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# The atomic and magnetic distributions in ferromagnetic $\text{Fe}_{0.865}\text{V}_{0.135}$

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## Abstract

Experimental results obtained for the atomic and magnetic distributions in the ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  system are presented. These results were obtained from the observed polarized neutron scattering from a single crystal at room temperature. The results are compared with those obtained from a first-principles density functional based theory. This theory can calculate both the atomic short-range order that exists in atomically disordered alloys and also determine the effect that fluctuations in the local chemical environment have on the magnetization in ferromagnetic alloys. The present neutron scattering results for the atomic correlations in the ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  system are in good agreement with those obtained from both a theoretical calculation and previous neutron scattering studies of FeV alloys. The current experimental results for the magnetic distribution in ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  are seen to accurately reproduce the result determined from the theoretical calculation.

## 1. Introduction

The mechanical, electronic and magnetic properties of alloys are dependent upon the electronic structure of the material. For the case of ferromagnetic binary metallic alloys, it is the electronic structure that determines both the distribution of the atoms upon the crystal lattice and the magnetic moment that each atom exhibits. Over recent years there has been significant progress in the area of first-principles calculations of the atomic and magnetic moment distributions in binary transition metal alloys. An *ab initio* description of metallic alloys based on the self-consistent field, Korringa–Kohn–Rostoker (KKR) coherent potential approximation (CPA) treatment of the electronic structure [1] has proved to be very successful for the study of the atomic and magnetic correlations in a variety of metallic alloys.

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Available from the theory is the atomic susceptibility,  $\alpha(\kappa)$  [2, 3], which describes the Fourier components of the atomic distribution that is present in the high temperature atomically disordered state. Importantly the theory self-consistently incorporates the magnetic state of the system into the calculation of  $\alpha(\kappa)$ , so a determination of the effect that changes to the magnetization have on the atomic correlations can be made. The magnetic moment distribution in ferromagnetic binary alloys can also be obtained from the theory via the calculated magneto-compositional response function,  $\gamma(\kappa)$  [4]. Both  $\alpha(\kappa)$  and  $\gamma(\kappa)$  can be experimentally determined from diffuse neutron scattering, so the validity of the theory may be determined from comparison with experimental results. The theory has been applied to the calculation of both  $\alpha(\kappa)$  [3, 5] and  $\gamma(\kappa)$  [4] for the ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  system primarily because the  $\alpha$ -FeV system has been extensively investigated, although a single-crystal study of  $\gamma(\kappa)$  has never been completed.

The existence of atomic short-range order in the  $\alpha$ -FeV system was first suggested by Nomura *et al* [6] on the basis of NMR experiments. Their qualitative results indicated repulsion between nearest neighbour vanadium atoms. The atomic correlations were further analysed by Mirebeau *et al* [7] who conducted diffuse neutron scattering measurements on  $\alpha$ -FeV polycrystalline alloys. The neutron scattering analysis was conducted on alloys quenched from the melt in the concentration range  $0.01 < c_V < 0.20$ , obtaining atomic short-range order corresponding to the paramagnetic state. It was observed that the amount of atomic short-range order increased as  $c_V$  increased. The scattering data indicated strong repulsion between the vanadium atoms for the first two shells, the size of this repulsion increasing with  $c_V$ . The vanadium atoms, pushed away from the first two shells, occupy the third shell with a probability greater than that given by a random distribution. In the fourth shell the occupation probability was concluded to be nearly random.

Cable *et al* [8] measured the diffuse nuclear neutron scattering from a single  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal to enable the atomic short-range order in the system to be more accurately determined. This crystal was quenched from an effective temperature of approximately 900 K, which is below the Curie temperature,  $T_C$ , of 1180 K. Therefore the observed atomic short-range order of the system was that present in the atomically disordered ferromagnetic state. The results for  $\alpha(\kappa)$  indicated atomic correlations that exist out to the eighth shell, with the observed correlations for the first three shells being similar to those obtained from the polycrystalline alloys. A subsequent first-principles theoretical calculation of  $\alpha(\kappa)$  for the  $\text{Fe}_{0.865}\text{V}_{0.135}$  system at a temperature above the theoretical chemical-transition temperature, but below the theoretical estimation of  $T_C$ , was made [5] to analyse the validity of the theory through comparison with the neutron data. Excellent quantitative agreement was achieved between the theoretically and experimentally obtained  $\alpha(\kappa)$ , with all experimentally observed features being reproduced from the theoretical calculation. The relatively long-ranged atomic interactions were interpreted as being due to a Fermi surface effect.

Previous neutron scattering investigations of the microscopic magnetic structure of ferromagnetic polycrystalline  $\alpha$ -FeV alloys in the concentration range  $0.01 < c_V < 0.20$  have shown that the vanadium atoms exhibit relatively large average moments,  $\mu_V$ , that are anti-parallel to the average moments of the iron atoms,  $\mu_{\text{Fe}}$  [9–11]. The results obtained for  $\gamma(\kappa)$  indicate that the presence of vanadium atoms in the first two shells of an atom decrease the size of the average moment, while the presence of vanadium atoms in the third shell increase the average moment.

The theoretical calculation of  $\gamma(\kappa)$  for chemically disordered ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  [4] indicates that the effect of the local environment upon both the iron and vanadium moments is limited to interactions from the first two neighbouring shells. As the iron content of the local environment of either an iron or vanadium atom increases, so too

does the magnitude of the moment at that site. Conversely, the magnitude of the moment of either an iron or vanadium atom decreases as the vanadium atomic concentration increases in its local environment. This behaviour is to be expected as the vanadium moment is an induced moment. The average moments were determined as  $2.075 \mu_B/\text{atom}$  on the iron sites and  $-0.724 \mu_B/\text{atom}$  on the vanadium sites [4]. These results are in close agreement with the values of  $(2.183 \pm 0.039) \mu_B/\text{atom}$  and  $(-0.82 \pm 0.08) \mu_B/\text{atom}$  for the average iron and vanadium moments in the Fe<sub>0.853</sub>V<sub>0.147</sub> system, determined via polycrystalline neutron scattering [11].

The theoretical calculation for  $\gamma(\kappa)$  has been directly compared with a preliminary experimental result determined from polarized neutron scattering from a single Fe<sub>0.865</sub>V<sub>0.135</sub> crystal [4]. This was the same crystal as was used by Cable *et al* [8] to obtain  $\alpha(\kappa)$ .  $\gamma(\kappa)$  determined from the neutron scattering data was not the same as the result determined via the theory. In particular, the experimental results lay well below the calculations and also below what would be expected from the bulk magnetic measurements of Aldred [12]. Due to the potential importance of the theory, a further polarized neutron scattering experiment was conducted in the hope of obtaining closer agreement between the experimentally and theoretically determined  $\gamma(\kappa)$ .

## 2. Theory

In binary alloys A<sub>c</sub>B<sub>1-c</sub>, the atomic configuration can be specified by  $\{\xi_i\}$  where  $\xi_i = 1$  (0) if there is an A (B) type atom located at lattice site  $\mathbf{R}_i$ . The thermal average of  $\xi_i$  determines the local concentration of A atoms at  $\mathbf{R}_i$ , that is  $c_i$ . The first-principles theory [2] can determine  $\alpha(\kappa)$  in the high temperature atomically disordered state where  $c_i = c$  for all  $\mathbf{R}_i$ , with the result taking the same form as that obtained by Krivoglaz [13] and Clapp and Moss [14, 15] for a binary alloy, where

$$\alpha(\kappa) = \frac{1}{[1 + c(1 - c)\beta V(\kappa)]}. \quad (1)$$

Here  $\beta = 1/k_B T$  and  $V(\kappa)$  is the lattice Fourier transform of the interchange potential in a pair potential model. In the first-principles theory,  $V(\kappa)$  is based on a mean field electronic description of the interchange energy [2] and, although it is equivalent to the random-phase approximation (RPA), it represents the real system more accurately as it is based on an electronic description of the system. The result for  $V(\kappa)$ , and therefore  $\alpha(\kappa)$ , can also indicate the importance of the various electronic effects on the ordering of a particular alloy.

For ferromagnetic atomically disordered alloys, the local moment at each lattice site is dependent upon the atomic species that occupies the site as well as the local environment. In the inhomogeneous CPA formalism [4] where long-range order is artificially induced into the system, the moment at each site is given by,

$$\mu_i = c_i \mu_i^A + (1 - c_i) \mu_i^B. \quad (2)$$

$\mu_i^{A(B)}$  is the inhomogeneous partially averaged CPA magnetic moment where the thermal average is taken with the site  $\mathbf{R}_i$  restricted to being occupied by an A (B) atom. The magneto-compositional pair response function,  $\gamma_{i,j}$ , specifies the response of the thermal average of the localized moment at  $\mathbf{R}_i$  due to a change of the concentration at  $\mathbf{R}_j$ , that is

$$\gamma_{i,j} = (\mu_A - \mu_B) \delta_{i,j} + c \gamma_A^{i,j} + (1 - c) \gamma_B^{i,j}, \quad (3)$$

where, from equation (2),  $\gamma_{A(B)}^{i,j} = \delta \mu_i^{A(B)} / \delta c_j$ . The functions  $\gamma_{A(B)}^{i,j}$  describe the change in the average moment of an A (B) atom located at  $\mathbf{R}_i$  due a change in the concentration at  $\mathbf{R}_j$

from the random CPA medium. Here  $\mu_{A(B)}$  are the average CPA moments of the A (B) atoms. For a high temperature atomically disordered alloy, a lattice Fourier transform can be taken, yielding [4]

$$\gamma(\boldsymbol{\kappa}) = (\mu_A - \mu_B) + c\gamma_A(\boldsymbol{\kappa}) + (1 - c)\gamma_B(\boldsymbol{\kappa}). \quad (4)$$

It is the response functions

$$\gamma_A(\boldsymbol{\kappa}) = \sum_{i,j} \gamma_A^{i,j} \exp[i\boldsymbol{\kappa} \cdot (\mathbf{R}_i - \mathbf{R}_j)], \quad (5)$$

and

$$\gamma_B(\boldsymbol{\kappa}) = \sum_{i,j} \gamma_B^{i,j} \exp[i\boldsymbol{\kappa} \cdot (\mathbf{R}_i - \mathbf{R}_j)], \quad (6)$$

together with  $\mu_A$  and  $\mu_B$ , that are determined via the theoretical calculation.  $\gamma(\boldsymbol{\kappa})$  is then determined from equation (4). These functions are important as they determine the local chemical environment effect upon the average moments of both of the constituent atoms.

The real space functions  $\gamma_{A(B)}^{i,j}$  can be determined from the calculated functions  $\gamma_{A(B)}(\boldsymbol{\kappa})$  using equations (5) and (6) defined over a distribution of  $\boldsymbol{\kappa}$  vectors. The microscopic magnetization of an alloy with any atomic distribution may then in principle be determined via the equation [4]

$$\mu_i = \xi_i \left[ \mu_A + \sum_{j \neq i} \gamma_A^{i,j} (\xi_j - c) \right] + (1 - \xi_i) \left[ \mu_B + \sum_{j \neq i} \gamma_B^{i,j} (\xi_j - c) \right]. \quad (7)$$

Provided that the induced moments are relatively small, this perturbative method can be used to provide a qualitative, if not quantitative, description of the magnetic structure that exists in ferromagnetic alloys. This procedure has been used to calculate the moments that occur in layered FeV structures from the calculated functions  $\gamma_{\text{Fe(V)}}(\boldsymbol{\kappa})$  [4]. If the result for  $\gamma(\boldsymbol{\kappa})$  has a cosine-like form between  $\boldsymbol{\kappa} = 0$  and the zone boundary, as do the results for the  $\text{Fe}_{0.865}\text{V}_{0.135}$  system reproduced in figure 4, only a small number of the  $\gamma_{A(B)}^{i,j}$  functions contribute to  $\gamma(\boldsymbol{\kappa})$ . In this case, changes in the size of the average moment only depend on concentration fluctuations at close neighbouring shells. Any deviation from this cosine form implies that more shells of atoms will be involved in the change of the moment.

### 3. Diffuse polarized neutron scattering from ferromagnetic materials

Polarized neutron scattering is a powerful tool in the investigation of both the atomic and magnetic structures of materials as the neutron polarization can be used to separate the nuclear and magnetic scattering. Hence polarized diffuse scattering can be used to simultaneously investigate both the atomic distributions and the magnetic moment disturbances in ferromagnetic and antiferromagnetic alloys [16]. The analysis of the various diffuse scattering contributions from polycrystalline alloys yields only values of the diffuse scattering averaged over the constituent crystal orientations. By using a single crystal, the diffuse scattering can be measured along a single crystal direction, or at a single position in reciprocal space. This results in it being possible to determine the distributions of nuclear and magnetic moment defects more accurately.

The total coherent elastic differential diffuse neutron scattering cross-section per atom for a magnetically saturated ferromagnetic  $A_cB_{1-c}$  binary alloy single crystal is given by [16]

$$\begin{aligned} \left( \frac{d\sigma}{d\Omega} \right)^P &= c(1-c)(b_A - b_B)^2 \alpha(\boldsymbol{\kappa}) + \gamma_0^2 c(1-c) f^2(\boldsymbol{\kappa}) \alpha(\boldsymbol{\kappa}) |\boldsymbol{\gamma}_\perp(\boldsymbol{\kappa})|^2 \\ &\quad - 2\gamma_0 c(1-c)(b_A - b_B) \alpha(\boldsymbol{\kappa}) f(\boldsymbol{\kappa}) \mathbf{P} \cdot \boldsymbol{\gamma}_\perp(\boldsymbol{\kappa}). \end{aligned} \quad (8)$$

$b_A$  and  $b_B$  are the nuclear scattering lengths of the two constituent atoms,  $\gamma_0$  is a constant equal to  $-0.269 \times 10^{-12} \text{ cm}/\mu_B$  and  $\mathbf{P}$  is the effective polarization of the incident neutron beam. The last two terms are derived with the assumption that the magnetic form factors,  $f(\boldsymbol{\kappa})$ , of the two atomic species are the same and independent of the local chemical environment [11]. This is an accurate approximation for transition metal alloys where the unpaired electron spin densities are similar. The first term of equation (8) results purely from nuclear scattering, while the second term results solely from the magnetization within the material. The third term, which is only observed for a polarized incident neutron beam, results from interference between the nuclear and magnetic scattered waves and results in magneto-compositional scattering.

All terms of equation (8) are dependent upon  $\alpha(\boldsymbol{\kappa})$  since this function specifies how the atoms are distributed about one another, which of course influences the spatial dependence of the diffuse scattering. Expressed in terms of the Cowley real space atomic short-range order parameters,  $\alpha(\boldsymbol{\kappa})$  becomes

$$\alpha(\boldsymbol{\kappa}) = \sum_{\mathbf{R}} \alpha(\mathbf{R}) \exp(i\boldsymbol{\kappa} \cdot \mathbf{R}), \quad (9)$$

where  $\mathbf{R}$  is a real space lattice vector spanning from an arbitrary origin and  $\alpha(\mathbf{R} = 0) = 1$ . Negative  $\alpha(\mathbf{R})$  implies the presence of ordering correlations of the two different atomic species over a distance  $\mathbf{R}$ , while positive  $\alpha(\mathbf{R})$  implies preference for like atoms to cluster.

Unlike the nuclear scattering lengths, the magnetic moment at each site is dependent upon the local environment. Thus  $\gamma(\boldsymbol{\kappa})$  is present in the magnetic contributions to the diffuse scattering since this function characterizes the environmental dependence of the moments.  $\gamma(\boldsymbol{\kappa})$  can be parametrized in the form

$$\gamma(\boldsymbol{\kappa}) = (\mu_A - \mu_B) + \sum_{\mathbf{R}} \phi(\mathbf{R}) \exp(i\boldsymbol{\kappa} \cdot \mathbf{R}), \quad (10)$$

where  $\phi(\mathbf{R} = 0) = 0$ . The parameters  $\phi(\mathbf{R})$  determine the change in the average moment due to the presence of A type atoms in the local environment, and from equation (3) they are given by

$$\phi(\mathbf{R}) = c\gamma_A^{i,j} + (1 - c)\gamma_B^{i,j}, \quad (11)$$

where  $\mathbf{R} = \mathbf{R}_i - \mathbf{R}_j$ . Note that in general only the parameters  $\phi(\mathbf{R})$  and not  $\gamma_A^{i,j}$  and  $\gamma_B^{i,j}$ , as is the case from the theory, can be uniquely determined from the magnetic diffuse scattering data.

As seen from equation (8), it is the component of  $\gamma(\boldsymbol{\kappa})$  that is perpendicular to the scattering vector,  $\gamma_{\perp}(\boldsymbol{\kappa})$ , that contributes to the neutron scattering cross-section. In most cases  $\gamma_{\perp}(\boldsymbol{\kappa}) = \gamma(\boldsymbol{\kappa})$  for all  $\boldsymbol{\kappa}$  since a saturating magnetic field is applied perpendicular to the scattering plane resulting in the magnetization of the material being perpendicular to all scattering vectors. Measuring the scattering with incident polarization parallel and anti-parallel to the sample magnetization allows each contribution to the scattering to be isolated.

#### 4. Experimental set-up

The long-wavelength multi-detector D7 neutron scattering spectrometer, located at the ILL facility in Grenoble, France, was used for this investigation. This instrument was specifically designed to investigate the diffuse scattering arising from the disorder in solids. Neutrons from the H15 cold neutron source at the ILL are monochromated by a focusing graphite monochromator crystal. The neutrons then pass through a beryllium filter which removes higher orders of the incident wavelength,  $\lambda/n$  where  $n = 2, 3, 4, \dots$ . For this investigation, an incident neutron wavelength of 3.02 Å was selected.

The  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal, which was the same crystal as used by Cable *et al* [8], had an ‘off-axis’ cylindrical shape. The ends of the crystal were perpendicular to the  $(1\bar{1}0)$  direction, which was at an angle of  $30^\circ$  to the cylindrical axis that lay along the  $(2\bar{1}1)$  direction. The crystal was placed in the spectrometer with the  $(1\bar{1}0)$  direction perpendicular to the scattering plane so that the scattering in the reciprocal space of the crystal, perpendicular to the  $(1\bar{1}0)$  direction, could be scanned.

The separation of the nuclear and magnetic contributions to the scattering was achieved by applying a saturating magnetic field of 4 T along the  $(1\bar{1}0)$  direction using a superconducting solenoid and taking measurements with the incident neutron polarization directed up and down relative to the scattering plane. It was assumed that the application of the field resulted in the domains aligning along the  $(2\bar{1}1)$  direction. Though the  $(2\bar{1}1)$  direction is close to the  $(1\bar{1}1)$  hard direction of the crystal, the large applied field of 4 T ensured that the magnetization of the crystal was aligned along the axis of the crystal. This resulted in the angle between the magnetization direction and the scattering vector being generally different for each scattering vector. Thus geometrical corrections were required to convert the measured function,  $\gamma_{\perp}(\kappa)$ , into the required magneto-compositional function,  $\gamma(\kappa)$ . It was also assumed that the spin directions of the neutrons, initially perpendicular to the scattering plane, were adiabatically altered by the resultant field produced by the crystal to being directed along the  $(2\bar{1}1)$  axis of the crystal. This meant that the direction of the polarization vector was dependent upon the crystal position.

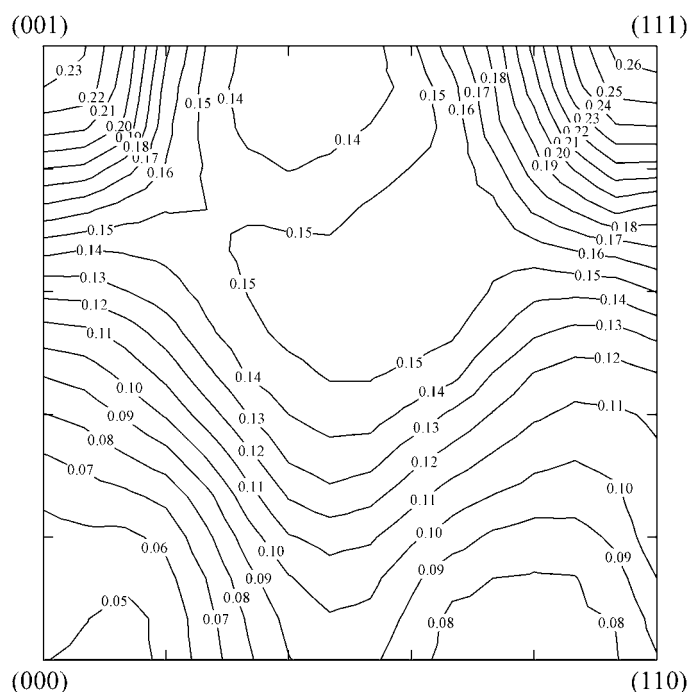
The effective neutron beam polarization was calculated by measuring the Bragg scattering intensity with incident neutron beam polarization directed parallel and anti-parallel to the crystal’s magnetization. The value obtained for the polarization was approximately equal to 36.3%, and was consistent at both the  $(110)$  and  $(\bar{1}\bar{1}0)$  reciprocal lattice positions.

The measurements were taken at room temperature with the 64 detectors arranged so as to allow scattering vectors of magnitudes up to about  $4 \text{ \AA}^{-1}$  to be scanned. With the detector angles fixed, the sample was rotated so that the scattering was measured in the  $(1\bar{1}0)$  reciprocal lattice plane of the  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal. The mechanical disc chopper was removed, resulting in no energy analysis being done. Background subtraction and absolute cross-sections were achieved by repeating the measurements using cadmium and vanadium samples with the same dimensions as the  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal. The intensity of the scattering from the cadmium and vanadium samples was measured using the same detector arrangement and rotating the samples through the same angles as were used for the  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal. Further data corrections were made to account for the attenuation of the neutron beam and multiple scattering.

The analysis of the scattering data relied on the assumption that the crystal did not contain any vacancies. This approximation can be justified by using experimental data for the vacancy formation energy in  $\alpha$ -Fe [17] to give an estimate of the vacancy concentration in the  $\text{Fe}_{0.865}\text{V}_{0.135}$  crystal. It is found that the vanadium concentration is greater than the vacancy concentration by about a factor of  $10^7$  in this system.

## 5. The atomic distribution in ferromagnetic $\text{Fe}_{0.865}\text{V}_{0.135}$

The nuclear contribution to the diffuse neutron scattering was isolated by measuring the scattering with incident polarization directed up and down relative to the scattering plane, together with equation (8). The result for the diffuse nuclear scattering in the  $(1\bar{1}0)$  plane, given by the first term of equation (8), is shown in figure 1. Here the scattering has been folded about the  $[001]$  and  $[110]$  symmetry axes, about which the scattering was observed to be symmetric. There is seen to be substantial structure, with large sharp peaks at the  $(001)$  and  $(111)$  positions which indicate the presence of anti-correlation for first-neighbour atomic



**Figure 1.** The diffuse nuclear neutron scattering from ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  in the  $(\bar{1}10)$  plane in units of  $\text{b sr}^{-1} \text{atom}^{-1}$  obtained from the observed polarized neutron scattering.

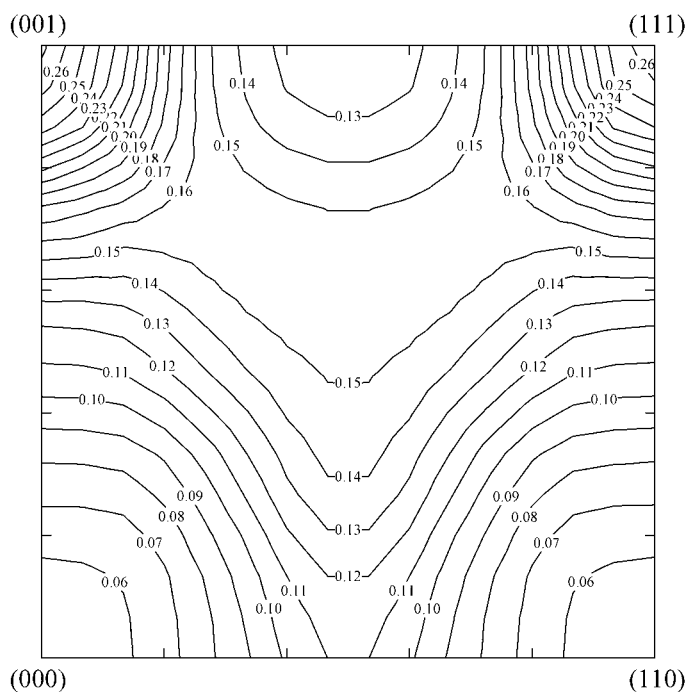
**Table 1.** Experimentally determined Cowley atomic short-range order parameters of ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  obtained from the present study.

Neighbour shell ( $R$ )	$\langle lmn \rangle$	$\alpha(R)$
1	$\langle 111 \rangle$	$-0.089 \pm 0.004$
2	$\langle 200 \rangle$	$-0.031 \pm 0.004$
3	$\langle 220 \rangle$	$0.032 \pm 0.004$
4	$\langle 311 \rangle$	$-0.003 \pm 0.002$
5	$\langle 222 \rangle$	$-0.006 \pm 0.004$
6	$\langle 400 \rangle$	$-0.004 \pm 0.004$
7	$\langle 331 \rangle$	$-0.007 \pm 0.002$
8	$\langle 420 \rangle$	$0.017 \pm 0.004$
9	$\langle 422 \rangle$	$0.002 \pm 0.002$

pairs, with the ordering being  $\beta$ -CuZn in nature [8]. The data shown in figure 1 were least-squares fitted to equation (9) and the first term of equation (8) to obtain the Cowley real space atomic short-range order parameters. The result for the ten-parameter nine-shell fit, required to reproduce the sharpness in the diffuse peaks at the (001) and (111) positions, is shown in figure 2. The parameters obtained from the fit are reproduced in table 1.

In a random alloy, where there are no atomic correlations over all distances  $R$ ,  $\alpha(R)$  will be equal to 0 for all  $R$ . For the ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  system, it is seen that there are significant atomic correlations between the atoms that extend out to the eighth shell. The currently obtained Cowley real space atomic short-range order parameters are in good





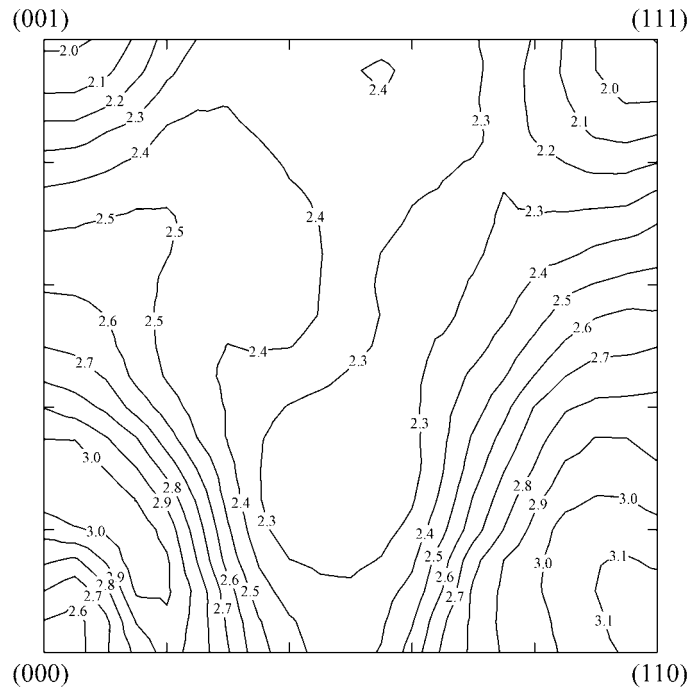
**Figure 2.** The least-squares fitted result for the diffuse nuclear neutron scattering from ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  in the  $(1\bar{1}0)$  plane in units of  $\text{b sr}^{-1} \text{atom}^{-1}$ . The Cowley atomic short-range order parameters obtained are shown in table 1.

agreement with the parameters obtained in the previous neutron scattering experiment from the same crystal conducted by Cable *et al* [8], as well as previous polycrystalline investigations [6, 7]. The nature of these observed atomic correlations in this system has been theoretically reproduced [3, 5]. In particular, figure 2(b) in the paper of Staunton *et al* [3] shows that the theoretical result for  $\alpha(\kappa)$  in the  $(1\bar{1}0)$  plane has the same structure as that determined from the experimental results, figure 1.

## 6. The magneto-compositional response function of $\text{Fe}_{0.865}\text{V}_{0.135}$

The magnitude of the magneto-compositional function,  $\gamma(\kappa)$ , shown in figure 3 in the  $(1\bar{1}0)$  plane, was obtained as follows. Firstly the difference between the measured diffuse scattering cross-sections with polarization parallel and anti-parallel to the crystal's magnetization direction was taken. This gave twice the third term of equation (8).  $\gamma(\kappa)$  was then isolated by dividing this difference by the fitted result for  $\alpha(\kappa)$  and the term  $4\gamma_0 c(1-c)(b_{\text{Fe}} - b_{\text{V}}) f(\kappa) |\mathbf{P}|$ . Figure 3 was obtained by folding the results for  $\gamma(\kappa)$  about the [001] and [110] symmetry axes, about which  $\gamma(\kappa)$  was observed to be symmetric.

Shown in figure 4 are cuts of  $\gamma(\kappa)$  along the three principal symmetry directions together with the results for  $\gamma(\kappa)$  obtained from the first-principles theoretical investigation [4]. It is seen that there is good agreement between the results obtained from theory and experiment except possibly near zero scattering vector where the experimental results seem to extrapolate below both the theoretical and bulk magnetization measurement [12] for  $\gamma(\kappa = 0)$ . Note that



**Figure 3.**  $\gamma(\kappa)$  of ferromagnetic Fe<sub>0.865</sub>V<sub>0.135</sub> in the (110) plane in units of  $\mu_B/\text{atom}$  obtained from the polarized neutron scattering.

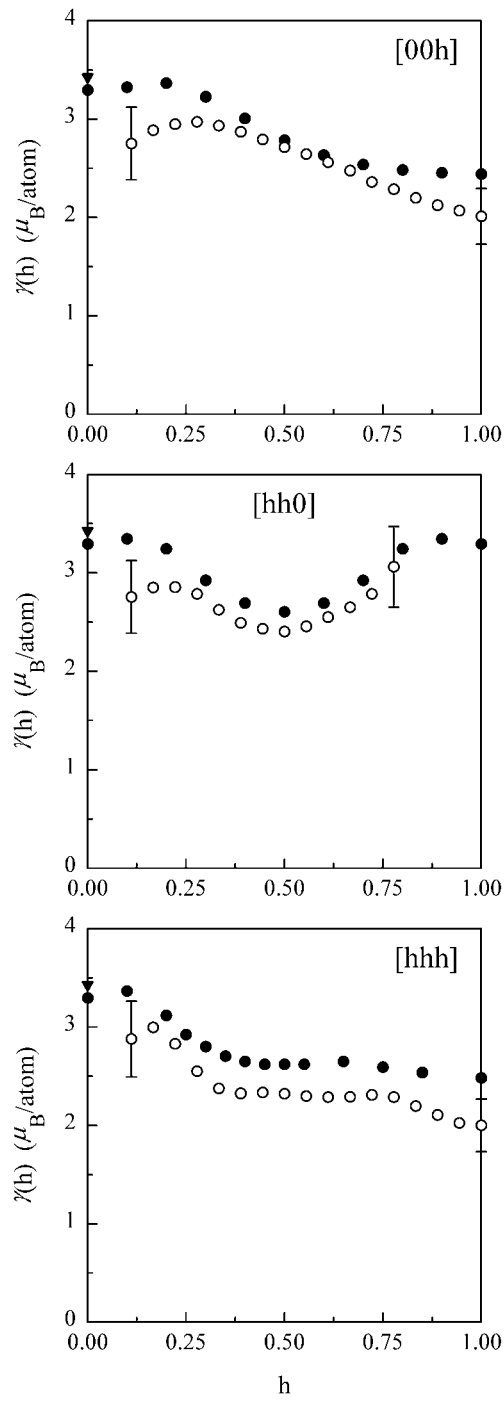
**Table 2.** Experimentally determined magnetic defect parameters of ferromagnetic Fe<sub>0.865</sub>V<sub>0.135</sub> obtained from the present study.

Neighbour shell ( <i>R</i> )	<i>(lmn)</i>	$\phi(R)$ ( $\mu_B/\text{atom}$ )
1	(111)	$0.067 \pm 0.007$
2	(200)	$0.047 \pm 0.007$
3	(220)	$-0.018 \pm 0.006$
4	(311)	$-0.003 \pm 0.005$
5	(222)	$-0.025 \pm 0.007$
6	(400)	$-0.010 \pm 0.007$
$\Delta\mu$ ( $\mu_B/\text{atom}$ )		$2.477 \pm 0.013$
$\mu$ ( $\mu_B/\text{atom}$ ) <sup>a</sup>		$1.782 \pm 0.027$
$\mu_{\text{Fe}}$ ( $\mu_B/\text{atom}$ )		$2.117 \pm 0.031$
$\mu_{\text{V}}$ ( $\mu_B/\text{atom}$ )		$-0.361 \pm 0.049$

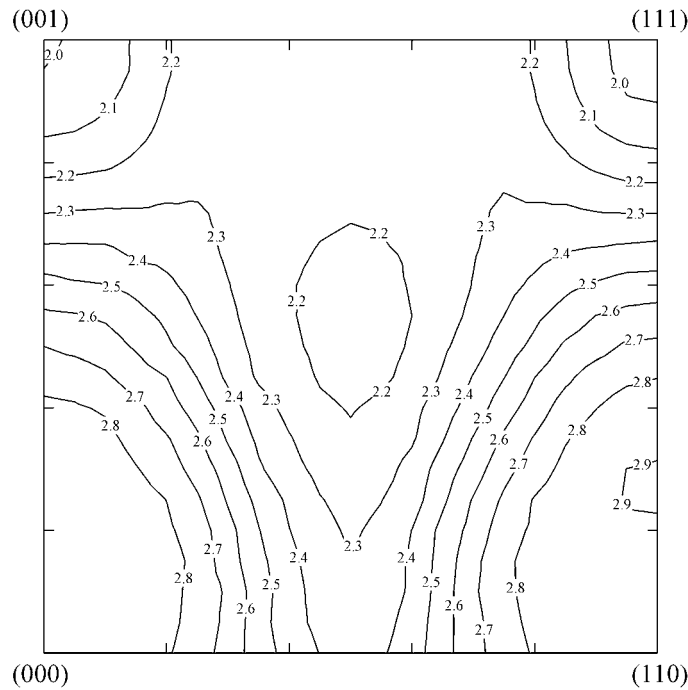
<sup>a</sup> From [12].

the results along the [hh0] direction are not continued to the (110) reciprocal lattice position due to the presence of a Bragg peak.

The results for  $\gamma(\kappa)$  shown in figure 3 were least-squares fitted to equation (10) out to the sixth shell. The result of the fit is shown in figure 5 and the resultant parameters are shown in table 2. The average moments on the iron and vanadium atoms were determined from the fitted result for the difference between the average moments of the constituent atoms,  $\Delta\mu$ , together with the value for the average moment,  $\mu$ , determined from the bulk magnetization measurements of Aldred [12].



**Figure 4.**  $\gamma(\kappa)$  of ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  along the three principal symmetry directions obtained from (○) the polarized neutron scattering data and (●) a first-principles theoretical calculation [4]. ▼ shows a bulk magnetization result [12]. Error bars show the uncertainty of the neutron scattering results, due mainly to the estimation of the effective polarization.



**Figure 5.** The least-squares fitted result for  $\gamma(\kappa)$  of ferromagnetic  $\text{Fe}_{0.865}\text{V}_{0.135}$  in the  $(1\bar{1}0)$  plane in units of  $\mu_{\text{B}}/\text{atom}$ . The magnetic defect parameters obtained are shown in table 2.

The theoretically determined parameters  $\gamma_{\text{Fe}}^1 = 0.096 \mu_{\text{B}}/\text{atom}$ ,  $\gamma_{\text{Fe}}^2 = 0.047 \mu_{\text{B}}/\text{atom}$ ,  $\gamma_{\text{V}}^1 = -0.165 \mu_{\text{B}}/\text{atom}$  and  $\gamma_{\text{V}}^2 = -0.057 \mu_{\text{B}}/\text{atom}$  yield, from equation (11), the parameters for the first two shells  $\phi(R = 1) = 0.062 \mu_{\text{B}}/\text{atom}$  and  $\phi(R = 2) = 0.033 \mu_{\text{B}}/\text{atom}$ . From table 2, these parameters are seen to be in good agreement with those determined from the neutron scattering experiment. Unlike the case for the theoretical result however, significant contributions from higher order shells are required to obtain a reasonable fit to the experimental data.

## 7. Discussion

It is clear from the results shown in figure 4 that the theory of Ling *et al* [4] describes very well the correlation between the distribution of atoms and moments in ferromagnetic  $\alpha$ -FeV alloys. Any discrepancy between the theoretical and experimental data is visible predominantly close to the (000) reciprocal lattice position. It is likely that it is the experimental data that are in error because the magneto-compositional response function should extrapolate to the rate of change of spontaneous moment with composition at zero wavevector. This is because at small wavevectors, the change of the average atomic moment due to changes of the local concentration is determined by the fluctuations in these quantities over macroscopic scales. Unfortunately, because a large applied magnetic field was necessary to overcome the demagnetization field caused by the large moment of the material, the experimental conditions could be quite different to those in the original modest field measurements of the change of moment with composition [12]. Because of this we measured the moment for a range of compositions around  $\text{Fe}_{0.865}\text{V}_{0.135}$  as a function of applied field up to 7 T [18]. There was

observed to be no significant difference between the changes in moment with concentration for high and low fields. Thus the presence of the high field should have a negligible effect on the magneto-compositional response of the system.

An experimental uncertainty was caused by the shape of the crystal used, where the cylindrical axis was not parallel to the normal of the scattering plane. The attempt to correct for this involved assuming that both the internal field and the polarization direction were directed along the axis of the crystal rather than perpendicular to the scattering plane and along the external field. It is clear that this arrangement was far from the ideal configuration of an ellipsoid with its major axis along the applied field. The consequences of this are a non-uniform field in the sample and possibly sharp changes of field direction near the sample's surface. The latter may partially account for the relatively low polarization of 36.3%, although the requirements on the degree of saturation of ferromagnets for low depolarization are quite severe even with an ideal geometry. The non-uniformity of the internal field is probably not that much of a problem given that the moment is a very weak function of the field.

The lack of energy analysis of the scattered neutrons will result in inelastic contributions to the observed scattering. This contribution to the scattering should however be relatively small due to the relatively high vanadium concentration of the alloy used, which results in a large amount of elastic diffuse scattering in comparison to the inelastic contributions [9]. This is verified by noting that the nuclear scattering obtained is similar to that observed from a triple-axis neutron scattering investigation from the same crystal [8].

As the agreement between theory and experiment for this system is very good, it would be beneficial to apply the theory to other ferromagnetic alloy systems. Unfortunately the theory is very computationally intense and it would be a major exercise to investigate another system. One possibility that could be of interest would be to calculate the magnetic distribution in an alloy that is still ferromagnetic, but close to the critical concentration for ferromagnetism. Because the theory uses the RPA it might fail in the same way as other mean field theories fail close to a critical point, the differences between theory and experiment possibly varying for different ferromagnetic systems. For instance nickel has less than one spin polarized electron per atom and phenomenological models such as that of Hicks [19] work quite well in describing the diffuse scattering right down to the critical concentration. There the assumption is that it is the *magnitude* of the moment on the magnetic species that is a function of the atomic environment. In iron alloys, where the average number of spin polarized electrons is in excess of two, the situation might be quite different. In this case there could well be a three-dimensional vector character to the moment, so the approach to the critical concentration might also involve transverse fluctuations.

## 8. Conclusions

The polarized neutron scattering observed from an  $\text{Fe}_{0.865}\text{V}_{0.135}$  single crystal has been used to characterize both the atomic and magnetic distributions that exist in this system in the ferromagnetic state. These results are consistent with previous experimental results obtained for ferromagnetic  $\alpha$ -FeV alloys and are also in good agreement with those obtained from a mean field first-principles theory. This theory can be used to calculate the atomic correlations in the high temperature atomically disordered state and also, for ferromagnetic materials, predict the dependence of the atomic magnetic moments on the local chemical environment. The experimental results presented here imply that this theory gives an accurate description of both the atomic short-range order and the dependence of the magnetic properties upon the local chemical environment for this ferromagnetic system.

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## References

- [1] Staunton J B, Johnson D D, Gyorffy B L and Walden C 1990 *Phil. Mag.* **B 61** 773
- [2] Ling M F, Staunton J B and Johnson D D 1994 *J. Phys.: Condens. Matter* **6** 5981
- [3] Staunton J B, Ling M F and Johnson D D 1997 *J. Phys.: Condens. Matter* **9** 1281
- [4] Ling M F, Staunton J B and Johnson D D 1995 *J. Phys.: Condens. Matter* **7** 1863
- [5] Staunton J B, Johnson D D and Pinski F J 1990 *Phys. Rev. Lett.* **65** 1259
- [6] Nomura M, Fujiwara H and Fujiwara Y 1975 *J. Phys. Soc. Japan* **38** 55
- [7] Mirebeau I, Cadeville M C, Parette G and Campbell I A 1982 *J. Phys. F: Met. Phys.* **12** 25
- [8] Cable J W, Child H R and Nakai Y 1989 *Physica B* **156–157** 50
- [9] Kajzar F and Parette G 1980 *Phys. Rev. B* **22** 5471
- [10] Mirebeau I and Parette G 1982 *J. Appl. Phys.* **53** 1960
- [11] Mirebeau I, Parette G and Cable J W 1986 *J. Phys. F: Met. Phys.* **17** 191
- [12] Aldred A T 1972 *Int. J. Magn.* **2** 223
- [13] Krivoglaz M A 1969 *Theory of X-Ray and Thermal Neutron Scattering by Real Crystals* (New York: Plenum)
- [14] Clapp P C and Moss S C 1966 *Phys. Rev.* **142** 418
- [15] Clapp P C and Moss S C 1968 *Phys. Rev.* **171** 754
- [16] Hicks T J 1995 *Magnetism in Disorder* (Oxford: Oxford University Press)
- [17] Korzhavyi P A, Abrikosov I A, Johansson B, Ruban A V and Skriver H L 1999 *Phys. Rev. B* **59** 11693
- [18] Robinson D J, Ling M F and Hicks T J 2001 *J. Magn. Magn. Mater.* **226–230** 1346
- [19] Hicks T J 1977 *J. Phys. F: Met. Phys.* **7** 481