Experimental report

19/04/2022

Proposal: 5-22-796 **Council:** 10/2020

Title: Structures and magnetism of the Li/ammonia intercalates of Fe3GeTe2 and Fe5GeTe2

Research area: Chemistry

This proposal is a new proposal

Main proposer: Simon James CLARKE

Experimental team: Stanislav SAVVIN
Machteld KAMMINGA

Local contacts: Stanislav SAVVIN

Samples: LiNH3Fe3GeTe2
LiND3Fe3GeTe2
KFe3GeTe2
KFe5GeTe2

Instrument	Requested days	Allocated days	From	To
D2B	2	2	16/06/2021	18/06/2021

Abstract:

This proposal is to measure the crystal and magnetic structures of new intercalates of the topical layered ferromagnets Fe3GeTe2 and Fe5GeTe2 obtained by intercalating lithium and ammonia between the iron germanium telluride slabs. The use of neutrons will enable location of light atoms of the intercalate and the measurement of additional low temperature magnetic Bragg scattering. These are chemical derivatives of a topical series of layered ferromagnetic compounds which offer a new route to property tuning.

EXPERIMENTAL REPORT

EXPERIMENT N° 5-22-796 INSTRUMENT D2B

DATES OF EXPERIMENT 16/06/2021 to 18/06/2021

TITLE Structures and magnetism of the Li/ammonia intercalates of Fe3GeTe2 and Fe5GeTe2

EXPERIMENTAL TEAM (names and affiliation)

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LOCAL CONTACT SAVVIN, Stanislav

Date of report 19/04/22

Structures and Magnetism of the Li/ammonia intercalates of Fe_3GeTe_2 and Fe_5GeTe_2

Recently several layered iron germanium tellurides [1, 2] have been reported that are ferromagnetic at or around ambient temperature and which may have encouraging physical properties – they have the highest Curie temperatures for bulk "van der Waals" type layered ferromagnets with strongly bonded slabs bound together by weak van der Waals interactions.

It has been shown that Na intercalation into $Fe_{3-\delta}GeTe_2$ is possible [3], but that this promotes some decomposition to sodium telluride and iron germanide products. We have now shown that intercalation of K or Li and ammonia into Fe_3GeTe_2 and the Fe-rich relative Fe_5GeTe_2 is possible, suggesting another way to decrease the dimensionality and potentially control the electron count and hence properties of these compounds. It represents a new chemical direction in the investigation of these topical compounds to complement investigations of monolayers, device fabrication and heterostructure formation.

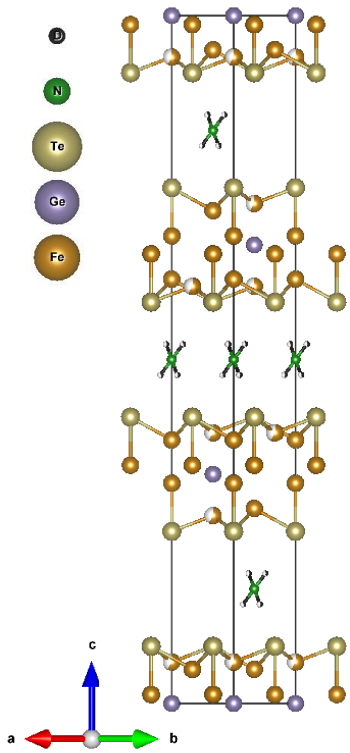

Figure 1. Structural model of intercalate $Li_x(NH_3)_yFe_5GeTe_2$.

The data collected on the D2B instrument in these experiments reveal the positions of the intercalated light atoms Li, H/D and N in between the iron germanium telluride slabs. Nitrogen atoms were refined to distorted octahedral sites formed by Te atoms of adjacent Fe_5GeTe_2 layers. The H and D atoms were located approximately 1 Å from the N atoms and have a linear N-H/D-Te geometry, as has been observed in many other ammonia intercalates [4]. (Fig. 1) Location of Li in the model is still in progress. Measurements taken at 10 K and ambient temperature on the same $Li_x(ND_3)_yFe_5GeTe_2$ sample reveals the absence of any magnetic peaks- indicating no long range ordering which eludes to complex magnetic states as reported for the parent compounds.

Potassium intercalates of Fe_5GeTe_2 and Fe_3GeTe_2, which were found to contain no ammonia, were also measured at 10 K and room temperature. The data collected of $K_xFe_5GeTe_2$ reveal two sets of Bragg peaks

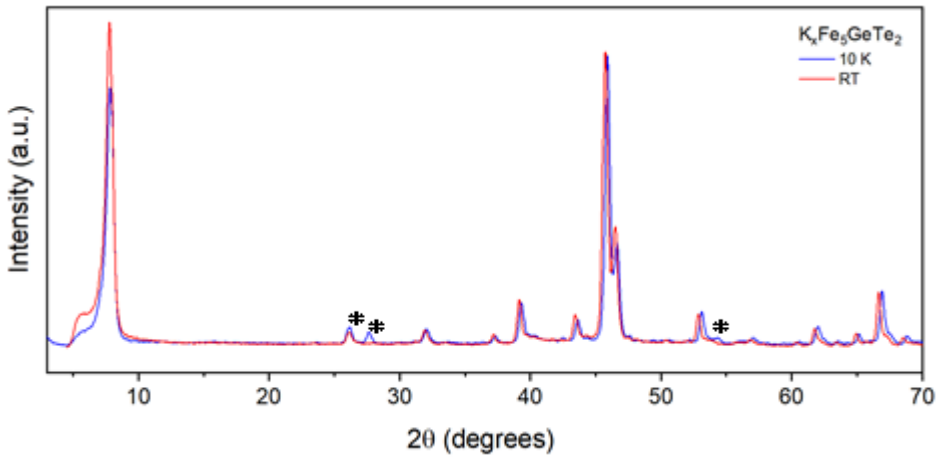

Figure 2. Raw D2B data for $K_xFe_5GeTe_2$ at 10 K and room temperature (RT). The data shows the emergence of three magnetic Bragg peaks marked by an asterisk (*).

at 10 K, one is likely to be ferromagnetic in nature and the other antiferromagnetic. (Fig. 2) Solution of the magnetic ordering is still in progress. The data collected of $K_xFe_3GeTe_2$ did not reveal any new Bragg peaks at 10 K but was used to confirm the nuclear structure of this new compound.

Overall the experiment was a success and we are grateful for the efforts of the local contact in running the experiment in full during the Covid-19 restrictions. Analysis is in progress. These compounds will also be explored using Mössbauer spectroscopy. The work carried out in this experiment will be published in an international journal and will form a significant part of the D.Phil thesis of Penny Hyde.

[1] Deiseroth, H.-J. *et al. Eur J. Inorg. Chem*. **2006**, *2006*, 1561.

[2] May, A. F. *et al. ACS Nano*, **2019**, *13*, 4436-4442.

[3] Weber, D. *et al. Nano Lett*. **2019**, *19*, 5031-5035

[4] Burrard-Lucas, M. *et al*, *Nature Mater*., **2013**, 12, 15–19.