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▶ **To cite this version:**

P. Wells, J. Smith. NEUTRON DIFFRACTION STUDY OF SHORT RANGE ORDER IN γ-MnNi. Journal de Physique Colloques, 1971, 32 (C1), pp.C1-70-C1-71. 10.1051/jphyscol:1971118 . jpa-00214002

HAL Id: jpa-00214002
https://hal.science/jpa-00214002

Submitted on 4 Feb 2008

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NEUTRON DIFFRACTION STUDY OF SHORT RANGE ORDER IN γ-MnNi

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Résumé. — Un monocristal de 80 % at MnNi a été obtenu par la méthode de Bridgman. C'est un antiferromagnétique cubique à faces centrées avec $T_N = 180$ °C et un moment magnétique par atome de manganèse de 1,5 ± 0,1 μ_B. Une étude par diffraction de neutrons révèle l'existence d'un pic diffus au voisinage de la position 100, dû à la fois à la diffusion nucléaire et magnétique. Les dix premiers paramètres d'ordre à courte distance ont été calculés. L'origine de la contribution magnétique est discutée en fonction de l'ordre à courte distance statique et de la diffusion par les magnons.

Abstract. — A single crystal of 80 at % MnNi has been grown by the Bridgman method. It is a face centered cubic antiferromagnet with $T_N = 180$ °C and a magnetic moment per manganese atom of 1.5 ± 0.1 μ_B. A neutron diffraction study has shown a diffuse peak about the 100 position to be due to both atomic and magnetic scattering. The first ten atomic short range order parameters have been calculated. The magnetic contribution to this diffuse peak is discussed in terms of static short range order and magnon scattering.

1. **Introduction.** — The face centered cubic γ-Mn structure may be retained at room temperature by quenching, from the γ-phase field, alloys of Mn with other transition or noble metals. Such alloys containing less than about 25 at % of Cu, Au, Co, Ni or Pd are antiferromagnetic (Meneghetti and Sidhu [1], Hicks and Browne [2], Hicks et al. [3] and Bacon and Cowlam [4]). The paramagnetic to antiferromagnetic transition is often accompanied by a martensitic shear transformation to a face centered tetragonal phase with $c/a \sim 0.96$ [1]. The MnNi and MnPd alloys, however, remain cubic on cooling through the Néel temperature T_N but transform to the tetragonal phase at some lower temperature [3]. The moment per manganese atom is reduced by the addition of Cu, Au and Ni but is increased by adding Pd [3]. Extrapolation to pure γ-Mn yields a moment of 2.4 μ_B in agreement with the neutron diffraction results of Smith and Vance [5] on hydrogen stabilized electrolytic γ-Mn. The magnetic structure was determined [1] to be of ferromagnetic 100 sheets coupled antiferromagnetically along the 001 direction, although Umebeyashi and Ishikawa [6] have suggested other possible structures. All neutron diffraction of γ-Mn alloys has shown a broad diffuse peak near the 100 position that has variously been attributed to magnetic S. R. O. [1, 7], magnon scattering [2] and atomic S. R. O. [4]. In order to study this discrepancy a single crystal of 80 at % MnNi was grown by the Bridgman method. It is antiferromagnetic with $T_N = 180$ °C and a moment per Mn atom of 1.5 ± 0.1 μ_B. At room temperature the alloy is still cubic. Neutron diffraction $\theta - 2\theta$ scans were obtained at room temperature along the directions of high crystal symmetry to locate the diffuse peak. The scattered intensity throughout the reciprocal unit cell was also measured at both low and high scattering angles to separate the atomic and magnetic contributions to the diffuse scattering.

2. **Diffraction Theory.** — For a binary alloy containing atomic fractions m_A and m_B of the two constituents, with scattering lengths b_A and b_B respectively, the differential cross-section for neutron scattering is

$$\frac{d\sigma}{d\Omega} = m_A\, m_B (b_A - b_B)^2 \sum_{i=0} \alpha_i \exp i(\mathbf{K}.\mathbf{R}_i) \quad (1)$$

where $\alpha_i = 1 - P_i/m_{A(B)}$ are the Cowley [8] S. R. O. parameters expressing the deviation from randomness of the c_i atoms in the i^{th} shell, distance R_i from a central atom, and P_i is the probability of an atom A(B) at R_i. Fourier inversion of this formula enables these individual α_i to be calculated from the measured values of the scattered intensity throughout the reciprocal unit cell.

Similarly, the diffuse magnetic scattering may be expressed as :

$$\frac{d\sigma}{d\Omega} = m_A \left(\frac{e^2\gamma}{mc^2}\right)^2 |f(\mathbf{K})|^2\, S(S+1) \times \times \sum_{i=0} m_i \exp i(\mathbf{K}.\mathbf{R}_i) \quad (2)$$

where $f(\mathbf{K})$ is the magnetic form factor, m_A the concentration of the magnetic species possessing a localized spin $\mathbf{S}$, and

$$m_i = \{ <\mathbf{S}_0.\mathbf{S}_i> - <\mathbf{S}_0>.<\mathbf{S}_i> \}/[S(S+1)] \quad (3)$$

Equation (2) reduces to the usual paramagnetic cross-section above the transition temperature where $<\mathbf{S}_i> = 0$.

3. **Results and discussion.** — The $\theta - 2\theta$ scan along [h00] (Fig. 1), shows that the diffuse peak is centered at the 100 position. The 100 peak is also more intense than the 300 and 500 peaks, but because of the form factor dependence of the magnetic scattering the 300 and 500 peaks must be due entirely to atomic S. R. O. scattering.

Fourier inversion of the scattered intensity throughout the reciprocal unit cell at high scattering angles around the 300 position yields the atomic S. R. O. parameters, α_i, for the first ten co-ordination shells as shown in table I. The large decrease in the magnitude of α_i beyond $i = 3$ indicates that ordering is significant only for a few neighbours. These broad

Article published online by EDP Sciences and available at http://dx.doi.org/10.1051/jphyscol:1971118

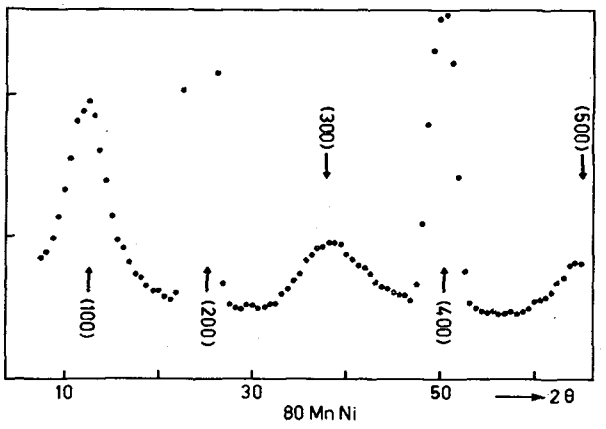

FIG. 1. — $\theta - 2\theta$ scan along [h00] in 80 at % MnNi ($T = 295$ °K).

TABLE I

Values of atomic S. R. O. *parameter* α_i (T = 295 °K)

i	α_i	i	α_i
0	1.000	6	− 0.007
1	− 0.047	7	− 0.001
2	0.062	8	0.003
3	− 0.008	9 a	0.003
4	0.001	9 b	− 0.001
5	0.006	10	0.001

Error ± 0.005

diffuse peaks are in contrast to the much sharper peaks found by Wells and Smith [9] in MnCu at the $1\frac{1}{2}0$ positions and where the ordering extends at least to the tenth shell.

The remaining magnetic contribution to the 100 peak may be from either static magnetic disorder or from magnon scattering or both. There is certainly some evidence for magnon scattering in MnNi alloys [10] although Elliot and Lowde [11] show that for a simple antiferromagnet this magnon scattering intensity will vary as $1/q_m^2$ away from the 100 position, where q_m is the magnon wave-vector. Figure 1 shows that the 100 peak does not have this pronounced cusp-like appearance and in electrolytic γ-Mn where magnon scattering should be evident, there is no diffuse peak [5]. In fact the diffuse peak always decreases with increasing manganese content. It thus appears that the major magnetic contribution arises from static disorder in the γ-Mn structure and increases with solute content. Assuming the spin on the manganese sites is localized, equation (2) may be used to calculate the m_i parameters (Table II).

TABLE II

Values of magnetic S. R. O. *parameter* m_i (T = 295 °K)

i	m_i	
0	1.00	
1	− 0.11	
2	0.21	Error ± 0.02
3	− 0.02	
4	0.10	

The temperature dependence of the 100 peak (Fig. 2) has the typical critical scattering maximum

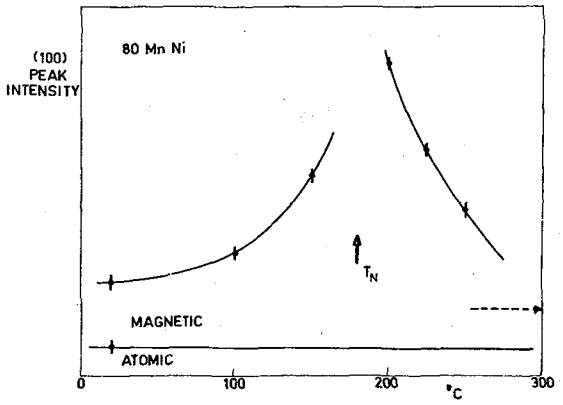

FIG. 2. — Temperature variation of 100 peak intensity. The dotted line shows the paramagnetic scattering estimated at 100 for a moment of 1. 5 μ_B.

expected at the Néel temperature. The respective contributions to this peak have been estimated.

Acknowledgements. This work was supported by a grant from the Australian Institute for Nuclear Science and Engineering. One of us (P. W.) was in receipt of a Commonwealth Postgraduate Research Scholarship.

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