# Investigation of the Magnetic Structure of FeCrAs

**W. Wu [1], A. McCollam [1], S. Julian [1], and I. Swainson [2]**

[1] Physics Department, University of Toronto, Toronto, ON, Canada M5S 1A7

[2] Canadian Neutron Beam Centre, National Research Council, Chalk River Laboratories, Chalk River, ON, Canada K0J 1J0

Ternary-metal arsenides with formula *MM'*As (*M, M'* = Cr, Mn, Fe, Co, Ni) usually show ferromagnetic or antiferromagnetic magnetic ordering below their corresponding critical temperatures. However, it was reported that FeCrAs is still paramagnetic at 4.2 K [1]. This compound has a $Fe_2P$-type crystal structure: hexagonal $P\bar{6}2m$ [2]. The space group ($P\bar{6}2m$) of this crystal and lattice parameters (a = 6.096 Å, c = 3.651 Å) of the unit cell were determined by R. Fruchart and L. Hollans et al. [2, 3]. Within this structure, there are two different types of atomic sites for metal atoms, *Mtet* and *Mpry*, with *Mtet* sites forming a corner-sharing triangular lattice. Mossbauer spectroscopy measurements showed that there is no magnetic ordering on the Fe atoms down to 4.2 K [1]. We postulated possible frustration as a cause of this lack of ordering.

Therefore neutron powder diffraction was undertaken to investigate possible frustration. We found that the two transition metals were strongly ordered over the two sites. Furthermore we found that in place of a lack of magnetic order, we found strong magnetic peaks which were indexed to a propagation vector of **k** = (1/3, 1/3, 0) corresponding to the K-point on the Brillouin Zone.

The peak at about 70° appears to be from an impurity phase. The best fit from a single basis function (BF) of the Cr atoms is $\psi_6$ of $\Gamma_6$. However, it doesn't appear to be a perfect description. Linear combinations of the BFs of $\Gamma_6$ are also allowed. The site symmetry of Fe is the same as that of Cr, so the BFs are common across the two sites. Therefore, we are investigating whether a very small contribution to the magnetic scattering from Fe may be at play, although this would contradict the Mossbauer study [1].

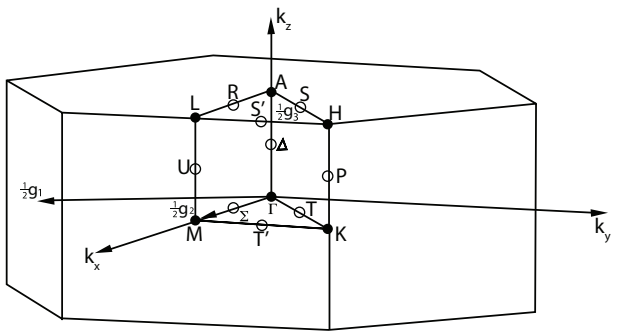


**Fig. 1** Brillouin Zone of the hexagonal primitive lattice.

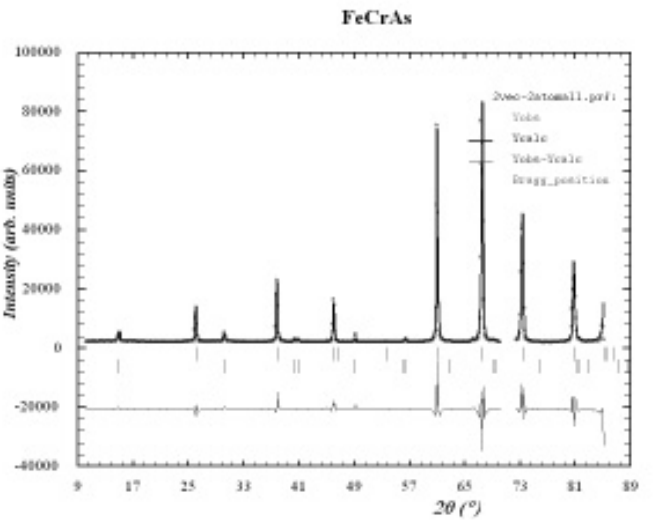


**Fig. 2** Fit to the observed neutron data, assuming only Cr moments. Lower tic marks are magnetic diffraction assuming $\Gamma_6\Psi_6$ (Table 3). Upper tic marks are the nuclear lattice, which has highly ordered Fe, Cr across the two sites.

| IR | BV | Atom | BV components | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | $m\|\|_a$ | $m\|\|_b$ | $m\|\|_c$ | $im\|\|_a$ | $im\|\|_b$ | $im\|\|_c$ |
| $\Gamma_2$ | $\psi_1$ | 1 | 4 | 0 | 0 | 0 | 0 | 0 |
| | | 2 | 0 | 4 | 0 | 0 | 0 | 0 |
| | | 3 | 2 | 2 | 0 | 3.464 | 3.464 | 0 |
| $\Gamma_3$ | $\psi_2$ | 1 | 0 | 0 | 4 | 0 | 0 | 0 |
| | | 2 | 0 | 0 | 4 | 0 | 0 | 0 |
| | | 3 | 0 | 0 | -2 | 0 | 0 | -3.464 |
| $\Gamma_4$ | $\psi_3$ | 1 | 2 | 4 | 0 | 0 | 0 | 0 |
| | | 2 | -4 | -2 | 0 | 0 | 0 | 0 |
| | | 3 | -1 | 1 | 0 | -1.732 | 1.732 | 0 |
| $\Gamma_5$ | $\psi_4$ | 1 | 0 | 0 | 4 | 0 | 0 | 0 |
| | | 2 | 0 | 0 | -2 | 0 | 0 | 0 |
| | | 3 | 0 | 0 | 1 | 0 | 0 | 1.732 |
| | $\psi_5$ | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | 2 | 0 | 0 | -3.464 | 0 | 0 | 0 |
| | | 3 | 0 | 0 | -1.732 | 0 | 0 | -3 |
| $\Gamma_6$ | $\psi_6$ | 1 | 4 | 0 | 0 | 0 | 0 | 0 |
| | | 2 | 0 | -2 | 0 | 0 | 0 | 0 |
| | | 3 | -1 | -1 | 0 | -1.732 | -1.732 | 0 |
| | $\psi_7$ | 1 | 0 | 2 | 0 | 0 | 0 | 0 |
| | | 2 | 1 | 1 | 0 | 1.732 | -1.732 | 0 |
| | | 3 | 2 | 0 | 0 | 0 | 0 | 0 |
| | $\psi_8$ | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | 2 | 0 | -3.464 | 0 | 0 | 0 | 0 |
| | | 3 | 1.732 | 1.732 | 0 | 3 | 3 | 0 |
| | $\psi_9$ | 1 | 1 | 1 | 0 | -1.732 | -1.732 | 0 |
| | | 2 | -1 | 0 | 0 | -1.732 | 0 | 0 |
| | | 3 | 0 | -1 | 0 | 0 | -1.732 | 0 |

Table 1: Basis vectors for the space group P -6 2 m with $\mathbf{k}_{13}$ = (.33333, .33333, 0). The decomposition of the magnetic representation *Fe* site (.60579, 0, .5) is $\Gamma_{Mag} = 0\Gamma^{\frac{1}{1}} + 1\Gamma^{\frac{1}{2}} + 1\Gamma^{\frac{1}{3}} + 1\Gamma^{\frac{1}{4}} + 1\Gamma^{\frac{2}{3}} + 2\Gamma^{\frac{2}{6}}$ The atoms of the nonprimitive basis are defined according to 1: (.60579, 0, .5), 2: (0, .60570, .5), 3: (.39421, .39421, .5).

***Fig. 3*** *Table of allowed basis vectors for the Cr sublattice.*

## References


[1] D.G. Rancourt, Thesis: Hyperfine Field Fluctuations in the Mossbauer Spectrum of Magnetic Materials: Application to Small Particles and to the Bulk Antiferromagnet $Fe_{(2-x)}Cr_{(x)}As$ (1984).

[2] R. Fruchart, Ann. Chim. 7, 563 (1982).

[3] L. Hollan, P. Lecocq, C. R. Acad. Sc. Paris, t. (260) (21), 6616 (1965).