Experimental report

16/12/2021

Proposal: 5-31-2839 **Council:** 10/2020

Title: Magnetic structures determination of ternary uranium germanides with U-zigzag chains: thermal and magnetic field dependence studies

Research area: Materials

This proposal is a new proposal

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Samples: U3TGe5 (T = Ti, V, Cr, Zr, Nb)
UT1-xGe2 (T = Fe, Co)
U6V4Al43

Instrument	Requested days	Allocated days	From	To
D1B	4	2	07/06/2021	09/06/2021

Abstract:

The U-zigzag chains encountered in the crystal structure of the uranium germanides UGe2, URhGe and UCoGe play a fundamental role on the coexistence of superconductivity and ferromagnetism in these very fascinating materials. Recently, we have discovered novel compounds characterized by such chains within two families, namely UT1-xGe2 and U3T'Ge5 (T and T' = transition metals), and presenting many crystallographic, magnetic and electrical similarities with the superconducting ferromagnets. Solving the magnetic structures of these intermetallics will help to understand the influence of the U-zigzag chains (U-U distances and angles) on their physical properties. Indeed, neutron diffraction experiments, including field dependence measurements, will help us in determining the origin of (i) the gapping of the Fermi surface of the ferromagnets U3TiGe5, U3ZrGe5, UFe0.40Ge2 and UCo0.45Ge2 (non-fully aligned moments vs. spin density wave), and (ii) the transition from ferromagnetism to antiferromagnetism to spin fluctuation when T' varies from column 4 to column 6 in U3T'Ge5 (with T' = Ti, Zr, V, Nb, Cr).

Experimental report on the proposal 5-31-2839: **Magnetic structures determination of ternary uranium germanides with U-zigzag chains: thermal and magnetic field dependence studies**

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1. Introduction

Understanding the coexistence of superconductivity and ferromagnetism, carried by the same atomic network, in the uranium germanides UGe_2 [1], URhGe [2] and UCoGe [3] is a hot topic for solid state physicists these last years. In addition to this coexistence, the re-entrance of superconductivity at elevated magnetic fields is a striking feature in this family. The presence of uranium zigzag chains in these compounds, locally breaking the inversion symmetry, seems to be of uttermost importance for occurrence of the ferromagnetic fluctuation induced spin-triplet superconductivity (see [4] for a review). At ambient pressure, the interatomic distance between the U-atoms is around 3.8 Å in UGe_2 with angles of 64° along the chains, while in UCoGe and URhGe the distances are much closer to the Hill limit for occurrence of magnetic ordering in uranium intermetallics (~3.5 Å) [5] and the angles much wider (~ 160°). Consequently, the orientation of the magnetic moments is different, being oriented in the U-chain direction in UGe_2 and perpendicular to it in the ternaries (**Fig. 1**).

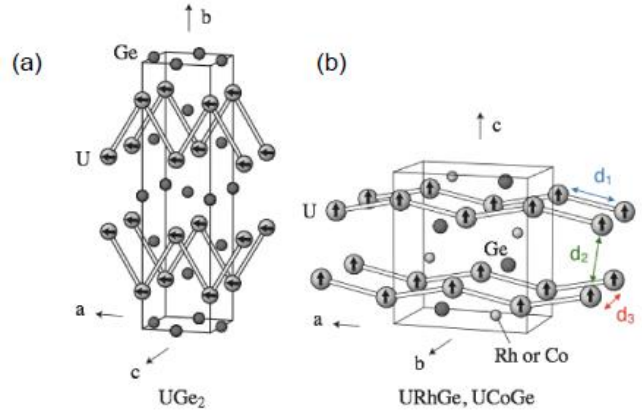

Fig. 1: Magnetic structures of the ferromagnetic superconductors (a) UGe_2 and (b) URhGe and UCoGe. For the sake of clarity, only the U-atoms are presented and the U-zigzag chains highlighted. Reproduced from [4].

These last years, two families of ternary uranium germanides, namely $UT_{1-x}Ge_2$ (T = Fe, Co, Ni, Ru, Os) [6-10] and $U_3T'Ge_5$ (T' = transition elements from columns 4, 5 and 6) [11-13] showing similar U-chain features and similarities of the magnetic and electrical behaviors with the aforementioned ferromagnetic superconductors were discovered and investigated.

By determining the magnetic structures of these ternary compounds and their thermal evolution in both the absence and application of an external magnetic field, we expect to better understand the role of the U-zigzag chains on the physical properties of the uranium germanides.

2. Neutron diffraction results

2.1. $UT_{1-x}Ge_2$ compounds

The $UT_{1-x}Ge_2$ (T = Fe, Co) compounds were investigated during this experiment. Rietveld refinement of the neutron powder diffraction data (λ = 2.52 Å) of $UCo_{1-x}Ge_2$ recorded in the paramagnetic state (T = 40 K) confirms the $CeNiSi_2$-type of structure ($Cmcm$) of this compound and the presence of weak quantity of the paramagnetic UGe_3 phase (AuCu3-type, $Pm\bar{3}m$) as impurity in the sample (~1 wt.%). The refinement of the Co content leads to the chemical composition $UCo_{0.39(2)}Ge_2$. This composition was fixed in the refinement of the magnetic structure from neutron powder diffraction data recorded in the magnetically ordered state (T = 2.9 K). Neutron powder diffraction data recorded at T = 2.9 K do not evidence the appearance of extra diffraction peaks, confirming the ferromagnetic behavior of $UCo_{0.39}Ge_2$. Difference pattern between data recorded in the paramagnetic (T = 40 K) and in the magnetic (T = 2.9 K) state shows a weak increase of the intensity of the *110*, *021*, *130* and *041/111* Bragg peaks and no apparent magnetic contribution to the *020* and *060* peaks, indicating that the magnetic moments are aligned along the *b*-axis. Rietveld refinement of the neutron powder diffraction data recorded at 2.9 K, shown in **Fig. 2**, leads to a magnetic moment of 0.69(14) μ_B per uranium atom in excellent agreement with magnetic data. However, the weakness of the magnetic contributions does not allow to investigate neither a potential canting of the magnetic moments at low temperature, nor a thermal evolution of the magnetic moment. A magnetic structure representation of $UCo_{0.39}Ge_2$ is shown in **Fig. 3**. Surprisingly, the moments are perpendicular to the U-chain direction while the chains are much closer from those in UGe_2 than those in U(Co,Rh)Ge. These results will be the subject of an upcoming publication [14].

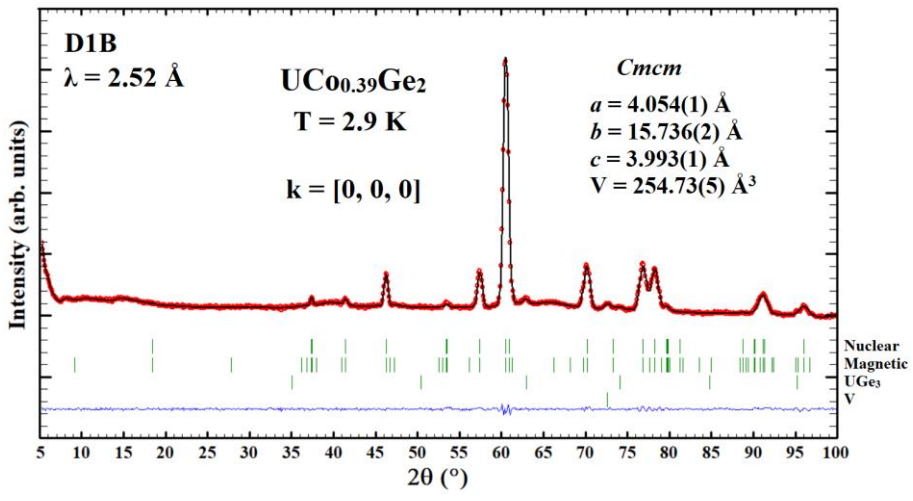

Fig. 2: Rietveld refinement of the neutron powder diffraction of $UCo_{0.39}Ge_2$ recorded at 40K

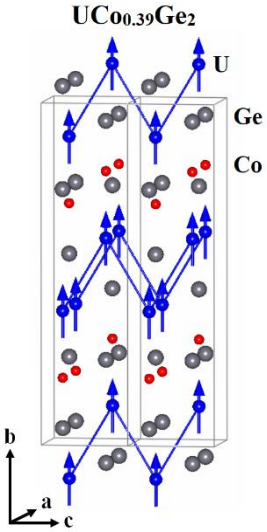

Fig. 3: Magnetic structure of $UCo_{0.39}Ge_2$

Analyses of the neutron powder diffraction data (λ = 2.52 Å) of $UFe_{1-x}Ge_2$ recorded with and without application of an external magnetic field are in progress but are so far locked by the atomic structure resolution, the latter showing incommensurate superstructure features.

2.2. U_3TGe_5 compounds

Note that due to the limited number of allocated days (2 instead of 4 requested in the proposal), only the U_3VGe_5 compound was investigated during this experiment. Neutron powder diffraction (NPD) data, recorded in field up (**Fig. 4**) and field down, are under investigations. They nevertheless enable us to confirm the antiferromagnetic behavior (T_N = 25 K) and metamagnetic transition of U_3VGe_5 (μ_0H > 1.5 T at 3 K) and to reveal that, in the absence of an external magnetic field, this compound is characterized by a commensurate magnetic structure with propagation vector k = [1/2, 0, 0] (**Fig. 5**).

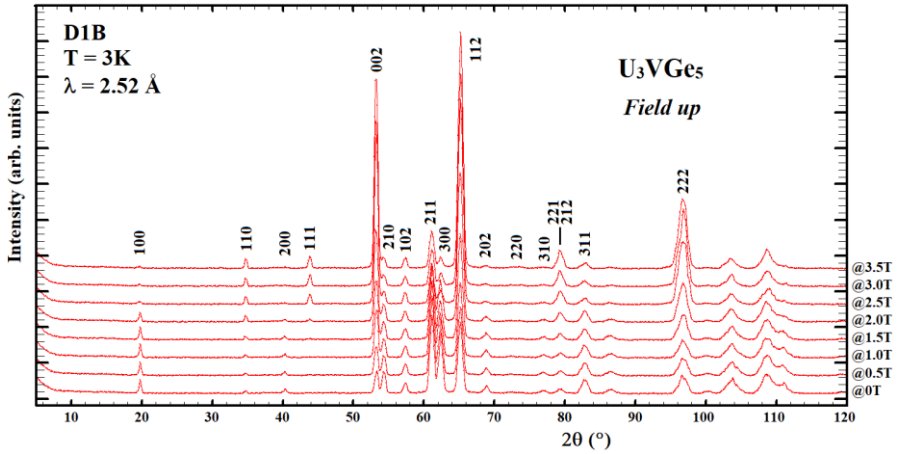

Fig. 4: NPD data of U_3VGe_5 recorded at T = 3K in field up

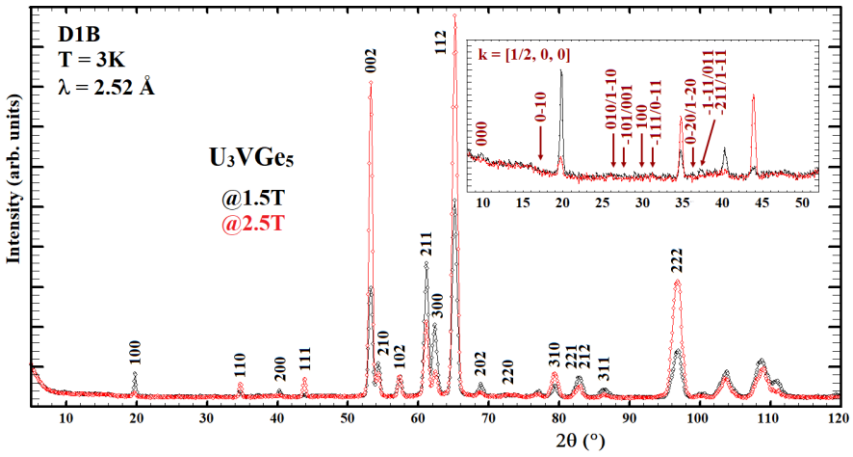

Fig. 5: NPD data of U_3VGe_5 at T = 3K and μ_0H = 1.5T and 2.5T

3. References

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