

## Magnetic-moment distribution and environmental effects around titanium impurities in nickel and iron matrix

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(Received 18 April 1979)

Results of elastic diffuse scattering of polarized neutrons with 4.25-Å wavelength on Ni-Ti with 3.87 and 7.72 at. % of Ti and Fe-Ti with 0.84, 1.33, and 1.73 at. % of Ti are reported. The data indicate quite different behavior of the impurity in the two matrices. In the nickel-based alloys the titanium atom has negligible magnetic moment while in the Fe-Ti alloys we observe a moment enhancement at the Ti sites at low impurity concentration. Also the environmental effects are different in these two alloys. In Fe-Ti alloys, these are negligible at low impurity concentration and appear at higher impurity concentration while in the Ni-based alloys we observe an opposite effect. These results are discussed within a band model using coherent-potential approximation and we obtain an overall good description of the magnetic-moment distribution in these two alloys except in the dilute limit in Fe-Ti alloys.

### I. INTRODUCTION

The elastic diffuse scattering of polarized neutrons is a useful tool to study the effect of impurities on the magnetic properties of a ferromagnetic matrix. It is well known that the addition of the element on the left-hand side of the 3d metal series (Sc, Ti, V, Cr) to the ferromagnetic metals (Fe, Co, Ni) diminishes the magnetic moment of the host metal. This diminution is qualitatively well understood in terms of the virtual bound states (VBS) model of Friedel<sup>1</sup>; in quantitative terms there are some discrepancies as discussed by several authors (see, e.g., Demangeat and Gautier<sup>2</sup>). The coherent-potential approximation (CPA) on the other hand allows one to make more detailed calculations of the magnetic-moment distribution and its variation with impurity concentration, as well as the effect of impurity on the band structure of the alloy. This is of special interest in the case of alloys with well-separated centers of gravity of the bands because of VBS formation. In the case of Fe-V alloys the CPA theory<sup>3,4</sup> predicts the existence of a large negative moment on vanadium which decreases rapidly (in absolute value) with impurity concentration whereas the Fe moment increases slightly at low V concentrations and thereafter decreases.<sup>3</sup> In the framework of the CPA this behavior of the magnetic moment is connected with a transfer of spin-up  $e_g$  electrons from the impurity to the host band. This transfer results in an increase of the magnetic moment of iron, asphericity parameter, and in the formation of a negative moment on vanadium. At higher impurity concentration this process vanishes

and the moments on both iron and vanadium as well as the asphericity parameter decrease.<sup>3</sup>

In order to study these effects more systematically we have undertaken, on the experimental side, polarized-neutron diffuse-scattering measurements and on the theoretical side the CPA calculations for Fe-Ti and Ni-Ti alloys. In these alloys the centers of gravity of the bands are more separated than in Fe-V alloys, the separation being more important for Ni-Ti alloys. Thus an important charge transfer from impurity to the host band should be expected.

On the other hand, it is interesting to compare the environmental effects around the titanium impurity in these two alloys. Comly *et al.*<sup>5</sup> pointed out, from the study of magnetic-moment disturbances around impurity sites in Ni-based alloys, that these are positive or negative depending on whether the VBS has formed or not. In an early study of Fe-Ti alloys by Collins and Low<sup>6</sup> on an alloy with 1–2 at. % of Ti and a more recent one by Child and Cable,<sup>7</sup> both being unpolarized-neutron diffuse-scattering measurements, such a magnetic-moment disturbance was not emphasized. The possibility of having short-range order was mentioned by Schurer *et al.*<sup>8</sup> in the hyperfine-magnetic-field study of an alloy with 3 at. % of Ti.

Recently we found, from diffuse scattering of polarized neutrons on two alloys with 2.88 and 4.92 at. % of Ti, a positive moment disturbance around impurity sites extending to the second shell of atoms.<sup>9</sup>

The magnetic-moment distribution and environmental effects in Ni-Ti alloys have been studied recently by Livet and Radhakrishna<sup>10</sup> by means of

polarized-neutron diffuse scattering on a sample with 2 at. % of Ti. The authors report a negative moment disturbance extending to the third shell of atoms but their data do not follow the curve plotted by Comly *et al.*<sup>5</sup> for several Ni-rich alloys.

The main difference between Ni- and Fe-rich alloys arises from the crystal structure and the consequent difference in the band structure; the first are fcc and the second are bcc. However the local environment is similar in both the alloys and the first shell of atoms, which is most perturbed, lies at the same distance ( $\sim 2.5$  Å) from the central atom. The second difference arises from the number of electrons filling the band and the resulting magnetic moment. The  $d$  band of Ni is nearly filled whereas that in iron contains about two electrons less and the bulk magnetic moments are  $0.58\mu_B$  and  $2.18\mu_B$  for Ni and Fe,

$$\left(\frac{d\sigma}{d\Omega}\right)_\epsilon = \left(\frac{d\sigma}{d\Omega}\right)_{\text{incoh}} + C_m C_i \left[ (\bar{b}_m - \bar{b}_i)^2 S(k) + \left( \frac{\gamma e^2}{2mc^2} f(k) \Delta\mu(k) \right)^2 + 2\epsilon (\bar{b}_m - \bar{b}_i) \left( \frac{\gamma e^2}{2mc^2} f(k) \Delta\mu(k) \right) \right], \quad (1)$$

where for a polycrystalline sample

$$S(k) = 1 + \sum_R N_R \alpha_R \frac{\sin kR}{kR} \quad (2)$$

and

$$\Delta\mu(k) = (\bar{\mu}_m - \bar{\mu}_i) S(k) + \sum_R N_R (1 - \alpha_R) (\delta\mu_{mi}^R - \delta\mu_{im}^R) \frac{\sin kR}{kR}. \quad (3)$$

In the expressions (1)–(3)  $k$  is the modulus of the scattering vector,  $k = 4\pi \sin\theta/\lambda$ ,  $f(k)$  is a magnetic form factor for the alloy,  $C_\alpha$  and  $\bar{b}_\alpha$  are the atomic concentration and nuclear coherent scattering length of the  $\alpha$  component of the alloy ( $\alpha = i, m$ ), and the subscripts ( $i, m$ ) refer to the impurity and matrix, respectively.  $\gamma e^2/2mc^2$  is the usual constant equal to  $0.2695 \times 10^{-12} \mu_B^{-1} \text{cm}$  and  $\sigma_{\text{incoh}}$  is the incoherent nuclear cross section of the alloy.  $\epsilon = \pm 1$  stands for the incident neutron spin direction parallel or antiparallel to the sample magnetization, respectively,  $S(k)$  is a function describing the chemical short-range order in which  $N_R$  is the number of near-neighbor atoms at a distance  $R$  from a central one, and  $\alpha_R$  is the short-range order parameter which measures the deviation from a perfect disorder.<sup>12</sup> The function  $\Delta\mu(k)$

respectively, at room temperature.

In this paper we report the results of polarized-neutron diffuse-scattering measurements on three Fe-Ti alloys with 0.84, 1.33, and 1.73 at. % of Ti and two Ni-Ti alloys with 3.87 and 7.72 at. % of Ti. The results of similar measurements on Fe-Ti alloys with 2.88 and 4.92 at. % of Ti have been reported previously.

## II. GENERAL EXPRESSIONS FOR THE DIFFUSE NEUTRON CROSS SECTIONS

According to Gautier<sup>11</sup> the elastic diffuse differential cross section of polarized neutrons from a disordered ferromagnetic binary alloy can be expressed as follows:

describes the local distribution of the magnetic moments due to the disturbances caused by the impurity atoms. In this function  $\bar{\mu}_\alpha$  is the average magnetic moment of an  $\alpha$ -type atom and  $\delta\mu_{\alpha\beta}^R$  is the averaged modification of the moment of an  $\alpha$ -type atom due to the presence of an atom of type  $\beta$  in the  $R$ th shell surrounding it.

The difference between the spin-dependent differential cross sections

$$\Delta \frac{d\sigma}{d\Omega} = \left( \frac{d\sigma}{d\Omega} \right)_+ - \left( \frac{d\sigma}{d\Omega} \right)_- = 4C_m C_i (\bar{b}_m - \bar{b}_i) \left[ \frac{\gamma e^2}{2mc^2} f(k) \Delta\mu(k) \right] \quad (4)$$

is directly proportional to the perturbation function  $\Delta\mu(k)$  and can be used to determine the difference between the individual average magnetic moments provided that the difference between the nuclear scattering lengths is sufficiently large.

The polarized-neutron method is favorable for studying the magnetic diffuse scattering from Fe-Ti and Ni-Ti alloys because the nuclear scattering lengths  $b_m$  and  $b_i$  have opposite signs (see Table I). But as it can be seen from Eq. (4) and the following one for the half sum of the spin-dependent differential cross sections

$$\frac{1}{2} \sum \frac{d\sigma}{d\Omega} = \frac{1}{2} \left[ \left( \frac{d\sigma}{d\Omega} \right)_+ + \left( \frac{d\sigma}{d\Omega} \right)_- \right] = \left( \frac{d\sigma}{d\Omega} \right)_{\text{incoh}} + C_m C_i \left[ (\bar{b}_m - \bar{b}_i)^2 S(k) + \left( \frac{\gamma e^2}{2mc^2} f(k) \Delta\mu(k) \right)^2 \right], \quad (5)$$

one cannot separate the nuclear and the magnetic contributions to the diffuse scattering. However this drawback of the polarized-neutron method can be eliminated if the value of the magnetic term ( $\gamma e^2/2mc^2$ ) ( $\bar{\mu}_m - \bar{\mu}_i$ ) compared to the value of the difference of the nuclear scattering lengths  $\Delta b = \bar{b}_m - \bar{b}_i$  is sufficiently small. In that case one can neglect the last term in Eq. (5) and the half sum  $\frac{1}{2} \sum d\sigma/d\Omega$  can be used to evaluate the short

TABLE I. Physical quantities used in the scattering-cross-section determination.

element	$\bar{b}$ ( $10^{-12}\text{cm}$ )	$\sigma_{\text{inc}}$ (b)	$\sigma_{\text{abs}}$ (b)	$\frac{2B}{\text{\AA}^2}$
Fe	0.951	0.4	6.01	0.71
Ni	1.03	4.725	11.12	0.59
Ti	-0.335	3.05	14.345	0.90
V	-0.052	5.07	12.2	1.14

range order function  $S(k)$ . This approximation is good for Ni-Ti alloys because  $\Delta\mu = \bar{\mu}_m - \bar{\mu}_i$  is small and  $\Delta b$  is large, but it is not applicable to Fe-Ti alloys where  $\Delta\mu$  is large and both the nuclear and the magnetic terms are comparable. In that case Eq. (4) can be rewritten as follows:

$$\Delta \frac{d\sigma}{d\Omega} = 4C_m C_i (\bar{b}_m - \bar{b}_i) \frac{\gamma e^2}{2mc^2} \times f(k) \left( \bar{\mu}_m - \bar{\mu}_i - \sum_R \beta_R N_R \frac{\sin kR}{kR} \right), \quad (6)$$

where

$$\beta^R = -(\bar{\mu}_m - \bar{\mu}_i) \alpha_R + (1 - \alpha_R) \delta\mu^R \quad (7)$$

with

$$\delta\mu^R = \delta\mu_{mi}^R - \delta\mu_{im}^R, \quad (8)$$

and the only information is the difference between the magnetic moments of the host and the impurity atoms. If however  $\alpha_R \equiv 0$  for all  $R$  then  $\beta_R = \delta\mu^R$ , the perturbation being purely magnetic. In other cases the method should be coupled with unpolarized-neutron or x-ray diffuse-scattering measurements in order to obtain the chemical short-range order parameters.

### III. EXPERIMENTAL PROCEDURE AND CORRECTIONS

The polarized-neutron diffuse-scattering measurements were performed on the multidetector spectrometer installed at the end of the cold-source neutron guide, Belenus II, of the reactor EL3 in Saclay.<sup>13</sup> The multidetector, made up of 400 cells covers a  $2\theta$  range of  $80^\circ$  with a resolution equal to  $12'$ .<sup>14</sup> With the Heusler  $\text{Cu}_2\text{MnAl}$  alloy polarizing monochromator mounted in a vertical permanent magnetic field of 2.4 kOe an incident beam of neutrons with wavelength of  $4.25 \text{\AA}$  and a polarization antiparallel to the applied field of 94% was obtained.<sup>15</sup> The reversal of the neutron polarization direction was achieved using the conventional resonance method.<sup>16</sup>

The polycrystalline samples of Ni-Ti alloys were prepared by Perrier de la Bathie from Cristaltech Grenoble and those of Fe-Ti alloys by the Department of Metallurgy in Saclay (DMECN) from 99.99% pure slabs. The alloy concentrations were determined by chemical analysis. In the case of Fe-Ti alloys, where the impurity concentration is low, this analysis was done taking the samples from the two ends of the ingot. The difference was found to be very small (see Table III).

The principal characteristics of the samples are given in Tables II and III. The bulk moments were determined by the extraction method on small parts cut from measured samples and the lattice constants were calculated using  $da/dc = 0.09a_{\text{Fe}}$  for Fe-Ti alloys (Arrott and Noakes<sup>17</sup>) and  $da/dc = 0.0985a_{\text{Ni}}$  for Ni-Ti alloys (combined data of Poole and Hume-Rothery<sup>18</sup> and Taylor and Floyd<sup>19</sup>). The saturation magnetization measurements of Fe-Ti alloys were performed at room temperature (RT) and the results follow the curve  $d\bar{\mu}/dc = -3.42\mu_B$ .<sup>9</sup> In the case of Ni-Ti alloys the bulk moments were determined at room and at liquid-helium temperatures. The low-temperature data agree well with the recent measurements by Gregory and Moody<sup>20</sup> and those at RT differ slightly from the values determined by Marian.<sup>21</sup> We note here that the value for the bulk moment given in Table II of the Ni-Ti alloy with 7.72 at. % of Ti corresponds to the magnetization in an

TABLE II. Lattice constants ( $\text{\AA}$ ) and magnetic moment distribution in Ni-Ti alloys. The magnetic moments are given in  $\mu_B$ .

at. % Ti	$a$	$\bar{\mu}$ (room temp.)	$\bar{\mu}$ (liquid-He temp.)	$\bar{\mu}_{\text{Ni}}$	$\bar{\mu}_{\text{Ti}}$
3.87	3.537	0.383(5)	0.444(5)	0.402(7)	-0.08(2)
7.72	3.551	0.185(8)	0.267(6)	0.21(1)	-0.09(4)

TABLE III. Lattice constants ( $\text{\AA}$ ) and magnetic moments ( $\mu_B$ ) in Fe-Ti alloys.

I analysis at. % of Ti	II analysis at. % of Ti	Average at. % concentration of Ti	$a$	$\bar{\mu}$	$\bar{\mu}_{\text{Fe}}$	$\bar{\mu}_{\text{Ti}}$
0.85	0.83	0.84(1)	2.868	2.146(8)	2.383(9)	-2.08(22)
1.30	1.36	1.33(3)	2.869	2.132(6)	2.383(8)	-1.42(23)
1.78	1.68	1.73(5)	2.87	2.118(7)	2.383(11)	-1.38(24)

external field of 13 kOe which was used in our diffuse-scattering measurements. The saturation magnetization is about 10% greater. From the RT value for  $\bar{\mu}_{\text{Ni}} = 0.583\mu_B$  and our value at 3.87 at. % of Ti we obtain  $d\bar{\mu}/dc = -5.1\mu_B$  while Marian's value at 4.84 at. % of Ti gives  $d\bar{\mu}/dc = -4.5\mu_B$ . The low-temperature measurements of Gregory and Moody<sup>20</sup> yield a value of  $d\bar{\mu}/dc = -4.3\mu_B$  if one considers only the part of the magnetization which changes is linear with titanium concentration (up to 8 at. % of Ti).

The diffuse-scattering measurements were performed on cylindrical specimens of diameters 5 and 6 mm for Fe-Ti and Ni-Ti alloys, respectively, mounted in a vertical magnetic field of 13 kOe perpendicular to the scattering vector. For the Fe-Ti alloys the measurements were done for one position of multidetector in the scattering vector range  $0.2 \leq k \leq 2 \text{\AA}^{-1}$  and for the Ni-Ti alloys on two positions ( $0.2 \leq k \leq 2.3 \text{\AA}^{-1}$ ). The measured intensities of scattered neutrons with up- and down-spin directions (flipper on and off, respectively) were put on an absolute scale by comparison with a vanadium standard of the same dimensions using the values from Table I for data conversion. Standard corrections for temperature effects, incomplete beam polarization and flipping efficiency, background, multiple-scattering effects, and transmission and absorption with spin-dependent  $\mu R$ 's were done. The absorption correction was made using the analytical formulas given by Rouse *et al.*<sup>22</sup> whereas for the multiple-scattering effects the formulas and table given by Blech and Averbach<sup>23</sup> were used. In our experimental set up (the polarization perpendicular to the scattering plane) and the scattering vector range the inelastic contribution arising from the spin-wave excitations are negligible and spin independent. This is peaked at small values of  $k$  for iron and nickel (Stringfellow,<sup>24</sup> see also discussion by Child and Cable<sup>7</sup>). The only contribution is that arising from phonon and magnetovibrational scattering. The first is spin independent and contributes only to the sum of differential cross sections while the second is spin dependent and contributes to both the sum and the difference of differential cross sections. In order to

evaluate this contribution we have performed similar measurements on pure nickel and iron samples. The results for  $\Delta(d\sigma/d\Omega)$  are plotted in Fig. 1. It is seen that this contribution is small in the case of nickel and is significant in the case of iron, especially at larger values of  $k$ . With the assumption that in our relatively dilute alloys corresponding contributions will be nearly the same as for the pure matrix (cf., Cable and Child<sup>25</sup>) we subtracted them from the measured cross sections for alloys.

#### IV. Ni-Ti ALLOYS

As mentioned in Sec. II, the magnetic term in the sum of differential cross sections [Eq. (5)] is negligible compared to the nuclear one in the case of Ni-Ti alloys. Thus using one half of this sum it was possible to determine the chemical short-range order.

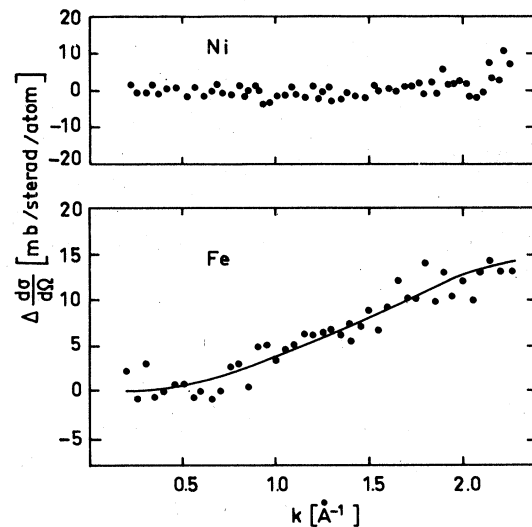


FIG. 1. Difference of differential cross sections for Ni and Fe. The line for Fe represents a fit of a formula  $F(k) = A(1 - e^{-Bk^2})f(k)$ , with  $A = 4.18 \text{ b}$ ,  $B = 0.0011 \text{ \AA}^2$ , and  $f(k) = 1 - 0.07k^2$ . The bars are the statistical errors only and each experimental point is an average of counts from 8 cells.

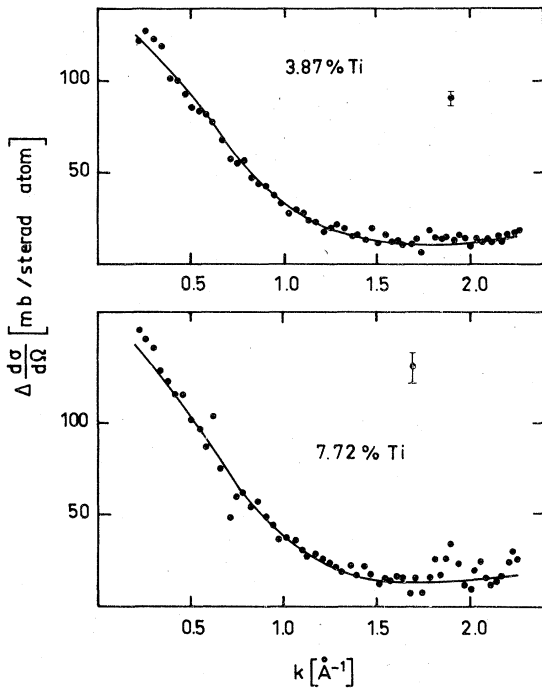


FIG. 2. Difference of differential cross sections for Ni-Ti alloys. The lines represent a fit as described in text. Other details as in Fig. 1.

parameters. The least-squares fit of Eq. (5) to experimental data showed that this order is negligible in the two alloy concentrations studied (see Table IV).  $\alpha_R$ 's thus obtained were used in fitting the formula (4) to experimental data of  $\Delta(d\sigma/d\Omega)$  shown in Fig. 2. In the fitting procedure we used an alloy magnetic form factor  $f(k) = 1 - 0.05k^2$  close to that of pure Ni. The least-squares-fitted parameters for magnetic-moment disturbance are also given in Table IV together with those for an alloy with 2 at. % of Ti studied by Livet and Radhakrishna.<sup>10</sup> All the results are coherent and indicate a decrease in the magnetic moment disturbance with increasing alloy concentration. The calculated values of  $\Delta(d\sigma/d\Omega)$  are plotted

in Fig. 2 (solid lines). The bars in Fig. 2 are the statistical errors only and the experimental values are averaged from eight cells of the multidetector.

### V. Fe-Ti ALLOYS

In the case of Fe-Ti alloys the magnetic term in Eq. (5) is not negligible in comparison to the nuclear one and the separation of the two terms is not possible. Thus we have used only the difference of differential cross sections and we fitted them using Eq. (6). The experimental values of  $\Delta(d\sigma/d\Omega)$  are plotted in Fig. 3 for all the alloys investigated in the present study. As before the bars denote the statistical errors only and the experimental values are the average over counts from eight cells of the multidetector.

In the least-squares fit of Eq. (6) to the experimental data we introduced the shells surrounding the central atom successively looking at the variation of  $\chi^2$  value. For all the alloys we have used the same magnetic form factor  $f(k) = 1 - 0.07k^2$  which is close to that of pure Fe (the same we used before for more concentrated alloys<sup>9</sup>). For the alloy with 0.84 at. % of Ti the value of  $\chi^2$  was not sensitive to the number of shells taken into consideration which indicates the absence of magnetic-moment disturbance. The data for the second alloy with 1.33 at. % of Ti were more sensitive to the fitting procedure and  $\chi^2$  value was slightly worse in the case without magnetic-moment disturbance. The most sensitive data were for the third alloy with 1.73 at. % of Ti. The lowest value of  $\chi^2$  for this alloy was obtained with two first shells of atoms indicating the presence of a magnetic-moment disturbance. In the last case the introduction of the third shell of atoms did not change the value of  $\chi^2$  modifying only slightly the values of  $\beta^{R1}$  and  $\beta^{R2}$  with much smaller value of  $\beta^{R3}$ . This behavior is well understood in the light of the fact that our measurements were performed in a limited scattering vector range. We note here that the value of  $\Delta\mu = \bar{\mu}_m - \bar{\mu}_i$  does not depend on the number of shells introduced in the computation; the parameters  $\beta^R$  show a tendency to cancel themselves, especially for the two first alloys.

TABLE IV. Averaged magnetic perturbation ( $\mu_B$ ) and short-range order parameters in Ni-Ti alloys.

at. % Ti	$\Delta\mu$	$\delta\mu^{R1}$	$\delta\mu^{R2}$	$\delta\mu^{R3}$	$\alpha_{R1}$	$\alpha_{R2}$	$\alpha_{R3}$
2 <sup>a</sup>	0.613(40)	-0.140(8)	-0.006(30)	-0.048(28)			
3.87	0.487(10)	-0.108(4)	-0.028(15)	-0.021(4)	-0.004(18)	0.016(82)	0.002(18)
7.72 <sup>b</sup>	0.299(11)	-0.067(4)	-0.027(18)	-0.010(5)	-0.011(7)	0.014(33)	0.003(7)

<sup>a</sup>Livet and Radhakrishna (Ref. 10).

<sup>b</sup>At  $H = 13$  kOe.

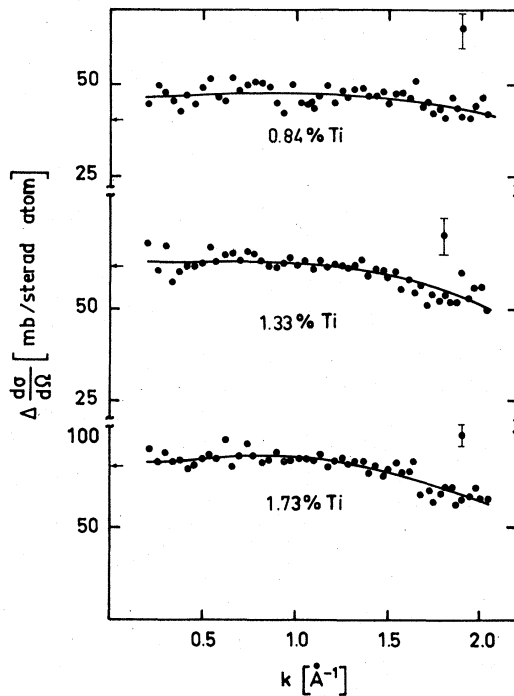


FIG. 3. Difference of differential cross sections for Fe-Ti alloys. The arrows indicate the difference of differential cross sections at  $k=0$  calculated from  $d\bar{\mu}/dc$  as described in text.

For these two alloys one can conclude that there is no magnetic-moment disturbance. Such moment disturbance occurs in the third alloy with 1.73 at. % of Ti. On the other hand the large values of  $\Delta\mu$  indicate existence of the magnetic-moment enhancement on Ti sites which decreases with increasing impurity concentration. The least-squares-fitted parameters are listed in Table V together with those for the two alloys measured previously<sup>9,26</sup> and calculated values of  $\Delta(d\sigma/d\Omega)$  are plotted in Fig. 3 (solid lines). We note here that in the measured alloys the perturbation is magnetic in origin, the sum of differential cross sections being almost flat. Thus the parameters

TABLE V. Averaged magnetic perturbation ( $\mu_B$ ) around a Ti impurity in Fe-Ti alloys.

at. % Ti	$\Delta\mu$	$\beta^{R1}$	$\beta^{R2}$
0.84	4.46(14)	0.09(11)	-0.06(15)
1.33	3.80(17)	0.07(8)	-0.04(12)
1.73	3.76(24)	0.08(6)	-0.03(3)
2.88 <sup>a</sup>	2.98(6)	0.046(16)	0.009(3)
4.92 <sup>a</sup>	2.75(9)	0.105(12)	0.006(5)

<sup>a</sup>Kajzar and Parette (Ref. 9).

listed in Table V (except those for an alloy with 4.92 at. % of Ti) represent the magnetic-moment disturbance. In the case of the alloy with 4.92 at. % of Ti the sum was slightly peaked at  $k=1.2 \text{ \AA}^{-1}$  indicating a possible presence of the chemical short-range order.<sup>26</sup>

## VI. INDIVIDUAL MAGNETIC MOMENTS

Combining the two sets of data, the bulk magnetic moments  $\bar{\mu}$  and the difference of average moments  $\Delta\mu$  as determined from the diffuse-scattering measurements, one can find individual average magnetic moments

$$\begin{aligned}\bar{\mu}_m &= \bar{\mu} + C_i \Delta\mu - \mu_{\text{diff}}, \\ \bar{\mu}_i &= \bar{\mu} - C_m \Delta\mu - \mu_{\text{diff}},\end{aligned}\quad (9)$$

where  $\mu_{\text{diff}}$  is the diffuse nonlocal magnetic moment seen in the polarized-neutron Bragg-scattering measurements.

For the Fe-Ti alloys we have assumed  $\mu_{\text{diff}} = -0.2\mu_B$ ,<sup>27</sup> the same for all Ti concentrations. In fact in similar Fe-V alloys<sup>28</sup> this value was found to be close to that of pure iron up to 5 at. % of V. In the case of Ni-Ti alloys the situation is more complicated. For pure Ni the value of  $\mu_{\text{diff}}$  is  $-0.105\mu_B$  as determined by Mook.<sup>29</sup> Moreover, there is no evidence to show how this value depends on the impurity concentration. This dependence should be significant because the average moment in these alloys decreases rapidly with concentration at room temperature. In order to avoid any introduction of an uncertainty in the data we have neglected the diffuse moment. The calculated values of individual magnetic moments for Ni-Ti alloys are given in Table II and those for Fe-Ti alloys in Table III. It is seen that in iron matrix titanium carries a large magnetic moment decreasing rapidly with increasing impurity concentration and coupled antiparallel to the host moment. This moment is much more important than that found for more concentrated alloys indicating a moment enhancement on impurity sites in the dilute limit. In Ni-Ti alloys the impurity atoms bear a small negligible negative moment. In fact the values given in Table II should be increased by the diffuse moment. For the alloy with 7.72 at. % of Ti there is an uncertainty connected with the fact that this alloy actually was not entirely saturated in an applied field of 13 kOe (the saturation value of bulk moment is about 10% higher than that reported in Table II). Thus the values given in Table II correspond to the magnetic moment at an external magnetic field of 13 kOe.

## VII. THEORETICAL CONSIDERATIONS

The coherent potential approximation (CPA) has been applied successfully to study the electronic

TABLE VI. Parameters used in CPA calculations (energy units are rydbergs).

	$U$	$J$	$J_{11}^N$	$J_{12}^N$	$J_{22}^N$	$W^0$	$N^0$	$\Delta$
Fe	0.295	0.028	0.0012	0	0	0.48	7.2	-0.03
Ni	0.11	0.011	0.0038	0	0	0.4	8.85	0.016
Ti	0.03	0.02	0	0	0	0.52 <sup>a</sup>	3	-0.16

<sup>a</sup>In bcc phase, in fcc phase  $W_{\text{Ti}}^0 = W_{\text{Ni}}^0 = 0.4\text{Ry}$ ,  $\Delta = -0.123\text{Ry}$ .

structure of disordered-3- $d$ -metal alloys. Within Hartree-Fock approximation for the Hubbard model it was possible to explain the concentration dependence of individual magnetic moments in several bcc Fe-based<sup>30</sup> and fcc Ni-based<sup>31</sup> alloys. Moreover the introduction of the orbital degeneracy<sup>32,33</sup> and calculation using a realistic density of states function allowed us also to explain the concentration dependence of the electronic specific heat and asphericity of the magnetic-moment distribution. These quantities are very sensitive to the shape of the density of states function used in the CPA calculations. We have performed also such calculations for Ni-Ti and Fe-Ti alloys. Up to now it was not done for these alloys and it seemed to us to be of interest because of the large charge difference between the alloy elements and occurrence of VBS.

Here we sketch briefly the method of calculation. More details are to be found in an earlier paper.<sup>3</sup>

The self-energy  $\Sigma_\mu^\sigma(Z)$  for a disordered binary  $A_{1-c}B_c$  alloy is obtained by solving the CPA equation

$$\Sigma_\mu^\sigma(Z) = \tilde{\epsilon}_{\sigma\mu} - [\epsilon_{A\sigma\mu} - \Sigma_\mu^\sigma(Z)] \times F_\mu^\sigma(Z) [\epsilon_{B\sigma\mu} - \Sigma_\mu^\sigma(Z)] , \quad (10)$$

where  $F_\mu^\sigma(Z)$  is the Slater-Koster function for the alloy. Within the Hubbard model and in the Hartree-Fock approximation the center of the gravity of the subband  $\mu$  with spin  $\sigma$  is

$$\epsilon_{i\sigma\mu} = \epsilon_{i\mu} + U_i n_{i-\sigma} + (U_i - J_i)(n_{i\sigma} - n_{i\sigma\mu}) \pm Z \sum_{i \neq A,B} [(1-C)J_{iA}^N(n_{A\uparrow\nu} - n_{A\downarrow\nu}) + CJ_{iB}^N(n_{B\uparrow\nu} - n_{B\downarrow\nu})] , \quad (11)$$

where following Sacchetti<sup>34</sup> we also introduced the nearest-neighbors exchange interaction.

In formula (11)  $\epsilon_{i\mu}$  are the centers of gravity of the subband  $\mu$ ,  $U_i$  is the intra-atomic Coulomb correlation energy,  $J_i$  is the intra-atomic exchange interaction energy,  $J_{ij}^N$  is the nearest-neighbor exchange-interaction energy,  $Z$  is the number of nearest neighbors,  $\pm$  signs refer to the up- and down-spin energies, respectively,  $C$  is the impurity concentration, the

indices  $i$  and  $j$  stand for the alloy elements  $A$  and  $B$ ,  $\mu$  for the subband, and  $\sigma$  for the spin direction,  $n_{i\sigma}$  is the total number of electrons on atom  $i$  with spin  $\sigma$

$$n_{i\sigma} = \sum_{\mu} n_{i\sigma\mu} \quad (12)$$

and  $n_{i\sigma\mu}$  is that in the subband  $\mu$ .

$$\tilde{\epsilon}_{\sigma\mu} = (1-C)\epsilon_{A\sigma\mu} + C\epsilon_{B\sigma\mu} \quad (13)$$

is average energy of electrons with spin  $\sigma$  in the subband  $\mu$ .

The Slater-Koster function  $F_\mu^\sigma$  is given by following equation:

$$F_\mu^\sigma(Z) = \int_{-\infty}^{\infty} \frac{\rho_\mu^0(\epsilon) d\epsilon}{Z - \Sigma_\mu^\sigma(Z) - \epsilon} , \quad (14)$$

where  $\rho_\mu^0(\epsilon)$  is the density of states function of the subband  $\mu$  before alloying.

Solving simultaneously the set of transcendental Eqs. (10) and (14) one obtains the partial density of states functions

$$\rho_{i\sigma\mu}(\epsilon) = -\frac{1}{\pi} \text{Im} \left[ \frac{F_\mu^\sigma(Z)}{1 - [\epsilon_{i\sigma\mu} - \Sigma_\mu^\sigma(Z) F_\mu^\sigma(Z)]} \right] \Big|_{Z=\epsilon+i0} \quad (15)$$

and corresponding occupation numbers

$$n_{i\sigma\mu} = \int_{-\infty}^{\epsilon_F} \rho_{i\sigma\mu}(\epsilon) f(\epsilon, T) d\epsilon , \quad (16)$$

where  $f(\epsilon, T)$  is the Fermi-Dirac distribution function, and  $\epsilon_F$  the Fermi energy in the alloy determined from the condition that the total number of electrons in the band is conserved

$$\begin{aligned} n^0 &= \sum_{\sigma} (1-C)n_{A\sigma} + Cn_{B\sigma} \\ &= \sum_{\sigma\mu} (1-C)n_{A\sigma\mu} + Cn_{B\sigma\mu} . \end{aligned} \quad (17)$$

The knowledge of the occupation numbers  $n_{i\sigma\mu}$  allows us to calculate the individual magnetic moments

$$m_i = \sum_{\mu} (n_{i\uparrow\mu} - n_{i\downarrow\mu}) , \quad (18)$$

the total magnetic moment

$$m = (1 - C)m_A + Cm_B, \quad (19)$$

as well as the asphericity parameter being the  $e_g$  part of the total magnetic moment

$$p = \frac{m_{e_g}}{m}. \quad (20)$$

In fact in cubic alloys we have to deal with twofold degenerate  $e_g$  orbitals and threefold degenerate  $t_{2g}$  orbitals with different spatial distribution of electron-spin density.

In the numerical calculations we have used the density of states for Ni calculated by Hodges *et al.*<sup>35</sup> and that for Fe derived from band-structure calculations by Tawil and Callaway<sup>36</sup> (the same we used for Fe-V alloys). For titanium in bcc phase we used the density of states for the neighboring element vanadium calculated by Wakoh and Yamashita<sup>37</sup> and in fcc phase that of Ni. As emphasized in an earlier paper<sup>3</sup> the only free parameter in the calculation is the difference between the centers of gravity of one sub-band

$$\Delta\mu = \epsilon_{B\mu} - \epsilon_{A\mu} \quad (\mu = e_g \text{ or } t_{2g}).$$

The others can be determined self-consistently if the electronic characteristics of pure elements are known. These are well known for pure Ni ( $\mu = 0.68\mu_B$  and  $p = 0.19$ )<sup>29</sup> and Fe ( $\mu = 2.37\mu_B$  and  $p = 0.53$ )<sup>27</sup>. There is no such information about Ti in bcc and fcc phases. We assumed that in both phases Ti is non-magnetic and the  $e_g$  subband lies lower, similar as in vanadium with 65% of  $e_g$  electrons. The last assumption has no influence on the magnetic-moment distribution. This can influence only the electronic specific heat, this one being mainly determined by the host band if the Fermi level lies below the virtual band as is the case, and the asphericity parameter. At least in the case of Ni-Ti alloys the impurity atoms bear a negligible magnetic moment and the asphericity is determined by host atoms. Thus this assumption has also no significant influence on the results. In the bcc phase one can expect that the electronic structure of titanium is similar to that of vanadium. Even if there are some small differences they do not influence significantly the results of calculations because of low Ti concentration (the bcc phase persists only up to about 13 at.% of Ti).<sup>38</sup> By analogy with vanadium we assumed that the  $3d$  band of Ti contains  $n_{Ti}^0 = 3$  electrons (cf., also Kajzar and Mizia<sup>39</sup>). The one free parameter from two  $\Delta\mu$ 's ( $\mu = e_g, t_{2g}$ ) we have chosen in such a way as to get  $d\bar{\mu}/dc$  in agreement with experimental values. All parameters used in the calculation are listed in Table VI. As we mentioned before the bcc phase in Fe-Ti alloys persists only up to about 13 at.% of Ti. In order to get a better picture of the concentration dependence of cal-

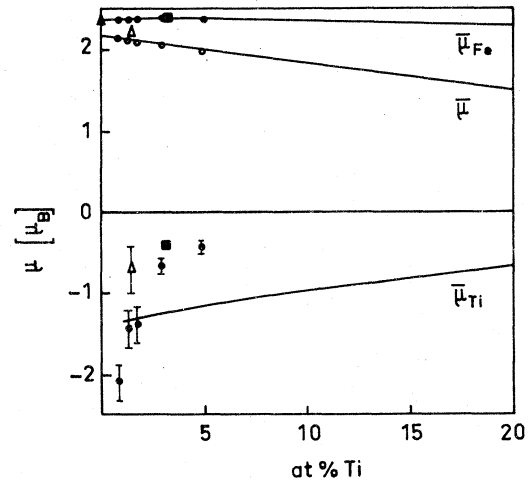


FIG. 4. Magnetic-moment distribution in Fe-Ti alloys. The solid lines are calculated values, ● - present study and Kajzar and Parette (Ref. 9), □ - Child and Cable (Ref. 7), Δ - Collins and Low (Ref. 6), ▲ - Shull (Ref. 27).

culated quantities we have performed our calculations up to 20 at.% of Ti. The results of computations of individual magnetic moments are plotted in Figs. 4 and 5 for Fe-Ti and Ni-Ti alloys, respectively. In both cases good overall agreement is seen between measured and calculated values except in the dilute limit in Fe-Ti alloys (Fig. 4). The calculated moment is smaller in absolute value than the measured one. Also the decrease of titanium moment is more important than the theoretical one. Increasing the value of Coulomb correlation energy  $U_{Ti}$  it is possible to obtain a larger moment on the impurity atom with however the same concentration dependence; the curve is only shifted. Even varying the parameter  $\Delta\mu$  it was not possible to get a more rapid decrease of titanium moment. It seems to us that if CPA gives a

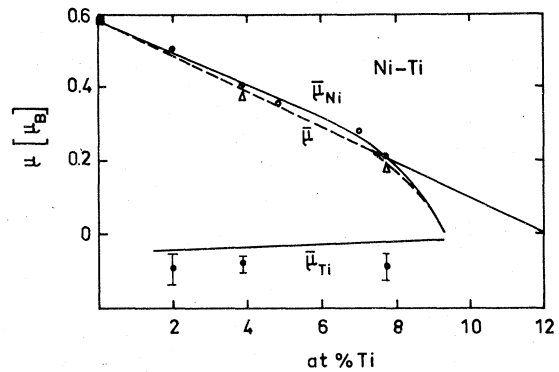


FIG. 5. Magnetic-moment distribution in Ni-Ti alloys. Solid lines represent calculated values, ○ - bulk moments [Marian (Ref. 21)], Δ - bulk moments (present study), ● - individual magnetic moments [Livet and Radhakrishna (Ref. 10) and present study], ■ - Mook (Ref. 29) ( $\mu_{spin} + \mu_{diff}$ ).



good description of concentration dependence of individual magnetic moments for more concentrated alloys, it fails in the dilute limit. In fact, starting from 1.73 at. % of Ti the concentration dependence of titanium moment is nearly the same (within errors) as predicted by CPA.

In the case of Ni-Ti the agreement between theory and experimental data is much better. The theory gives a small negligible negative magnetic moment on titanium atoms in agreement with experimental data. Also the calculated concentration dependence of the bulk moment is in good agreement with experimental data. A small disagreement is seen for the alloy with 7.72 at. % of Ti. This is probably due to the fact that our sample was not entirely saturated and we have neglected the diffuse moment. According to the value of  $d\bar{\mu}/dc$  the ferromagnetism in Ni-Ti alloys disappears at  $C_{\text{crit}} \approx 11$  at. % of Ti, whereas our calculation yields for  $C_{\text{crit}}$  a lower value ( $\sim 9.3$  at. % of Ti). In fact, in the neighborhood of the critical concentration, the ferromagnetic solution matches the paramagnetic one and can explain why  $C_{\text{crit}}$  is lower than the experimental one and why the calculated variation of  $d\bar{\mu}/dc$  is no more linear for the concentrations above 8 at. % of Ti. However the extrapolated value of  $d\bar{\mu}/dc$  (dashed line in Fig. 5) gives a nearly correct value of  $C_{\text{crit}}$ .

The electronic specific heat, which is directly proportional to the number of electrons at the Fermi level  $\rho(\epsilon_F)$

$$\chi = \frac{2}{3} \kappa^2 \rho(\epsilon_F) \quad (21)$$

where  $\kappa$  is the Boltzmann constant, is plotted in Figs. 6 and 7 for Ni-Ti and Fe-Ti alloys respectively. The experimental data for Ni-Ti alloys are taken from Gregory and Moody.<sup>20</sup> For Ni-Ti alloys we have obtained a good description of electronic specific heat

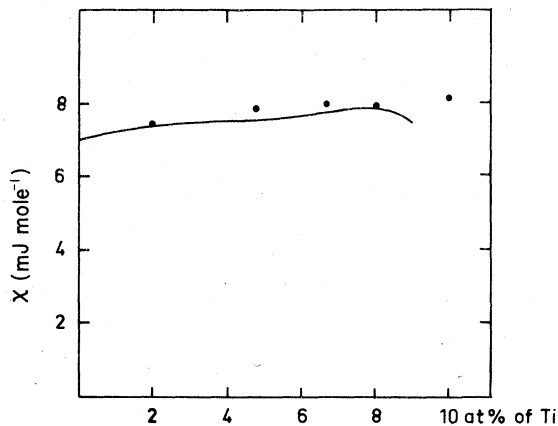


FIG. 6. Electronic specific heat in Ni-Ti alloys. Solid lines represent calculated values and the points are measured values by Gregory and Moody (Ref. 20). The data have been adjusted for the corresponding value of pure nickel.

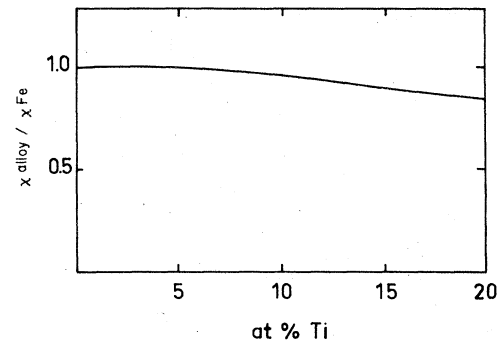


FIG. 7. Calculated ratio of electronic specific heat of alloy to that of pure iron in Fe-Ti alloys.

up to 8 at. % of Ti. Above this concentration the calculated specific heat decreases while the experimental data show a nearly constant behavior. This disagreement is due to the transition from the ferromagnetism to the paramagnetic state and corresponding lowering of the number of electrons at the Fermi level while the experimental data were taken at liquid-helium temperature where ferromagnetism persists at over 15 at. % of Ti (Gregory and Moody<sup>20</sup>).

In the case of Fe-Ti alloys the electronic specific heat decreases more slowly than in Fe-V alloys. The fact is in agreement with experimental data (quoted by Gautier<sup>11</sup>). Also we got for Fe-Ti alloys a constant decrease of  $\chi$  up to 20 at. % of Ti while in Fe-V alloys, it reaches a minimum at 10 at. % of V.

The calculated concentration dependence of the asphericity parameter  $p$  is plotted for both alloys in Fig. 8. For Ni-Ti alloys we obtained a slight increase of  $p$  up to 3 at. % of Ti. Such an increase of the asphericity parameter was observed in an alloy with 2 at. % of Ti by Livet and Radhakrishna<sup>40</sup> who found  $p = 0.205(p_{\text{Ni}} = 0.19)$ .<sup>29</sup> Above 3 at. % of Ti the calculated asphericity parameter decreases.

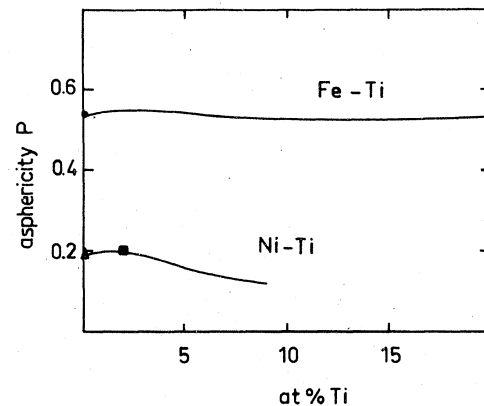


FIG. 8. Calculated variation of the asphericity parameter in Fe-Ti and Ni-Ti alloys (solid lines). • - Shull (Ref. 27), ▲ - Mook (Ref. 29), and ■ - Livet and Radhakrishna (Ref. 10).

To our knowledge there is no experimental data for the concentration dependence of the asphericity parameter in Fe-Ti alloys. Our calculations give a slightly different behavior of  $p$  as a function of the alloy concentration than in Fe-V alloys.<sup>3</sup> Similarly to the case of Fe-V alloys this parameter increases at low impurity concentration. However this increase is less pronounced than in Fe-V alloys and stops at about 5 at. % of Ti where  $p$  starts to decrease, and above 15 at. % of Ti we obtained again a slight increase of  $p$ . The last result may play a role in destabilizing the bcc phase of Fe-Ti alloys.

### VIII. DISCUSSION

We have performed polarized neutron-elastic diffuse-scattering measurements on two Ni-Ti alloys with 3.87 and 7.72 at. % of Ti and three Fe-Ti alloys with 0.84, 1.33, and 1.73 at. % of Ti. These measurements together with bulk magnetization data allowed us to determine the average individual magnetic moments, magnetic-moment disturbance, and in the case of Ni-Ti alloys the chemical short-range order, found to be negligible. The present data together with the previous ones<sup>9</sup> indicate quite different behavior of Ti impurity in both matrices. The main differences are the following: (i) The value of the impurity moment. In an iron matrix, impurity atoms bear a large negative moment decreasing rapidly with increasing alloy concentration. In contrast in the nickel matrix the Ti moment is negligible. (ii) The magnetic-moment disturbance has opposite signs in these alloys and is more extended in Ni-Ti alloys, up to the third shell of atoms. In Ni-based alloys the magnetic-moment disturbance decreases with increasing alloy concentration while in iron matrix this occurs at higher impurity concentration (starting from 1.73 at. % of Ti).

The experimental data together with performed CPA calculations show the existence of VBS in both alloys. The charge transfer from the impurity to the host atoms is more important in the Ni-Ti alloys as expected.

The difference in the impurity behavior in both matrices can be associated with three factors: (i) Different crystal structures resulting in a different local environment. As we mentioned before, in our opinion this is a less important point. In fact, the first shell, which is the most perturbed is distant in both alloys by nearly the same value,  $R_1 \approx 2.5 \text{ \AA}$ . (ii) Different number of electrons in the  $3d$  bands of Ni and Fe, the first being nearly filled, the second containing about two electrons less. (iii) Different electron transfer from the impurity to the host band. As we mentioned before this transfer is more important in Ni-Ti alloys and tends to rapidly fill the band of nickel.

In the light of above remarks we think that the sign of the magnetic-moment disturbance caused by

impurities is not connected with the question of the creation of VBS as pointed out by Comly *et al.*<sup>5</sup> but rather with the value of impurity moment and the number of electrons in the band. If there is no chemical short-range order and the impurity moment is large one observes a negligible or small positive moment disturbance confined to the first shells of atoms. This is a case of Fe-Ti, Fe-V,<sup>6</sup> and low-concentration Fe-Cr,<sup>6,41</sup> Fe-Mn,<sup>6</sup> Ni-Mn,<sup>6,25</sup> and Ni-Fe alloys.<sup>6</sup> In this case we have to do with a type of compensation of magnetic-moment disturbance around impurity and host atoms. If however, the impurity moment is very small or negligible, we have an important and negative magnetic-moment disturbance extended in the space as is observed in Ni-Ti, Ni-Cr,<sup>42</sup> Ni-Ru,<sup>43</sup> and low-concentrated Ni-Pd alloys.<sup>44</sup> In these alloys, due to the charge transfer from impurity to the host band, the host magnetic moment decreases in neighboring impurity shells. In Ni-Pd alloys<sup>44</sup> the magnetic-moment disturbance decreases with increasing impurity concentration and changes sign at 25 at. % of Pd. At the same time the Ni and Pd moments increase. The situation is however more complicated for the chemical short-range order. A better understanding of this phenomena needs more systematic studies with the use of polarized neutrons which allows correct determination of the sign of quantities under question.

Our CPA calculations give a good overall description of magnetic-moment distribution in both alloys. The agreement is better in the case of Ni-Ti alloys. For Fe-Ti alloys we got smaller values of impurity magnetic moment at lowest titanium impurity in disagreement with experimental values. In Fig. 9 we plotted the observed and calculated values of the difference between iron and titanium moments. This difference is independent of the assumption of diffuse moment. In fact Eqs. (9) attribute the same value of  $\mu_{\text{diff}}$  to Fe and Ti sites which can be incorrect. As it is seen from Fig. 9 the agreement is slightly better although the calculated difference also varies more slowly with concentration than the observed ones. At higher concentration of titanium the calcu-

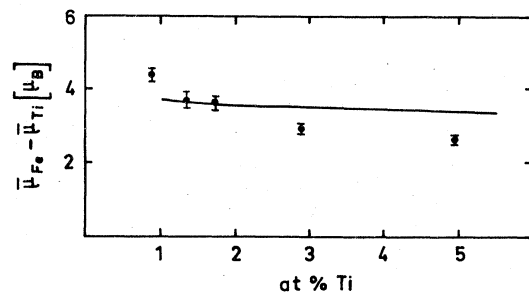


FIG. 9. Calculated and observed concentration dependence of  $\bar{\mu}_{\text{Fe}} - \bar{\mu}_{\text{Ti}}$  (solid line) in Fe-Ti alloys.

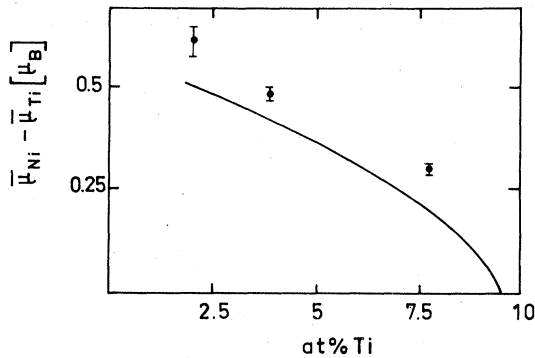


FIG. 10. Calculated concentration dependence of  $\bar{\mu}_{Ni} - \bar{\mu}_{Ti}$  (solid line) in Ni-Ti alloys. • - Livet and Radhakrishna (Ref. 10) (2 at.% Ti), and present study.

lated variation of  $\mu_{Fe} - \mu_{Ti}$  is again in good agreement with experimental values although there is a difference between calculated and observed values. A similar plot for Ni-Ti alloys is given in Fig. 10. The observed variation of  $d\bar{\mu}/dc$  with titanium concentration is in good agreement with the calculated one. The difference between calculated and observed values can be attributed to the neglect of diffuse moment in our calculation (we assumed a Ni moment equal to  $0.583 \mu_B$  which is the bulk moment).

For the last alloys the experimental data are available only starting from 2 at.% of Ti. These results seem to indicate that CPA gives a good description of magnetic-moment distribution in both alloys at higher impurity concentrations. This fails at the very dilute limit as is the case for Fe-Ti alloys with 0.84 at.% of Ti. This can be well understood taking into account the fact that CPA is a theory analogous to molecular-field approximation. It assumes the existence of an average field constant in the alloy. If this assumption can work well in more concentrated alloys, it fails at dilute limit where impurities are well separated and a local modification of the potential occurs connected with a local modification of the band structure.

We note here that Campbell and Gomès<sup>45</sup> have also obtained a large negative moment on titanium impurity in the dilute limit ( $\approx -2\mu_B$ ) from the VBS concept in good agreement with our value at 0.84 at.% of Ti.

Marshall<sup>46</sup> has shown that the magnetic-diffuse-scattering cross section of unpolarized neutrons from a dilute alloy at zero scattering vector value is proportional to the average magnetization variation with alloy concentration

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{mag, diff}} (k=0) = C_i C_m \left( 0.2695 \frac{d\bar{\mu}}{dc} \right)^2. \quad (22)$$

In the case of diffuse scattering of polarized neutrons an analogous formula has been given by Medi-

TABLE VII. Calculated and extrapolated values of  $\Delta(d\sigma/d\Omega)(k=0)$  in mb for Ni-Ti alloys.

at.% of Ti	$\left( \Delta \frac{d\sigma}{d\Omega} \right)_{\text{calc}}$	$\left( \Delta \frac{d\sigma}{d\Omega} \right)_{\text{extrapol}}$
2	147	100
3.87	279	137
7.72	535	159

na and Garland<sup>47</sup>

$$\Delta \frac{d\sigma}{d\Omega} (k=0) = 1.078 C_i C_m (b_i - b_m) \frac{d\bar{\mu}}{dc} S(0). \quad (23)$$

This formula takes into account a possible short-range order in the alloy neglected in Eq. (22) and should be verified also at more concentrated alloys.

The calculated values of  $\Delta(d\sigma/d\Omega)(k=0)$  using Eq. (23) and  $d\bar{\mu}/dc = -3.42 \mu_B/\text{atom}^9$  for Fe-Ti alloys are indicated by arrows in Fig. 3. It is seen that Eq. (23) is well verified for all alloy concentrations. However in the case of Ni-Ti alloys we observe a departure from this law increasing with alloy concentration. In all cases the calculated value of  $\Delta(d\sigma/d\Omega)(k=0)$  is higher than the measured difference of differential cross sections extrapolated to  $k=0$ . Even at 2 at.% of Ti Livet and Radhakrishna<sup>10</sup> observed such departure although these authors used too small an absolute value of  $d\bar{\mu}/dc$  ( $-3.6 \mu_B/\text{atom}$ ).

In Table VII we compare the extrapolated from experimental data and the calculated values of  $\Delta(d\sigma/d\Omega)$  using Eq. (23) and  $d\bar{\mu}/dc = -5.1 \mu_B/\text{atom}$  as determined in the present study including also the data for the alloy studied by Livet and Radhakrishna.<sup>10</sup> It is seen that the difference between calculated and experimental data increases rapidly with impurity concentration. Similar behavior was also observed by Cable and Medina<sup>42</sup> in Ni-Cr alloys. These authors attributed it to some nonlocal effects in Ni-Cr alloys. Similar effects are to be expected in Ni-Ti alloys although we think that in this case the value of  $d\bar{\mu}/dc$  is not constant and depends on the alloy concentration as it was observed at low temperature by Gregory and Moody<sup>20</sup> for  $C_{Ti} > 8$  at.%.

#### ACKNOWLEDGMENTS

The authors would like to thank Professor J. Friedel from Université Paris-Sud and Dr. J. W. Cable from ORNL for useful discussions and suggestions, as well as Professor Barbier, Director of Laboratoire Louis Néel of CNRS in Grenoble for permission to make the bulk magnetization measurements in his laboratory and M. Barlet for technical assistance in performing them.

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