Calculating muon sites in the iron pnictide FeCrAs using density functional theory

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Abstract

Using muon-spin spectroscopy (μ^+SR) we have searched for the proposed hidden spin-liquid phase in the iron pnictide FeCrAs. Zero-field μ^+SR measurements indicate a magnetic phase transition at T_N=105(5) K. We do not find any evidence for the spin-liquid phase, but instead observe glassy behaviour, with a glass freezing transition at T=20 K. Using density functional theory we propose three muon stopping sites in this compound and assess the degree of distortion induced by the implanted muon.

Introduction

FeCrAs has been described as a 'non-metallic' metal. Heat capacity measurements show Fermi liquid like specific heat but the resistivity has non-metallic character[1].

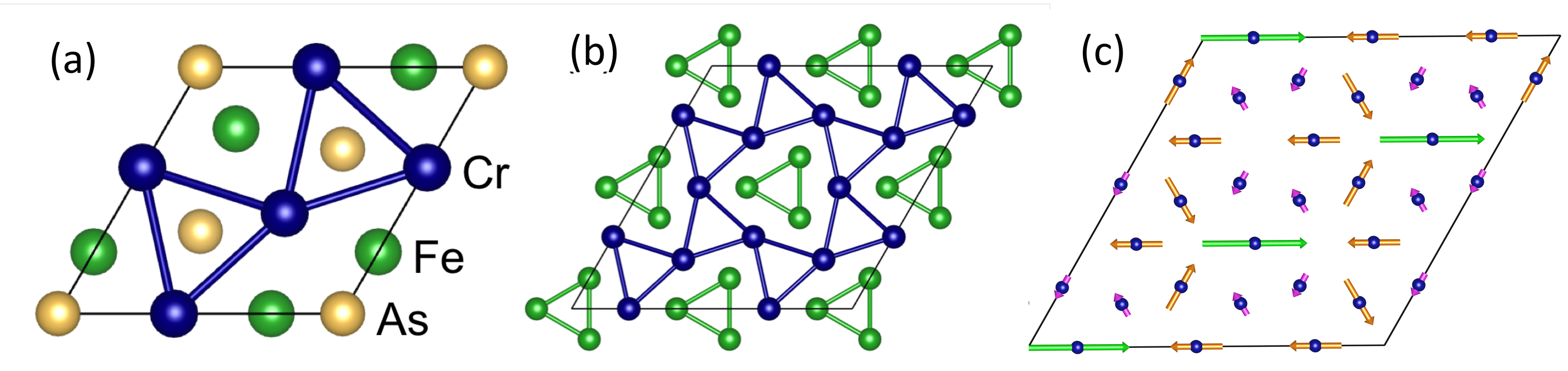

Figure 1: Structure of FeCrAs, showing (a) the unit cell, (b) Fe trimers and Cr distorted kagome lattice, (c) magnetic structure[2].

The Cr magnetic moments have been found to order at T_N=125 K, despite the strong geometric frustration[2]. It was suggested that the electronic state on the Fe sublattice is a spin liquid phase that survives in the presence of the magnetic Cr sublattice[3].

Muon-spin spectroscopy

To search for the proposed *hidden spin-liquid* phase, we have carried out zero-field (ZF) muon-spin spectroscopy (μ^+SR) at PSI [Figure 1(i)] and ISIS [Figure 1 (ii)][4].

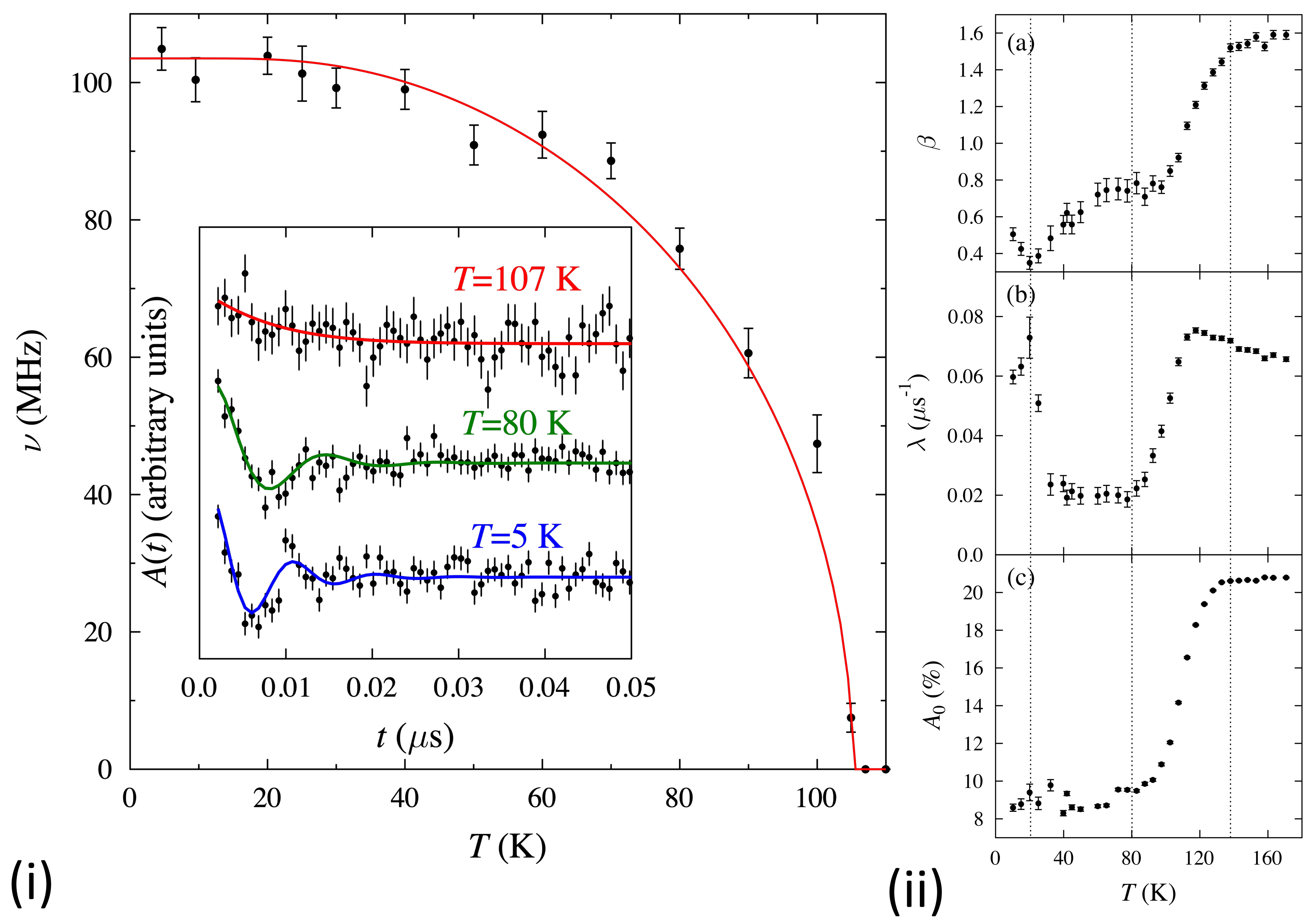

Figure 2: (i) Temperature dependence of the muon precession frequency for the asymmetry spectra measured at PSI (inset). (ii) Temperature dependence of various parameters for a stretched exponential fit to data measured at ISIS.

Long range magnetic order is indicated by the presence of oscillations in the asymmetry for temperatures below 105 K [Fig. 1(i), inset]. No purely relaxing component is required to describe the spectra, which might be in the case for a spin-liquid phase.

Using ZF μ^+SR at ISIS [Figure 1(ii)], we searched for missing fractions of the asymmetry across the magnetic transition. Taking the initial asymmetry lost across the transition to be 2/3 of the magnetic fraction leaves 3% of the initial asymmetry below the transition unaccounted for. This is not large enough to rule in favour of a spin-liquid phase. The behaviour of the relaxation rate indicates a glass freezing transition at T=20 K.

Muon site calculations

Much recent progress has been made in calculating muon stopping sites using density functional theory (DFT)[5]. We determine muon sites in FeCrAs from structural relaxations of a 2x2x2 supercell. Calculations are carried out using the plane-wave basis-set code CASTEP[6] within the DFT generalised gradient approximation (GGA). We identify three distinct stopping sites: two in the Cr layer and one in the Fe layer. The calculated sites show good agreement with the minima in the electrostatic potential of the unperturbed structure (Figure 3). The muon does not introduce significant distortions to the lattice, so we expect it to faithfully probe the magnetism in this system.

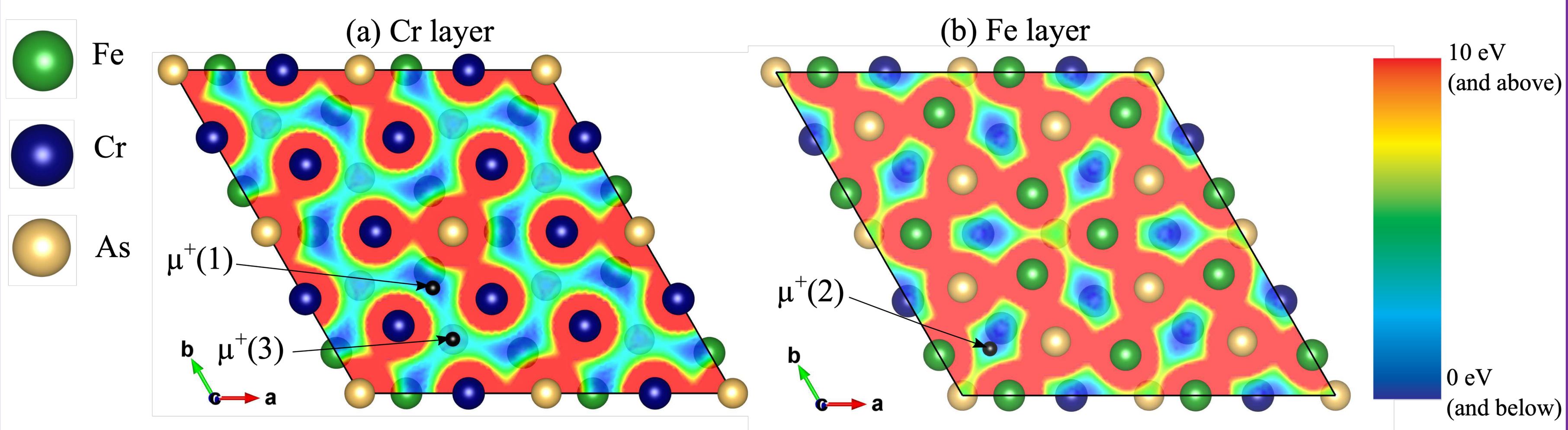

Figure 3: Muon stopping sites in (a) the Cr layer and (b) the Fe layer show good agreement with the minima in the electrostatic potential.

Using the known magnetic structure [see Figure 1(c)] from neutron diffraction experiments[2], we have calculated the dipolar field expected at each of the muon sites. The non-collinear magnetic structure means muon situated in the same crystallographic site are not necessarily magnetically equivalent. The average field and width of field associated with each site are shown in Table 1. The average field for the lowest energy site is in reasonable agreement with the measured muon precession frequency.

Site no.	Muon position	Relative energy (eV)	Dipolar field (MHz)	Field width (MHz)
1	Cr layer, inside hexagon	0.00	88	44
2	Fe layer	0.12	29	9
3	Cr layer, inside triangle	0.40	50	18

Table 1: The calculated average dipolar field (expressed in terms of the muon precession frequency $\nu=\gamma_\mu B/2\pi$) and the field width at each of the muon sites.

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