Experimental report

10/01/2022

Proposal: EASY-751 **Council:** 10/2020

Title: Crystal structure of a newly discovered LaFeSiX compound with an orthorhombic lattice at room temperature.

Research area: Materials

This proposal is a new proposal

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Experimental team:

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Samples: LaFeSiX

Instrument	Requested days	Allocated days	From	To
D1B	2	2	17/02/2021	18/02/2021

Abstract:

The discovery of superconductivity in tetragonal (T) LaFeSiH in 2018 extended the field of iron-based superconductors beyond the chalcogenides and pnictides [PRB 97, 100504(R) (2018)].
The pairing mechanism of iron-based superconductors is still debated in the literature. A proposed mechanism is related to spin-fluctuations since superconductivity emerges at the quantum critical point where the antiferromagnetic (AFM) ground state of the parent compound is destroyed by doping. The low temperature AFM ordering of the parent compound is accompanied by a structural transition from a T symmetry into an orthorhombic (O) system.
We have synthesized a compound with nominal composition LaFeSiX (X = unknown light element) which crystallizes in an O lattice at room temperature (RT). The observation of O symmetry (by XRD) at RT is unexpected. The identification of the light element X and its atomic position is crucial in understanding this new phase. Synthesis was done at HP-HT using BH3NH3 as hydrogen source through thermal decomposition. Since the structure is so different, a different light element than H is expected to have entered the structure. We propose to use NPD to determine it.

The experiment involved the acquisition of two diffraction patterns, using 2 different wavelengths. The best pattern is shown in figure 1.

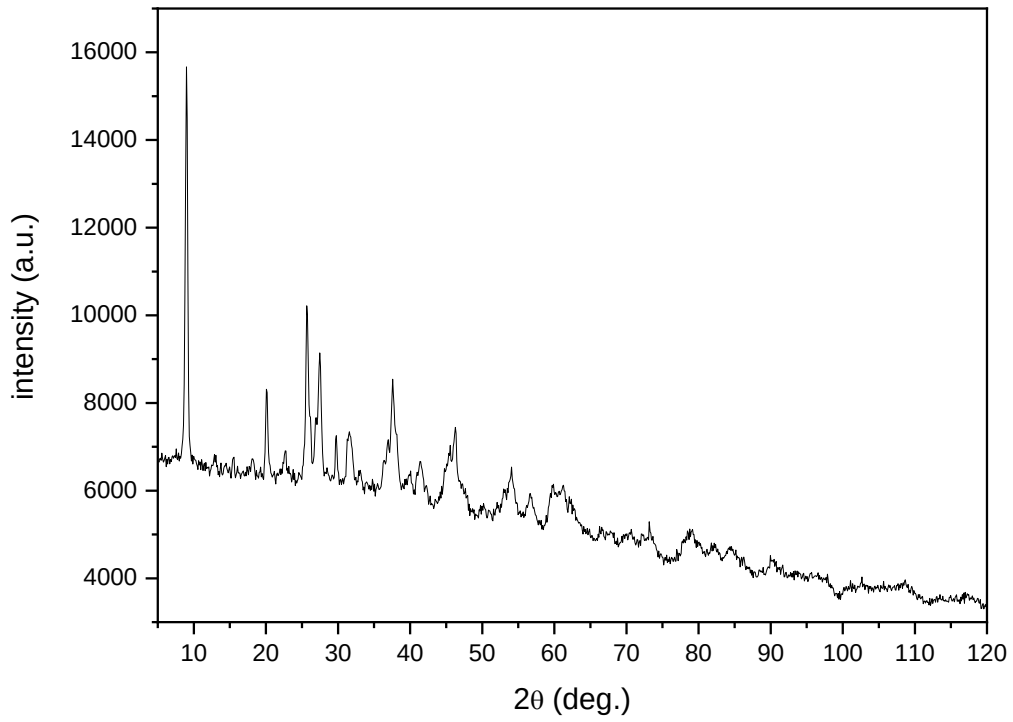

Figure 1: The neutron powder diffraction pattern acquired using a wavelength of 1.28 Ang.

The data was fitted using a le bail fit obtaining an orthorhombic unit cell corresponding to a = 5.7104 Ang., b = 5.8490 Ang. and c = 8.1558 Ang. as also observed using a lab source.

Moving to Rietveld refinement, however, did not yield reliable determination of the atomic positions due to the low crystallinity of the sample in combination with a large background, possibly from hydrogen.