTRODUCTION

In this paper a local model is used to calculate the value of g', the effective magnetomechanical ratio, in Fe-Ni alloys. The present model combines the local Fe and Ni magnetizations, as determined (for a given alloy composition) from nuclear-scattering studies,[1-3] with Einstein-de Haas–effect measurements[4] of g' for the pure ferromagnetic Fe and Ni metals. The resulting calculated g' values are in good agreement with the room-temperature effective alloy g' values experimentally determined on slow-cooled samples by Scott.[4]

In the past Tsuya[5] and Wangsness[6] have derived expressions for the effective g' in an alloy in terms of the g' values and saturation magnetizations of the pure metals. They assumed that the individual g' values and magnetizations per atom are the same as for the constituent metals, and that the component atoms have their magnetic moments parallel throughout each domain. The calculated g' values for their model were well outside the reported errors in Scott's measured g' values[4] (see Fig. 1) for Fe-Ni. Because Scott has reported the experimental g' values to an accuracy of about 0.2%, a comparison of calculated g' values with the experimental g' values is a very sensitive test of the model.

We assume (as did Tsuya and Wangsness) that the g' values of the pure ferromagnetic metals remain unchanged upon alloying, despite the fact that the wave functions of the magnetic electrons change with composition. This change is evident from the composition dependence of the local magnetic moments.[2]

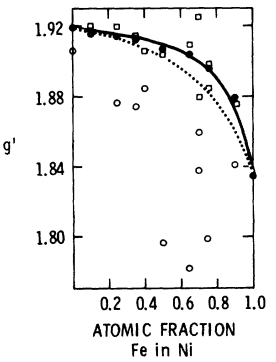

FIG. 1. Magnetomechanical ratios as a function of atomic fraction of iron in nickel. □, g' values calculated with *a* local moments. O, g' values calculated with *b* set of moments. ···, curve obtained using Tsuya-Wangsness relation with a magnetization ratio of 4.0. •, measured magnetomechanical ratios. Solid line is obtained using a magnetization ratio of 8.2.

To develop the present model we need to enumerate some of the experimental facts already determined about these alloys. Magnetic-disorder-scattering[2] and the nuclear-disorder-scattering studies[1,2] of the Fe-Ni alloys have established the following.

(i) For a given alloy, Fe_xNi_{1-x}, a constituent atom can be said to possess a particular atomic state with a characteristic moment $\mu_{Fe}(x)$ for iron and $\mu_{Ni}(x)$ for nickel. (This implies that *only* two moments exist at a given composition, associated with the two constituent atoms.)

(ii) The local magnetic moments vary with the composition of the alloy.

Since differences in the absolute value of the magnetic-scattering length are obtained from the nuclear-scattering technique, there are two sets of moments which are consistent with the neutron data.[2] Both sets of magnetic moments are considered here; we shall see that only one set is consistent with the g' results.

Indirect evidence from studies of the saturation magnetization,[7] magnetic anisotropy,[8] specific heat,[9] electrical resistance,[10] and total neutron cross section[11] have shown that

(iii) short-range order may exist over much of the concentration range of the Fe-Ni alloys.

Direct evidence of short-range order has been obtained[12] for Ni_3Fe, but the order parameter is difficult to determine because Fe and Ni have very similar scattering amplitudes for either x rays or neutrons.

From results (i) and (ii) above and the values of g' for pure ferromagnetic Fe and Ni, we calculate the effective g' values over the entire composition range. From a comparison of the measured and calculated g' values we then *estimate* the value of

the first short-range order parameter (assuming its effect to be much larger than that of the other short-range order parameters) as a function of composition.

The plan of the remainder of this paper is as follows. In Sec. II we describe the way in which the calculated g' values were obtained and compare this with other methods. In Sec. III we present the results, and in Sec. IV we state the conclusions.

II. g' CALCULATION

To obtain the calculated values of g' as a function of composition we have used the previously obtained relationship[13] between g' and the total (M_T) and spin (M_s) magnetizations:

$$g' = (2M_T/2M_T - M_s) \quad . \tag{1}$$

The neutron results[1-3] have been analyzed to give local moments, using an expression of the form

$$M_T(x) = x_{\mathrm{Ni}}\mu_{\mathrm{Ni}}(x) + x_{\mathrm{Fe}}\mu_{\mathrm{Fe}}(x) \quad , \tag{2}$$

where x_{Ni} is the number fraction of Ni atoms and x_{Fe} the number fraction of Fe atoms ($x_{\mathrm{Ni}} + x_{\mathrm{Fe}} = 1$).

To obtain the total spin magnetization we then assume for a given atom (Fe or Ni)

$$M_{s,\mathrm{Fe}} = 2x_{\mathrm{Fe}}\mu_{\mathrm{Fe}}(g'_{\mathrm{Fe}} - 1)(g'_{\mathrm{Fe}})^{-1} \quad , \tag{3}$$

where g'_{Fe} is the magnetomechanical ratio of *pure* ferromagnetic iron (the appropriate values being used for the Ni case). Hence we write

$$M_s = 2[x_{\mathrm{Fe}}\mu_{\mathrm{Fe}}(g'_{\mathrm{Fe}} - 1)(g'_{\mathrm{Fe}})^{-1} + x_{\mathrm{Ni}}\mu_{\mathrm{Ni}}(g'_{\mathrm{Ni}} - 1)(g'_{\mathrm{Ni}})^{-1}] \quad , \tag{4}$$

where we assume that the component atoms have their magnetic moments parallel within each domain.

Table I shows the two sets, *a* and *b*, of local moments μ_{Fe} and μ_{Ni} obtained from the neutron-scattering work. Taking the pure ferromagnetic values[4] $g'_{\mathrm{Fe}} = 1.919$ and $g'_{\mathrm{Ni}} = 1.835$, we then use Eq. (3) to obtain the local spin moments shown. Of the ten calculated g' values, the data for three values ($x_{\mathrm{Fe}} = 0.35,\ 0.65,\ 0.75$) were obtained from a least-squares fit of the neutron-scattering local moments, since no actual scattering measurements were available at these compositions.

A plot of the two sets of calculated g' values as well as of the measured g' values is shown in Fig. 1. In addition, the dashed line represents the theoretical curve from the Tsuya-Wangsness model[4] of g' in Fe-Ni alloys, using a magnetization ratio of 4. The solid curve is obtained from the same theory using a saturation magnetization ratio of 8.2.

If we assume that the difference $\Delta g'$ between the calculated and the measured g' values is exclusively due to short-range order, we can estimate the magnitude of α_1, the first short-range order parameter,[14] which would lead to this difference.

We relate α_1 to the probability p_1 of finding a nickel atom at a nearest-neighbor distance from an iron atom; thus[14]

$$\alpha_1 = \frac{1 - p_1}{1 - x} \quad , \quad x = x_{\mathrm{Fe}} \quad .$$

(Note: if $\alpha_1 < 0$, unlike neighbors are more probable.) We can write

$$\Delta g' = g'_{\mathrm{exp}} - (2M_T/2M_T - M_s)$$

TABLE I. Fe-Ni magnetic data. Local magnetic moments of iron, μ_{Fe} (*a*) and (*b*), of nickel, μ_{Ni} (*a*) and (*b*), local spin moments of iron, $\mu_{s,\mathrm{Fe}}$ (*a*) and (*b*), local spin moments of nickel, $\mu_{s,\mathrm{Ni}}$ (*a*) and (*b*), total spin moments M_s, (*a*) and (*b*), total magnetization M_T, calculated g' using *a* magnetic moments, g'(*a*), calculated g' using *b* magnetic moments g'(*b*), experimental values of g', g'_{expt} and first short-range order parameter, α_1, all with increasing at.% Fe in Ni. The (ord) refers to an ordered sample, (*a*) to an annealed one, and (*q*) to a quenched sample. The values of local and total moments at 10, 30(*a*), 30(*q*), 60, and 90 at.% Fe were obtained from Ref. 2. The values at 25(ord), 25, and 50 at.% Fe were obtained from Ref. 3. The experimental g' values were obtained from Ref. 4.

	μ_{Fe} (μ_B)		μ_{Ni} (μ_B)		$\mu_{s,\mathrm{Fe}}$ (μ_B)		$\mu_{s,\mathrm{Ni}}$ (μ_B)		M_s (μ_B)			g'			
at.% Fe	(*a*)	(*b*)	(*a*)	(*b*)	(*a*)	(*b*)	(*a*)	(*b*)	(*a*)	(*b*)	$M_T(\mu_B)$	(*a*)	(*b*)	g'_{expt}	α_1
0														1.835	
10	2.58	−0.78	0.64	1.01	2.48	−0.748	0.587	0.927	0.776	0.760	0.83	1.878	1.843	1.880	−0.027
25	3.13	−0.25	0.63	1.70	3.00	−0.240	0.578	1.560	1.18	1.11	1.25	1.899	1.799	1.895	−0.003
25 (ord)	3.10		0.68		2.974		0.624		1.21		1.29	1.885			
30 (*a*)	3.02	−0.06	0.63	1.94	2.90	−0.058	0.580	1.78	1.28	1.23	1.33	1.927	1.860		
30 (*q*)	2.66	0.06	0.63	1.75	2.55	0.058	0.580	1.61	1.17	1.14	1.25	1.880	1.838		
35	2.93	0.16	0.65	2.03	2.81	0.154	0.596	1.86	1.37	1.27	1.44	1.910	1.783	1.904	−0.006
50	2.54	0.87	0.78	2.30	2.44	0.835	0.716	2.11	1.58	1.47	1.66	1.904	1.797	1.908	0.00
60	2.44	1.34	0.83	2.48	2.34	1.29	0.760	2.28	1.71	1.69	1.80	1.905	1.885		
65	2.43	1.45	0.84	2.62	2.33	1.39	0.771	2.40	1.79	1.75	1.87	1.914	1.876	1.912	−0.007
75	2.42	1.72	0.87	2.86	2.32	1.65	0.798	2.62	1.94	1.89	2.03	1.920	1.878	1.914	−0.062
90	2.41	2.14	0.93	3.26	2.31	2.05	0.853	2.99	2.17	2.15	2.26	1.920	1.905	1.915	−0.074
100														1.919	

and, by recalculating M_T and M_s using all possible nearest-neighbor arrangements m ($m=8$ for the bcc phase and $m=12$ for the fcc phase), we obtain[14]

$$\Delta g'(x) = g'(x)_{\text{exp}} - \left(\frac{\sum_{n=0}^{m} \binom{m}{n} [\, xY^{m-n}(1-Y)^n \mu_{\text{Fe}}(x) + (1-x)(1-Y)^{m-n} Y^n \mu_{\text{Ni}}(x)]}{\sum_{n=0}^{m} \binom{m}{n} \{xY^{m-n}(1-Y)^n [\mu_{\text{Fe}}(x)/g'_{\text{Fe}}] + (1-x)(1-Y)^{m-n} Y^n [\mu_{\text{Ni}}(x)/g'_{\text{Ni}}]\}} \right) ,$$

where $Y = 1 - x\,(1-\alpha_1)$. In this expression we assume the local iron and nickel moments are the result of the local configuration. These local-moment values we have obtained from the a-set neutron-scattering local moments,[2] their values being obtained from the appropriate concentration values (or interpolations thereof) in Table I. We believe the close comparison of the calculated and measured g' values serves to confirm the reliability of these assumed local moments. Collins, Jones, and Lowde have also compared their individual magnetic moments as given in Table I with comparable determinations from nuclear-disorder scattering by Shull and Wilkinson[15] and have found generally good agreement. The values[16] of α_1 which satisfy the $\Delta g'$ expression for different values of x are shown in Fig. 2.

Based upon the concept of a fixed local g' value for Fe and Ni we may also obtain the local electronic oribital moments as a function of alloy composition, as shown in Fig. 3. For this purpose we have assumed that the local orbital moments of iron, $M_{o,\text{Fe}}$, and nickel, $M_{o,\text{Ni}}$, are related to the local spin moments and the pure-metal g' values by

$$M_{o,\text{Fe}} = \left(\frac{2 - g'_{\text{Fe}}}{2g'_{\text{Fe}} - 2} \right) M_{s,\text{Fe}}(x)$$

and

$$M_{o,\text{Ni}} = \left(\frac{2 - g'_{\text{Ni}}}{2g'_{\text{Ni}} - 2} \right) M_{s,\text{Ni}}(x) \quad .$$

III. RESULTS

From a comparison of the ten calculated g' values we conclude that the a set of local moments is the one which is consistent with the measured g' values. While the calculated g' values for set a do not fall entirely within the experimental error of the measured g' values, this is not surprising, since the experimental error of the neutron work is much larger.

For all compositions considered the value of α_1 obtained was zero or negative, with the largest absolute value of the high-Fe-concentration side. The α_1 values have the same *sign* but are smaller in magnitude than the values reported for quenched Ni_3Fe specimens.[12]

The local electronic orbital moment in Ni appears to increase very slightly with increasing iron. In the fcc region, the local electronic orbital moment of iron is fixed at $\sim 0.1\mu_B$.

IV. CONCLUSIONS

Our results indicate that for these alloys the magnitude of the local atomic g' does not change upon alloying, although the effective g' value does, due to changes in the magnetic moments of the magnetic electrons of the constituents. The large difference in g' values at 30 at.%, of course, results from the different degrees of order in the annealed sample as compared with the quenched sample.[2] It has been suggested[17,18] that the Fe-Fe nearest-neighbor moments could be antiferromag-

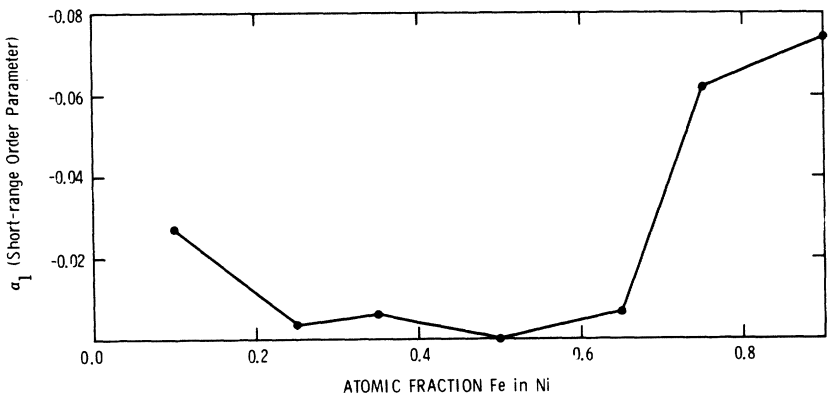

FIG. 2. First short-range order parameter as a function of the atomic fraction of iron.

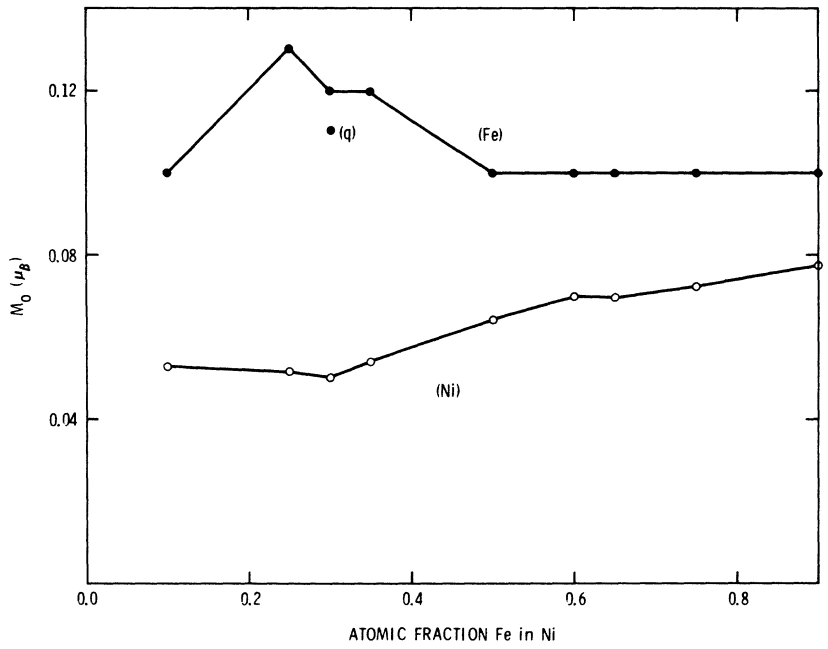

FIG. 3. Local electronic orbital moments as a function of the atomic fraction of iron.

netically coupled in this composition region, to account for the change in M_T and hence in g'.

We conclude that the local moment of ferromagnetic Ni remains less than one-half the Fe value and is relatively constant over much of the composition range. On the other hand, the local moment of Fe appears to peak at $\sim 3.1\mu_B$ around 30 at.% Fe, in the ordered samples, and then to level off $\sim 2.5\mu_B$ beyond 50 at.% Fe. This leveling off at higher Ni concentration is in contradiction to earlier extrapolations for μ_{Fe} given by Bardos, Aldred, and Beck.[19] Our conclusions also do not agree with Lomer and Marshall's original *theoretical* predicted values[20] of the local moments in the Fe-Ni alloys.

Some obvious criticisms may be leveled against the present analysis. To obtain the local moments from the neutron-scattering work,[2] the polarization of the conduction electron was neglected. If this were significant it would imply that our good agreement between calculated and measured g' values was fortuitous.

That there is some degree of short-range order in these alloys can probably not be questioned. Its magnitude, however, appears always to be less than that observed[14] when Cu dilutes Ni.

It is interesting to compare the dilution of Ni with Fe to dilution with Cu. In the present case our results confirm that no minimum number of atoms is required to obtain a magnetic Fe-Ni cluster and a very narrow *range* of local moments if any, must be present due to different numbers of nearest and second nearest neighbors of a given constituent. This is exactly opposite to the apparent wide distribution of local moments in the Cu-diluted Ni alloys.[14] Also, in these Ni-Fe alloys the local g' values or, in effect, the coupling of local spin and orbital components remain constant while in Cu-Ni only the orbital component remains constant.[14]

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