Experimental report

31/08/2015

Proposal: 5-31-2317 **Council:** 4/2014

Title: Magnetic structure in intermediate-valent compound Ce2RuZn4

Research area: Physics

This proposal is a new proposal

Main proposer: Karel PROKES

Experimental team: Karel PROKES
Steffen HARTWIG

Local contacts: Thomas HANSEN

Samples: Ce2RuZn4

Instrument	Requested days	Allocated days	From	To
D20	2	1	25/09/2014	26/09/2014

Abstract:

We propose to perform neutron diffraction experiment on a trivalent/intermediate-valent ordered cerium based compound Ce2RuZn4. There are two different Ce crystallographic positions wit radically different nearest-neighbor (NN) distances. For one of the sites (called Ce2) is the separation to NN Ru atoms (=260 pm) even smaller than the sum of the covalent radii of 289 pm. Magnetic bulk and specific heat experiments show that this intermetallic compound orders magnetically at 2 K. First principles calculations suggest that a sizable moment of about 0.6 muB resides only on one half of Ce atoms, namely at the Ce1. Due to the size of magnetic moments involved and the low temperature at which one needs to perform the experiment we ask for two days on the high-flux instrument D20.

Scientific Background

Ternary intermetallic compounds in the system Ce-Ru-*X*, where *X* is an element of the third, fourth, or fifth main group, have been intensively studied in recent years. This is due to the fact that these materials exhibit peculiar structural and physical properties, where the transition-metal ruthenium seems to play a key role. In comparison to related compounds with other transition metals, ruthenium often shows extremely short Ce-Ru distances, even much shorter than the sum of the covalent radii. This situation is realized also in Ce_2RuZn_4 for which ab-initio calculations predict that the Ce2 site (Fig. 1) does not carry any magnetic moment[1].

The purpose of the recent study using D1A and D20 that was published in PRB [2] was to determine the magnetic structure of this material that exists below T_N = 2.3 K. In particular, we wanted to verify the prediction that Ce2 site is indeed without a long-range magnetic order. Magnetic bulk measurements are indeed in agreement with this prediction. The experiment was carried out using a standard orange-type cryostat above T_N and in temperatures down to 1.7 K.

Results

The differential spectrum shown in Fig. 2 shows very tiny but well defined additional Bragg reflections that are due to magnetic order. All of them are indexable with an incommensurate propagation vector q_m = (0.384, 0.384, 1/2).

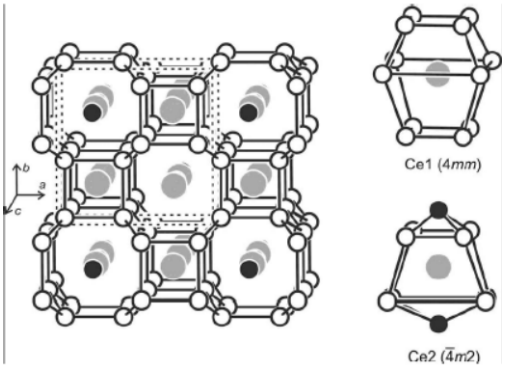

Fig. 1: Schematic representation of the crystal structure of Ce_2RuZn_4 with two Ce sites. Ce2 site is supposed to remain paramagnetic to the lowest temperatures.

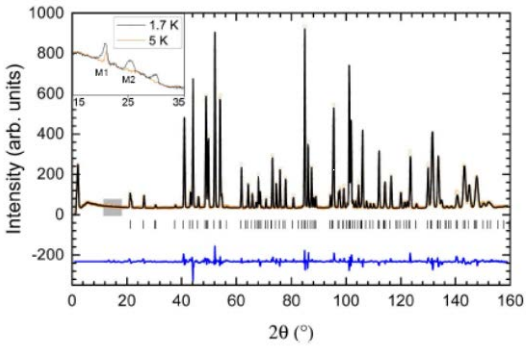

Fig. 2: Refinement of the powder diffractogram obtained on Ce_2RuZn_4 using D1A instrument. The inset shows data related to the grey area obtained using D20 at 1.7 and 5 K, respectively.

Group analysis shows that there are four 1-D irreducible representations. One of them cannot explain observed magnetic intensities at all, one gives a very large magnetic moment on the non-magnetic Ce site and the two remaining ones lead the same agreement (Fig. 3) between the experimental and calculated profiles. The two modulated magnetic structures although having different coupling of Ce1 moments within one unit cell are physically equivalent. This follows from the

existence of different Ce chains that build a co0mplicated 3D network and are not in insets of Fig. 3 easily visible. Assuming that the Ce2 site does not carry any substantial moment, Ce1 magnetic moments are confined to the (110)-type planes and transversely modulated with an amplitude of 1.77(3) μB.

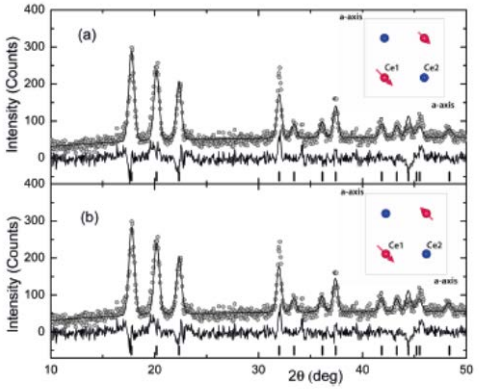

Fig. 3: Best fits to the differential ("1.7-5K") powder diffractogram obtained on Ce_2RuZn_4 using D20 instrument and two different irreducible representations. The inset show the corresponding magnetic structures

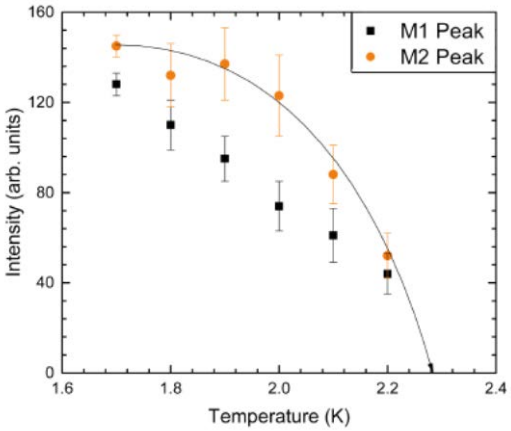

Fig. 4: The temperature dependence of the Bragg intensities of the two first magnetic reflections (see inset of Fig. 2).

However, one point needs to be still clarified. The two lowest-lying magnetic reflections have different temperature dependencies (see Fig. 4). This suggests either small contribution from Ce2 sites or a c-axis component residing on the Ce1 site that could be produced by e.g. subtle crystal structure distortion not detected in the present experiment.

References

[1] V. Eyert, et al., Phys. Rev. B **78** (2008) 214420.
[2] S. Harwig, et al., Phys. Rev. B **92** (2015) 024420