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μSR and neutron diffraction studies of $U(Ni_xCu_{1-x})_2Si_2$ magnetic structure

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Abstract

Neutron powder diffraction and zero-field μSR studies of $U(Ni_xCu_{1-x})_2Si_2$ with $x = 0$ and 0.25 have been performed. These compounds have different types of AF ordering below $T_N \sim 120$ K. Muon precession has been observed in both samples. Neutron diffraction together with μSR analysis have shown us changing between incommensurate phase and simple AF with the changes of temperature. Possible mechanisms of magnetic ordering are discussed.

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Keywords: Muon spin precession; Neutron diffraction; Intermetallic compounds

1. Introduction

UNi_2Si_2 belongs to the family of uranium-based intermetallides, crystallizing in $ThCr_2Si_2$-type structure (space group I4/mmm). It orders antiferromagnetically at $T_N = 125$ K and exhibits different AF phases below T_N. Magnetic moment possesses only at uranium ions, and all phases consist of ferromagnetic basal planes of uranium moments parallel to the *c*-axis. Replacing Ni by Cu leads to changes in magnetic structure and in T_N. Previous neutron diffraction experiments [1,2] showed quite complicated phase diagram. The main features are following:

- ordered magnetic moments are found on the uranium ions,
- magnetic moments are along the tetragonal axis,
- magnetic structures characterized by propagation vector $k = (0, 0, k_z)$,
- the commensurate structure are formed by stacking of equivalent ferromagnetic uranium basal planes along *c*-axis:

Simple AF:	$k = (0,0,1) : + - + -$
Ferri:	$k = (0,0,2/3) : + + - + + -$
AF-IA	$k = (0,0,1/2) : + + - -$

In comparison with $x = 0.25$, the magnetic phase diagram is most complicated. At $0 < T < 100$ K, a coexistence of several magnetic phases was supposed in Ref. [2].

μSR, being a local probe technique, can provide complementary to the neutron diffraction information since it allows one to determine the local magnetic field in the crystal lattice, which is directly connected with the real magnetic moment of the atoms.

2. Experimental details

Polycrystalline samples of UNi_2Si_2 and $U(Ni_{0.25}Cu_{0.75})_2Si_2$ were prepared by arc-melting of the initial components in an Ar atmosphere. The samples were annealed at $T = 800\,^{\circ}C$ for 1000 h. Neutron diffraction experiments were performed at the DMC diffractometer at the SINQ spallation source at Paul Scherrer Institute (PSI) [3]. Incident wavelength was $\lambda = 2.59$ Å. Zero-field μSR

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experiments were performed with the GPD instrument also at PSI.

3. Results

3.1. UNi_2Si_2

Our neutron diffraction data show that the sample crystallized in a tetragonal body centered lattice with I4/mmm space group and unit cell parameters $a = b = 3.96\,\mathring{A}$ and $c = 9.51\,\mathring{A}$. The sample magnetically orders at the temperature $T < T_N \sim 125\,K$. At low temperature the magnetic structure is a simple AF $(+-+-)$ (see Fig. 1) but in the temperature region of $50 < T < 100$ it changes to commensurate structure AF-IA and with a increasing of the temperature higher than 100 K to incommensurate AF with $k = (0, 0, k_z)$, where k_z is slightly vitiated around 0.75.

The muon spin precession in zero external magnetic field was observed below T_N. The signal has one component at $T < 50\,K$, two components with two different muon precession frequencies F1 and F2 (see Fig. 2) at the temperature more than 50 K. Both frequencies decrease until $T = 100\,K$, where F1 vanishes and F2 has a small peculiarity. Above $T = 100\,K$ there is only one muon precession frequency F2, which disappears at T_N.

3.2. $U(Ni_{0.25}Cu_{0.75})_2Si_2$

Neutron diffraction experiments have shown that the sample ordered antiferromagnetically (simple AF) below 120 K. No other magnetic phases have been found. The muon spin precession in zero external field was also observed. The signal has only one component (see Fig. 2). The frequency slightly changes in whole temperature range below T_N and has only one weak peculiarity around 100 K.

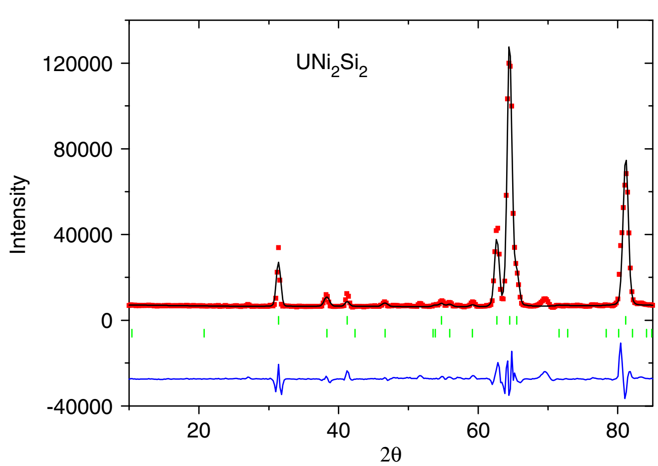

Fig. 1. Neutron diffraction pattern of UNi_2Si_2 at $T = 15\,K$. Experimental points, the calculated profile and the difference curve are shown. Rods show positions of nuclear peaks (upper row) and magnetic satellites for the AF-type structure (lower row). Small peak at the $2\vartheta \sim 70$ belongs to impurity.

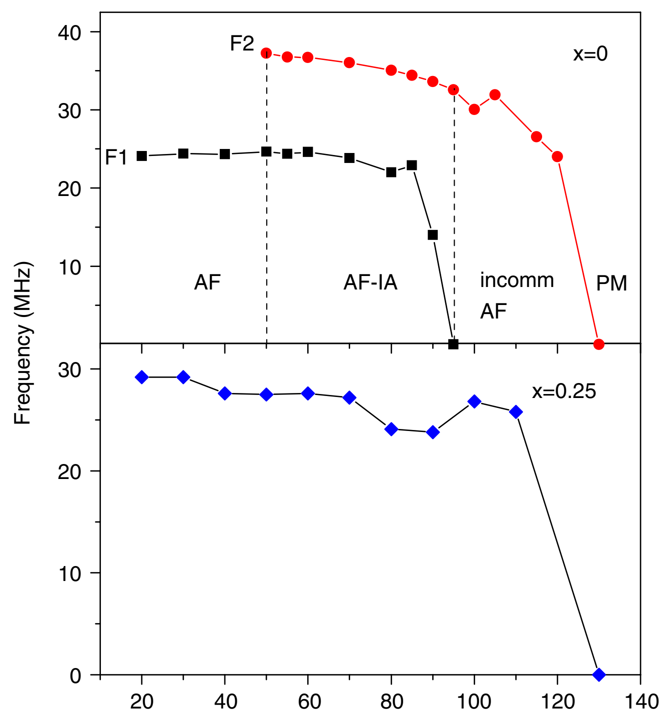

Fig. 2. Temperature dependence of the muon precession frequencies F1, F2 in zero external field in UNi_2Si_2 (close symbols) and $U(Ni_{0.25}Cu_{0.75})_2Si_2$ (open symbols).

4. Discussion

Possible muon sites for the crystal structures of $ThCr_2Si_2$ type were discussed in Refs. [4,5]. A comparison of the dipole magnetic fields in the AF state at the different muon sites showed that the muon site $(0\frac{1}{2}\frac{1}{8})$ agrees with the experimental precession frequency, as it was found for the UPd_2Ge_2 [5,6]. Values of magnetic moments, defined by neutron diffraction correspond with values, defined from μSR experiment $m = F/\alpha$, where $\alpha = 13.9\,MHz/\mu_B$.

As already described in our previous works [5,6], muon sites in crystal lattice are crystallographically equivalent but in case of commensurate square modulation the main contribution to the dipolar field is different for different muon positions, therefore we observed two different precession frequencies.

According to the theoretical predictions based on RKKY [2], a most probable magnetic structure in system $U(Ni_xCu_{1-x})_2Si_2$ at the $x < 0.25$ is AF and $x < 0.25$ is AF-IA. Our experiments (both neutron diffraction and muon precession) show that the magnetic structure of $U(Ni_{0.25}Cu_{0.75})_2Si_2$ is simple AF below $T_N \sim 125\,K$. One-component precession means that all muon sites are equivalent and there are no additional magnetic satellites in neutron pattern. We suppose that a mixture of several magnetic phases observed in Ref. [1] is only due to inhomogeneous distribution of Cu in the sample.

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