A 'first-principles' theory for magnetic correlations and atomic short-range order in paramagnetic alloys. II. Application to CuMn

1994 J. Phys.: Condens. Matter 6 6001

(http://iopscience.iop.org/0953-8984/6/30/017)

J. Phys.: Condens. Matter 6 (1994) 6001–6010. Printed in the UK

A 'first-principles' theory for magnetic correlations and atomic short-range order in paramagnetic alloys: II. Application to CuMn

M F Ling†, J B Staunton† and D D Johnson‡

† Department of Physics, University of Warwick, Coventry, UK

‡ Computational Materials Science Department, Sandia National Laboratories, Livermore, CA, USA

Received 25 March 1994, in final form 20 May 1994

Abstract. We illustrate our 'first-principles' theory for magnetic correlations and atomic short-range order in paramagnetic alloys with an application to a $Mn_{15}Cu_{85}$ alloy, well known for its spin-glass behaviour at low temperatures. Our results indicate some unusual antiferromagnetic correlations, as also found experimentally. We provide a consistent interpretation of the extensive magnetic and atomic neutron-scattering data.

1. Introduction

In the preceding paper I [1] we have described the details of our 'first-principles' theory for both the magnetic and compositional correlations which grow in a compositionally disordered alloy in its paramagnetic phase as it is cooled. We have provided expressions for the compositional correlation function $\alpha(q)$ and the paramagnetic susceptibility $\chi(q)$ and have shown how they are dependent upon the electronic structure of this phase. Paramagnetic spin fluctuations are modelled in terms of 'local moments' and can have a profound effect upon the electronic structure and hence can affect the atomic short-range order (ASRO) which develops. In this paper we illustrate our theory by applying it to a specific alloy. The calculations of $\alpha(q)$ and $\chi(q)$ can be compared directly with results from non-spin-flip (or nuclear) and spin-flip (or magnetic) neutron-scattering experiments, respectively. It should be noted that our theory for the paramagnetic susceptibility neglects any correlations between the atomic occupations of the sites and this will be an important consideration for the comparison with experiments on certain annealed crystalline samples. Consequently, before detailing both the calculations and the comparison with experiment, we comment on some relevant issues in the next section. The following section describes the application to the $Mn_{15}Cu_{85}$ alloy upon which there are extensive neutron data. The final section summarizes the key findings.

2. Considerations for comparison of theory and experiment

Plainly, some attention has to be paid to the history and method of crystal sample preparation. The theory is based on the electronic structure in the high-temperature, paramagnetic state. Therefore, our calculations should be compared ideally with neutron-scattering experiments

0953-8984/94/306001+10$19.50

performed on crystals at high temperatures, *in situ*, above any compositional ordering temperature. This is not usually experimentally feasible and, instead, crystals are used which have been fast quenched from a high temperature. The experiments are then conducted at the lower temperature. Since the diffusion time of atoms in the alloys at room temperature is much longer than both the electronic 'hopping' time and the rate of variation of the 'local-moment' spin fluctuations, such a fast-quenched alloy crystal will maintain for a long time the compositional correlations determined by its electronic and magnetic structures appropriate to the temperature from which it is quenched. (Of course, the quenching may not be sufficiently uniform throughout the bulk crystal due to its size but this does not alter the consideration that follows.) On the other hand, the magnetic correlations will pertain to the system at the lower temperature albeit with the compositional disorder 'frozen in', essentially because of the difference in time scales of the response. An illustrative example is given by the case of the alloy $Fe_{0.865}V_{0.135}$, a single crystal of which was subjected to some unpolarized neutron-scattering experiments by Cable *et al* [7]. This alloy (which has a high Curie temperature, T_c, of 1180 K) was quenched from temperatures a couple of hundred degrees below T_c to room temperature. It followed that the atomic short-range order was supported by the spin-polarized electronic structure of the ferromagnetic alloy. Indeed a detailed interpretation of the data was given in these terms [8]. If this experiment were to be repeated with the single-crystal sample being quenched from temperatures in excess of the Curie temperature, then the atomic short-range order might change since it would be supported by the electronic structure of the paramagnetic state. Of course, the magnetic correlations in the paramagnetic phase would be only available from an experiment conducted at a temperature above the Curie temperature.

In many experiments, fast-quenched crystals are subject to lengthy annealing at some intermediate temperatures before measurements are taken. It is well established that the annealing process can greatly enhance atomic short-range order in alloys like Mn_cCu_{1-c} [9–12]. Therefore, it would not be appropriate to compare directly experimental measurements of the magnetic correlations on annealed crystals with our calculations at present even if the intermediate temperature is above any magnetic ordering temperature (as in the case of Mn_cCu_{1-c}). Evidently, if a detailed comparison of our theory for the paramagnetic susceptibility is to be made, it is essential that the bulk of the crystal is quenched uniformly. In other words, the data from polarized neutron-scattering experiments are obtained from single crystals quenched quickly from the higher temperature. In this way, strong effects of the compositional correlations that can affect the magnetic fluctuations can be neglected. Due to the size of the crystal samples, it has to be born in mind that cooling may not have occurred sufficiently uniformly throughout its bulk so that the growth of ASRO in parts of the crystal is avoided. This seems to be a fairly common problem and a detailed and informative study of the effects of the lack of uniform cooling in AuFe has been carried out by Anderson and Chen recently [13].

3. Application to a copper–manganese alloy

We have applied our theory to an $Mn_{15}Cu_{85}$ alloy owing to the large number of reports of neutron-scattering data with which we can compare our results [9–11, 12, 14–17, 19]. CuMn and other noble metals alloyed with low concentrations of magnetic transition-metal atoms, such as AgMn and AuFe, have been extensively studied over the years for their spin-glass properties. Notwithstanding the intense theoretical and experimental efforts to understand spin-glass materials, their strange magnetic behaviour is still something of a

puzzle [14, 15, 20]. A spin-glass material is usually defined as possessing frozen-in magnetic moments below some freezing temperature T_f, and hence a peak in its frequency-dependent susceptibility. It also lacks periodic long-range magnetic order at low temperatures and has remanence and magnetic relaxation on macroscopic time-scales below T_f when there are changes to the applied magnetic field [21]. Traditional spin-glass theories have been based on the model suggested by Ruderman, Kittel, Kasuya, and Yoshida (RKKY) [22] where the 'spin–spin' interactions are mediated by the conduction electrons. Recently Werner [15] suggested that new polarized neutron-scattering data lent support to an alternative theory proposed by Overhauser [23] that the unusual magnetic behaviour of **Cu**Mn was due to a mechanism of interacting, static spin-density waves (SDWs) arising from nested sheets of Fermi surface. This interpretation, though, is not uncontroversial [14].

Over the years, especially with the advent of polarized neutron-scattering techniques, a general picture of the compositional and magnetic structures of **Cu**Mn has begun to emerge. The experimental results can be summarized as follows. Unpolarized neutron-scattering experiments have found that some degree of ASRO [9–12, 14, 15] exists in most **Cu**Mn single crystals and the action of heat treatment is known to enhance ASRO in these crystals [9–12]. Heat-treated **Cu**Mn is thought to be comprised roughly of small clumps of partially ordered Cu–Mn alloy. Polarized neutron-scattering experiments on these crystals have found both ferromagnetic correlations characterized by peaks in the cross-section around $q = 0$, but the main feature which is observed indicates strong antiferromagnetic correlations signified by peaks around $q = (1, \frac{1}{2}, 0)$. In addition, Cable *et al* [11] have also found incommensurate peaks around the $(1, \frac{1}{2}, 0)$ position at low temperatures. It is claimed that the ferromagnetic correlations are inherent to the atomically short-range ordered clumps which are assumed to behave like tiny ferromagnets. On the other hand, the main antiferromagnetic peaks at $(1, \frac{1}{2}, 0)$ are usually interpreted to be a reflection of the ASRO and the ferromagnetic clumps [11, 14, 15] though the justification for this interpretation is not clear. The spin–spin correlations characterized by incommensurate peaks around $(1, \frac{1}{2}, 0)$ are usually construed to have come from the nesting of sheets of Fermi surface [11, 15, 24]. The incommensurate peaks, however, are observed only below the spin-freezing temperature, in a region where our theory for the high-temperature, paramagnetic state is no longer applicable. The neutron data from powdered crystals quenched rapidly from high temperatures show the dominant $(1, \frac{1}{2}, 0)$ antiferromagnetic peaks only.

Using the complete 'first-principles' theory described in I, we now present our theoretical results for $Mn_{0.15}Cu_{0.85}$ and try to interpret some of the experimental measurements. We note that the paramagnetic state for this alloy consists of local moments associated with the Mn sites only, and according to the theory the magnetic susceptibility is approximately of the form (equation (14) of I)

$$\chi(q) \simeq \frac{c^2\bar{\mu}^2(\beta/3)}{[1-(\beta/3)c(J^{mm}_{\mathrm{Mn,Mn}}(q)-\Lambda^{m}_{\mathrm{Mn}})]} \tag{1}$$

and the atomic pair-correlation function

$$\alpha(q) = \frac{\beta c(1-c)}{(1-\beta c(1-c)S^{(2)}(q)} \tag{2}$$

where $c = 0.15$. The magnetic susceptibility $\chi(q)$ (and the effective moment–moment interactions, $J^{mm}_{\mathrm{Mn,Mn}}$) and the compositional correlation function $\alpha(q)$ (and the atomic interchange energy, $S^{(2)}(q)$) have been calculated. Our calculated $\chi(q)$ (and $J^{mm}_{\mathrm{Mn,Mn}}(q)$) do

indeed possess the unusual antiferromagnetic correlations characterized by $(1, \frac{1}{2}, 0)$ peaks in q-space at high temperatures. The absolute instability to the antiferromagnetic state is found to be 200 K. In figure 1 $\chi(q)$ is shown for this alloy at a temperature of 295 K. This is in fine accord with both compatible neutron experiments performed at that temperature on fast-quenched powdered crystals [9] and shows the main feature found in experiments on well annealed single crystals at temperatures above 180 K [14, 15]. In fact, it seems that this $(1, \frac{1}{2}, 0)$ peak in the magnetic response is characteristic of Cu–Mn alloys for a range of concentrations, as well as other similar noble-metal, spin-glass alloys at temperatures 100 K or so above T_f [24].

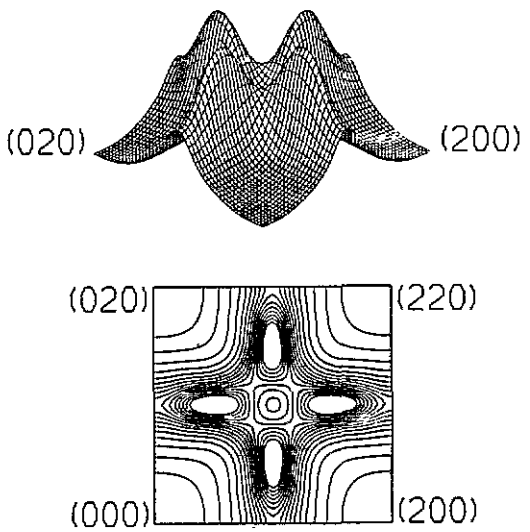

Figure 1. The paramagnetic susceptibility $\chi(q)$ of $Cu_{85}Mn_{15}$ at 295 K for the $q_z = 0$ plane in atomic units. In the 3D plot, the corner facing the reader is the $q = (0, 0, 0)$ position.

Interestingly, we find that these calculated magnetic interactions can be fitted very well by a lattice Fourier transform of a damped, RKKY-like interaction, $J^{mm}_{ij;\mathrm{Mn,Mn}} = J_0 \cos(2k_F|\boldsymbol{R}_i - \boldsymbol{R}_j|)\exp(-\lambda|\boldsymbol{R}_i - \boldsymbol{R}_j|)/(k_F|\boldsymbol{R}_i - \boldsymbol{R}_j|)^3$ in which $J_0 = 0.149$ Ryd, $\lambda = 0.22a_0^{-1}$ and $k_F = 0.42a_0^{-1}$ (a_0 is the Bohr radius). Comparing with a similar RKKY-like interaction (without damping) for a pair of Mn impurities embedded in pure Cu, the magnetic interactions in this concentrated alloy are also oscillatory but, on the average, somewhat shorter ranged. For j belonging to sites in the first nine nearest-neighbour shells of site i, $J^{mm}_{ij;\mathrm{Mn,Mn}}/c = -29.05$, 9.71, 3.25, −0.61, −1.19, −0.67, −0.12, 0.17 and 0.23 mRyd. Evidently neighbouring Mn atoms in this alloy interact antiferromagnetically whilst next-nearest neighbours interact ferromagnetically.

It is worth seeking an explanation as to why the interactions $J^{\mathrm{Mn,Mn}}(q)$ in this concentrated alloy have $(1, \frac{1}{2}, 0)$ maxima and in real space resemble RKKY-like model interactions. In an alloy where every Mn atom has, on average, more than one Mn nearest neighbour, it is pertinent to ask why 'direct' Mn–Mn interactions seem relatively unimportant compared to indirect interactions apparently mediated by the alloy's s free-electron-like states and usually relevant to very dilute alloys. The answer lies in a combination of competing, electronic effects which we have described in another short

publication [25]. The central idea is that the competing effects arise from the different degrees of hybridization of the t_{2g} and e_g components of Mn d-states with the Cu host which plays an important, mediating role. In figure 2(a) we show the compositionally averaged density of states of $Mn_{15}Cu_{85}$, and figure 2(b) shows the t_{2g} (solid) and e_g (dotted) components of density of states of the Mn(⇑) and Mn(⇓) d-electron density of states. Note the 'local exchange splitting' which is shown for the density of states associated with the Mn sites. As detailed in [25], the Cu host essentially 'fixes' the Fermi energy relative to the Mn d-states in such a way that the direct Mn–Mn magnetic interactions are at the cross-over between being ferromagnetic and antiferromagnetic. (A 'rule of thumb' is that roughly half-filled states imply antiferromagnetic interactions whereas near filling means ferromagnetic ones [30]). This enhances the relative importance of the intermediary role played by the Cu host and consequently the Mn-Mn interactions are roughly RKKY like even in such a concentrated alloy as $Mn_{15}Cu_{85}$. Furthermore the different degrees of hybridization of the t_{2g} and e_g Mn states with Cu mean that the former contribute a marginal antiferromagnetic effect (closer to being half filled) whereas the latter provide a ferromagnetic component to the Mn–Mn magnetic interactions. The competition between these two aspects further reduces the direct Mn–Mn interactions. We found that these features are robust in that changing the Cu concentration, either less or more, will produce the same general behaviour. Indeed the neutron-scattering data of Cable *et al* [11] show the same general features for both 15% and 25% Mn alloys, namely dominant structure around $(1, \frac{1}{2}, 0)$ points in wave-vector space for the magnetic correlations.

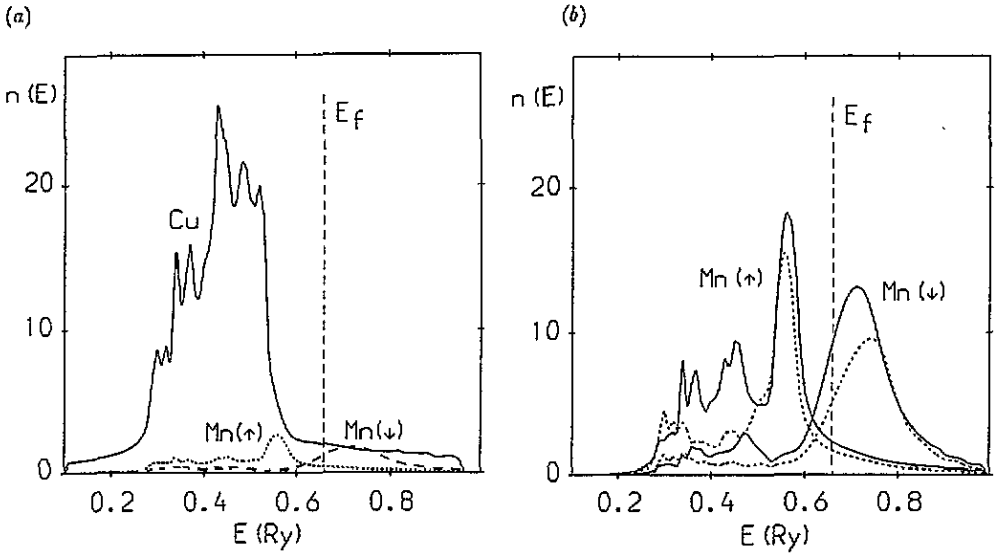

Figure 2. (a) The compositionally averaged density of states of $Cu_{85}Mn_{15}$ and its resolution into components associated with Cu (solid) and Mn sites weighted by concentration, in units of states/atom/Rydberg/spin. The Mn contribution is resolved into that for electrons with spins polarized parallel (⇑) (dotted) and anti-parallel(⇓) (dashed) to the orientation of the local moment on the Mn site. (b) t_{2g} (solid) and e_g (dotted) components of density of states of the Mn(⇑) and Mn(⇓) d-electron density of states with the weighting with respect to concentration removed.

Next, we turn to our calculation of compositional correlations. Our theory predicts a spinodal temperature of 1000 K. $\alpha(q)$ for the $q_z = 0$ plane at $T = 1250$ K is shown in figure 3. The inference that the alloy tends, on average, to cluster compositionally is

consistent with both phase diagrams and thermochemical data [26]. Besides the dominant clustering correlations shown by the $q = 0$ peak, weaker $(1, \frac{1}{2}, 0)$-ordering correlations are also visible, as found experimentally. It is these finite-q peaks which Cable *et al* and some other workers [11, 14, 15] have interpreted as giving rise to the magnetic peaks also at that same wave-vector although we have suggested a different origin for these magnetic peaks from our calculations.

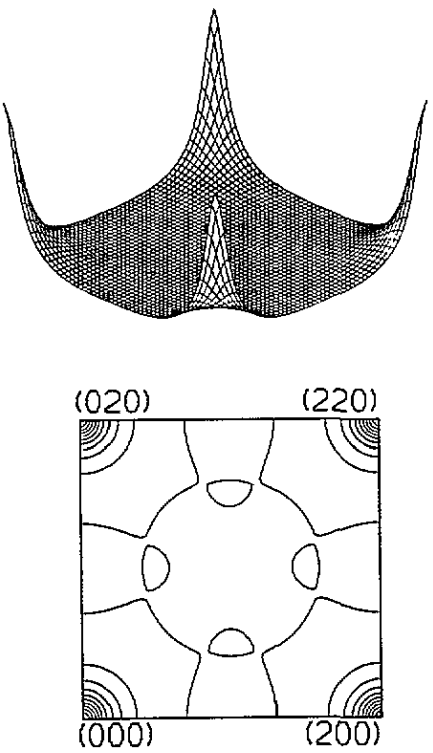

Figure 3. The compositional response $\alpha(q)$ of $Cu_{85}Mn_{15}$ at 1250 K for the $q_z = 0$ plane in atomic units. In the 3D plot, the corner facing the reader is the $q = (0, 0, 0)$ position.

The origin of the compositional clustering can also be understood from the underlying electronic structure of the alloy. A look at the density of states (see figure 2(a)) reveals that the d-states are mostly occupied, and following well known, band-filling arguments [2–6], we can see that the alloy should phase segregate. Most diffuse unpolarized neutron-scattering data [11, 15] have been interpreted with attention being paid to the intensity in the $(1, \frac{1}{2}, 0)$ region, although a more complete comparison of our results with experiment necessitates small angle neutron and X-ray scattering measurements. Since our calculation indicates strong compositional clustering correlations, consistent with thermochemical data, it would be very interesting from a material science point of view to investigate the cause of the growth of atomic short-range order in these alloys under heat treatment [11]. This is, of course, outside the scope of the current theory.

We have also calculated the compositional correlations for a non-magnetic (i.e. no 'local moments' in the paramagnetic state) $Mn_{15}Cu_{85}$ in order to check the importance of the local

exchange splitting of the electronic structure for the compositional correlations in this alloy. Figure 4 shows the compositionally averaged density of states of this alloy. As expected a single virtual-bound-state-like peak containing Mn-related states is seen above the host copper d-states. We find that such a non-magnetic $Mn_{15}Cu_{85}$ alloy would also cluster but with a much higher transition temperature than its 'local moment' counterpart, 3100 K as compared with 1000 K. This is the first piece of evidence from explicit calculations that the introduction of a local exchange splitting of the underlying electronic structure of the paramagnetic alloy has a dramatic effect upon its compositional correlations. We expect a similar effect in many alloys where at least one of the atomic species can support a local moment in the paramagnetic state, i.e. many iron, cobalt, and manganese alloys.

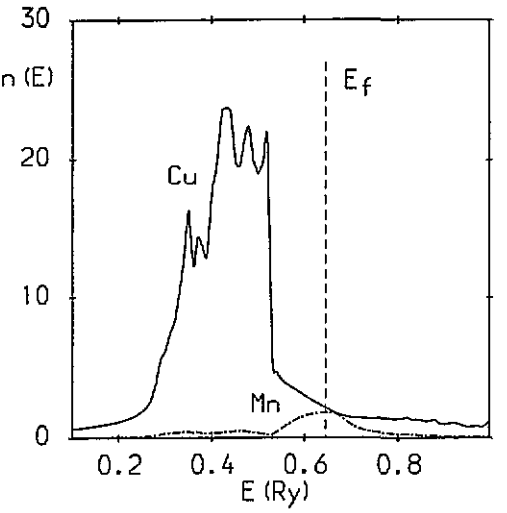

Figure 4. The compositionally averaged density of states of a *non-magnetic* $Cu_{85}Mn_{15}$ and its resolution into components associated with Cu (solid) and Mn (dashed) sites weighted by concentration, in units of states/atom/Rydberg/spin.

As mentioned above, the polarized neutron-scattering experiments have shown that in general two types of magnetic correlation exist in **Cu**Mn alloys. One is ferromagnetic characterized by peaks around $q = (0, 0, 0)$, and the other stronger one is antiferromagnetic with peaks around $q = (1, \frac{1}{2}, 0)$. This latter feature is contained in our theory and shown to be a property of the alloy when the compositional configurations are averaged over. We now use our calculations to sort out some apparently conflicting experimental evidence. Some experimental data have been interpreted to show that magnetic interactions between a pair of Mn impurities in **Cu**Mn are antiferromagnetic if the two impurities are nearest neighbours (NNs) but ferromagnetic if they are next-nearest neighbours (NNNs) separated by a Cu nearest neighbour [9, 10, 14, 16, 17]. Analysis of some other measurements have suggested the contrary picture [14, 18, 19]. Recent experimental results by Clad *et al* [27] appear to have reaffirmed the former. Both impurity calculations [28] and our alloy calculations of $J^{mm}_{ij,\mathrm{Mn,Mn}}$ are also consistent with the former picture.

Our calculations of $\chi(q)$ for the compositionally disordered alloy have shown the origin of the main $(1, \frac{1}{2}, 0)$ peak in the polarized neutron-scattering data. In addition, from our calculated interactions $J^{mm}_{ij,\mathrm{Mn,Mn}}$ given above, we can also deduce that the atomically short-range-ordered clumps in the heat treated **Cu**Mn crystals possess ferromagnetic correlations.

In these clumps each Mn atom, on average, has a Cu atom as first-nearest neighbour and a greater than average chance of an Mn atom as next-nearest neighbour. These Mn NNNs interact ferromagnetically, and hence the polarized neutron-scattering cross-section has some additional weight around $q = (0, 0, 0)$ in these samples.

Several workers [11, 14, 15] have attributed the relatively broad magnetic peak at $q = (1, \frac{1}{2}, 0)$ to the ferromagnetic clumps of ordered Cu–Mn alloy which interact antiferromagnetically. A more drastic conclusion about these ferromagnetic clumps is that they are '...the "building blocks" out of which the spin-glass state is established and they should be considered theoretically' [19]. This conclusion is to some extent similar to Wohlfarth's idea that the superparamagnets are responsible for the glassy magnetic behaviour in some of the spin-glass materials [29]. Our calculations, however, suggest that the observed antiferromagnetic correlations, marked by the broad $(1, \frac{1}{2}, 0)$ peaks, are a property of $Mn_{15}Cu_{85}$ when the effects of all the compositional configurations are averaged over. In other words, such antiferromagnetic correlations in **Cu**Mn alloys have their origin in the underlying electronic structure of the compositionally disordered phase [25]. We find that this antiferromagnetic peak at $q = (1, \frac{1}{2}, 0)$ is robust over a wide range of temperatures in the calculations and we expect it to persist to some extent in the form of a broad peak at $(1, \frac{1}{2}, 0)$ even as clumps of compositionally ordered Cu and Mn atoms begin to develop under heat treatment and reveal their presence in the form of peaks at $(0, 0, 0)$ in the polarized neutron-scattering cross-section. Our interpretation would appear to contradict that of Werner and Mydosh [14, 15], though the possibility that the ferromagnetic clumps are also responsible for the antiferromagnetic peaks at or around $q = (1, \frac{1}{2}, 0)$ at low temperatures cannot be ruled out by our theory. Since spin-glass behaviour in **Cu**Mn has been partly attributed to the interactions between the ferromagnetic clumps by some workers, it would be helpful to resolve this discrepancy. We propose, therefore, that further neutron-scattering experiments be carried out on single crystals which have been fast-quenched from high temperatures, as uniformly as possible, and without annealing at a lower temperature so that the amount of ASRO in these samples is as small as possible. If our interpretation is correct then only the antiferromagnetic peaks around $q = (1, \frac{1}{2}, 0)$ should be observed. Moreover, if these crystals are then annealed at a few hundred degrees centigrade as before [15, 17] for different lengths of time and the experiment repeated after each anneal, then, in addition to the antiferromagnetic $(1, \frac{1}{2}, 0)$ peaks, a peak around $q = (0, 0, 0)$ would develop, its importance growing as the anneal time is increased.

4. Conclusion

We have applied our theory in the first instance to an $Mn_{15}Cu_{85}$ spin-glass alloy. Our calculation of the paramagnetic susceptibility indicates antiferromagnetic correlations characterized by peaks at $q = (1, \frac{1}{2}, 0)$ in q-space, which is in good agreement with polarized neutron-scattering experiments. We find that the effective interaction in real space between the Mn local moments can be fitted very well by a damped oscillatory RKKY-like model interaction, albeit with a somewhat shorter range than a similar RKKY-like interaction for a pair of Mn impurities embedded in pure Cu. We have associated a new combination of competing, electronic effects with the unusual antiferromagnetic interaction [25], which we claim is robust over a wide range of temperatures. Our description appears to be at variance with the earlier interpretation of polarized neutron data that the antiferromagnetic correlations showing up as peaks at $q = (1, \frac{1}{2}, 0)$ arise from the magnetic interaction between the ferromagnetic clumps thought to exist in heat-treated **Cu**Mn alloys [11, 14, 15]. Even

though the calculated magnetic correlations agree well with experiment, our theory cannot rule out such a mechanism. Given the importance attached to such interactions for our understanding of this class of spin-glass materials [14, 19, 29], we propose that new neutron-scattering experiments be performed to verify the effect of atomic short-range order, or the lack of it, on these unusual antiferromagnetic correlations.

Our compositional correlation function, $\alpha(q)$, peaks at $q = (0, 0, 0)$, indicating that the alloy tends to cluster. In addition, weaker $(1, \frac{1}{2}, 0)$-ordering correlations can also be seen. The dominant clustering result is in fine agreement with thermochemical data [26]. In unpolarized neutron-scattering measurements attention has been mainly paid to the peaks at $q = (1, \frac{1}{2}, 0)$, whilst the clustering peaks at $q = (0, 0, 0)$ can only be observed in careful small-angle neutron experiments. From a material science point of view, it would be very interesting to investigate how heat treatment can promote the growth of atomic short-range order in what should be a predominantly clustering crystal.

That the topology of our calculated magnetic and atomic correlations agrees well with experimental data, as well as the temperature scales for the onset of these correlations, lends credence to our interpretation of the 'spin-glass' and chemical behaviour found in this class of alloys. The suggestions for experimental verification will not only benefit the experimental understanding of these systems but also validate (or refute) the above interpretations in terms of the disordered-local-moment picture used in our model of the paramagnetic, chemically disordered alloy.

Acknowledgments

This work was supported in part by the SERC in the UK and by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Science through a new-initiative grant under contract No DE-AC04-94AL85000 with Sandia.

References

[1] Ling M F, Staunton J B and Johnson D D 1994 *J. Phys.: Condens. Matter* submitted
[2] Gyorffy B L, Johnson D D, Pinski F J, Nicholson D M and Stocks G M 1989 *Alloy Phase Stability, NATO-ASI Series E163* ed G M Stocks and A Gonis (Dordrecht: Kluwer) pp 421–68
Stocks G M, Nicholson D M, Shelton W A, Gyorffy B L, Pinski F J, Johnson D D, Staunton J B, Ginatempo B, Turchi P E A and Sluiter M 1993 *Statics and Dynamics of Alloy Phase Transformations, NATO-ASI Series* ed A Gonis and P E A Turchi (New York: Plenum)
[3] Ducastelle F 1989 *Alloy Phase Stability, NATO-ASI Series E163* ed G M Stocks and A Gonis (Dordrecht: Kluwer) pp 293–328
[4] Staunton J B, Johnson D D and Pinski F J 1994 *Phys. Rev.* B at press
[5] Johnson D D, Staunton J B and Pinski F J 1994 *Phys. Rev.* B at press
[6] Pettifor D G 1978 *Solid State Commun.* **28** 621–3; 1979 *Phys. Rev. Lett.* **42** 846–50
[7] Cable J W, Child H R and Nakai Y 1990 *Physica* B **156&157** 50
[8] Staunton J B, Johnson D D and Pinski F J 1990 *Phys. Rev. Lett.* **65** 1259
[9] Gray E M, Hicks T J and Smith J H 1982 *J. Phys. F: Met. Phys.* **12** L189
[10] Harders, Hicks T J and Smith J H 1983 *J. Phys. F: Met. Phys.* **13** 1263
Harders, Hicks T J, Smith J H and Wells P 1983 *J. Phys. F: Met. Phys.* **13** 1017
[11] Cable J W, Werner S A, Felcher G P and Wakabayashi N 1982 *Phys. Rev. Lett.* **49** 829; 1984 *Phys. Rev.* B **29** 1268
Tsunoda Y and Cable J W 1992 *Phys. Rev.* B **46** 930; 1985 *J. Appl. Phys.* **57** 3753
[12] Clad R, Kuentzler R and Pfeiler W 1990 *J. Phys.: Condens. Matter* **2** 6593
[13] Anderson J P and Chen H 1994 *Metall. Trans.* submitted
[14] Mydosh J A 1988 *J. Appl. Phys.* **63** 5415

[15] Werner S A 1983 *Comment. Condens. Matter Phys.* **15** 53; 1983 *Solid State Commun.* **56** 457
[16] Davis J R, Burke S K and Rainford B D 1980 *J. Magn. Magn. Mater.* **15–18** 151
[17] Ahmed N and Hicks T J 1974 *Solid State Commun.* **15** 415; 1975 *J. Phys. F: Met. Phys.* **5** 2168
[18] Davis J R and Hicks T J 1979 *J. Phys. F: Met. Phys.* **9** 753
[19] Morgownik A F J and Mydosh J A 1983 *Solid State Commun.* **47** 321; 1983 *Solid State Commun.* **47** 325
[20] Anderson P W 1988 *Phys. Today* 9
[21] Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 801
[22] Ruderman M A and Kittel C 1954 *Phys. Rev.* **96** 99
Kasuya T 1956 *Prog. Theor. Phys.* **16** 45
Yoshida K 1957 *Phys. Rev.* **106** 893
[23] Overhauser A W 1960 *J. Chem. Solids* **13** 71
[24] Koga K and Ohshima K 1993 *J. Appl. Phys.* **73** 5457
[25] Ling M F, Staunton J B and Johnson D D 1994 *Europhys. Lett.* **25** 631–6
[26] Hultgren R, Desai P D, Hawkins D T, Gleiser M, Kelley K K and Wagman D D (eds) 19– *Selected Values of Thermodynamic Properties of Binary Alloys* (Metals Park, OH: American Society for Metals)
[27] Clad R, Kuentzler R, Migschitz M and Pfeiler W 1992 *J. Magn. Magn. Mater.* **104–7** 1593
[28] Podloucky R, Zeller R and Dederichs P H 1980 *Phys. Rev.* B **22** 5777
Oswald A, Zeller R, Braspenning P J and Dederichs P H 1985 *J. Phys. F: Met. Phys.* **15** 193
[29] Wohlfarth E P 1980 *J. Phys. F: Met. Phys.* **10** L241; and references therein
[30] Heine V and Samson J 1983 *J. Phys. F: Met. Phys.* **13** 2155