Experimental report

30/04/2020

Proposal: 5-23-729 **Council:** 4/2019

Title: Hydrogenation of LaFeSi precursor and Crystal and magnetic structure of superconducting LaFeSiH

Research area: Physics

This proposal is a new proposal

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Experimental team: Pierre TOULEMONDE
Laura CHAIX

Local contacts: Thomas HANSEN
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Samples: LaFeSiH
LaFeSiD

Instrument	Requested days	Allocated days	From	To
D20	3	0		
D2B	2	2	16/09/2019	18/09/2019
D1B	2	0		

Abstract:

Last year, a new iron based superconductor, free of toxic elements like As or Se, has been discovered in Bordeaux/France: LaFeSiH, with Tc = 10K. It is isostructural to the well known antiferromagnet LaFeAsO, a parent compound of the superconducting iron-based pnictides discoverd in 2008.
The first objective (A) of our proposal is to follow the hydrogenation (preferentially deuteration, to decrease the incoherent background in the patterns due to hydrogen) process of the precuror, LaFeSi, and the desorption of D in a full deuterated LaFeSiD sample by in-situ neutron powder diffraction (and thermogravimetry).
In the second objective (B), we propose to perform high resolution NPD on superconducting LaFeSi(H,D) to (1) determine for the first time precisely Ts, the temperature associated to its tetragonal -> orthorhombic transition, and (2) check for long range magnetic order below Ts.

Experimental report for ILL experiment n°: 5-23-729

Title : Hydrogenation of LaFeSi precursor and Crystal and magnetic structure of superconducting LaFeSiH

Instrument : D2B

Dates of experiment : 16/09/2019 to 18/09/2019

Experimental Team :	**Institut**
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Local Contact : NASSIF Vivian

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In 2017, a new iron based superconductor, free of toxic elements like As or Se, has been discovered in Bordeaux/France: LaFeSiH, with T_c = 10K [Bernardini *et al.* Phys.Rev. B 97, 100504(R) (2018)]. It is isostructural to the well known antiferromagnet LaFeAsO, a parent compound of the superconducting iron-based pnictides discovered in 2008. At 15 K and low pressure (~1 kbar), in the diamond anvil cell, some of the Bragg peaks measured by synchrotron x-ray diffraction (XRD) showed a slight broadening, suggesting an orthorhombic lattice at low temperature.

The first objective (A) of our proposal, i.e. to follow the hydrogenation process of LaFeSi, and the desorption of D in a full deuterated LaFeSiD sample by in-situ neutron powder diffraction (NPD) and thermogravimetry, was not accepted by the review committee. Only the second objective (B) was accepted. This objective (B) was (1) to determine precisely T_s, the temperature associated to the expected tetragonal to orthorhombic transition, and (2) to check for long range magnetic order below T_s, by high resolution NPD on superconducting LaFeSi(H,D).

The corresponding experiment was performed at D2B instrument using a monochromatic beam at λ= 1.594Å for regular temperature steps between 2 K and 300 K. The splitting of Bragg peaks due to the expected structural transition at low temperature was not observed; furthermore no new nuclear diffraction peaks were shown (Fig.1). We conclude that the small orthorhombicity measured previously at ESRF at 15 K by XRD and 1 kbar was an artefact and maybe due to a pressure gradient in the cell.

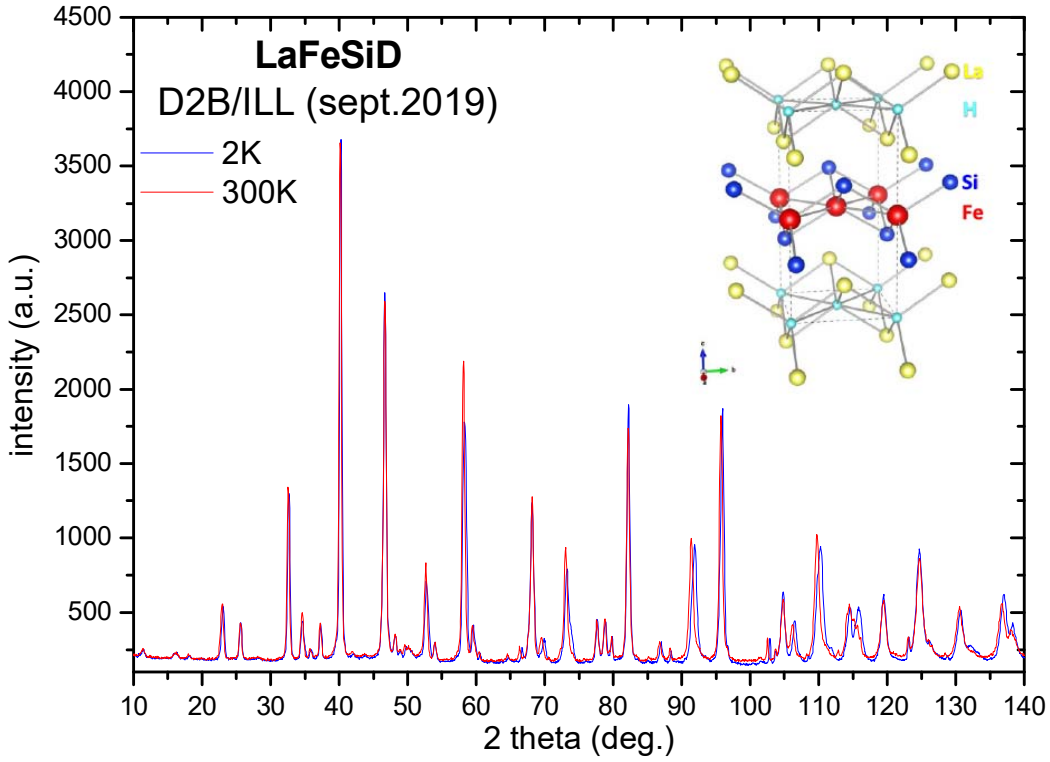

Fig. 1 : D2B NPD patterns of LaFeSiD measured at 2 K and 300 K at λ = 1.594 Å.

In addition, no new magnetic peaks associated with the expected long range antiferromagnetic order was observed. The temperature changes of the lattice parameters were determined (Fig.2). While c-axis decreases continuously from 300K to 2K, the a-axis shows a small increase below 50-100K which is not well understood. Further experiments are needed to explain the origin of such behavior.

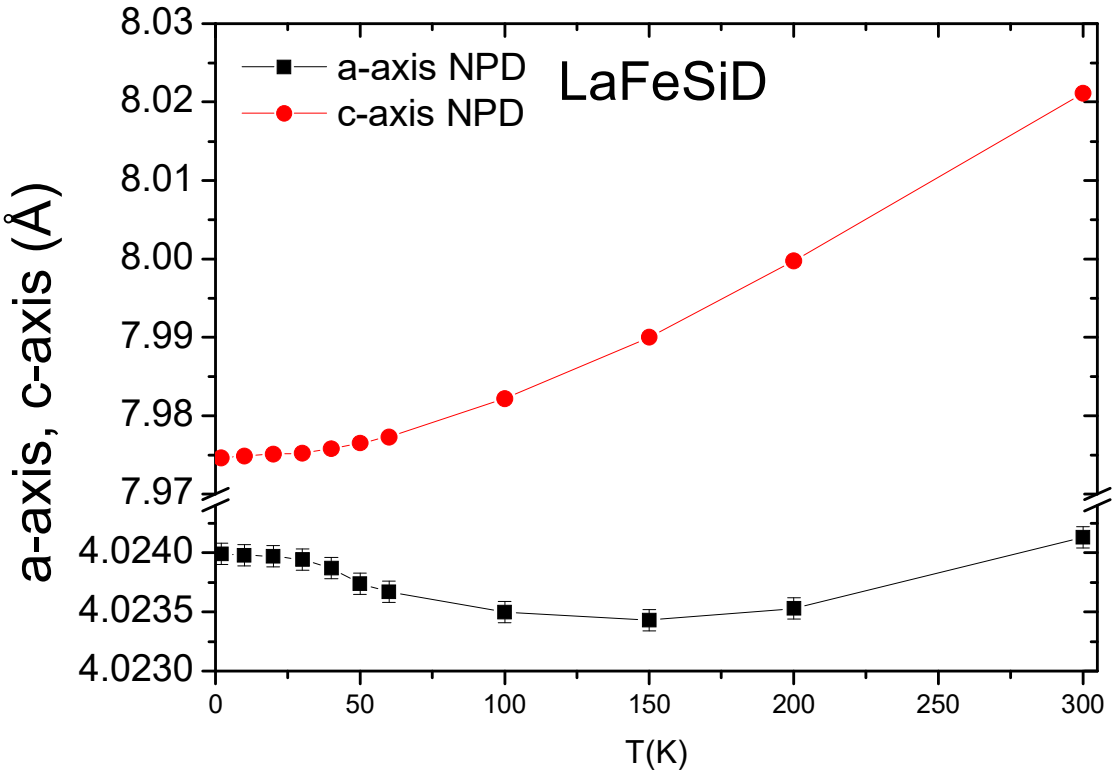

Fig. 2 : Temperature dependence of refined lattice parameters for LaFeSiD obtained from D2B NPD patterns.