Experimental report

04/10/2022

Proposal: EASY-1017 **Council:** 4/2021

Title: Structure determination of Lu1.5Ca1.5Ga5011.25

Research area: Materials

This proposal is a new proposal

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Experimental team:

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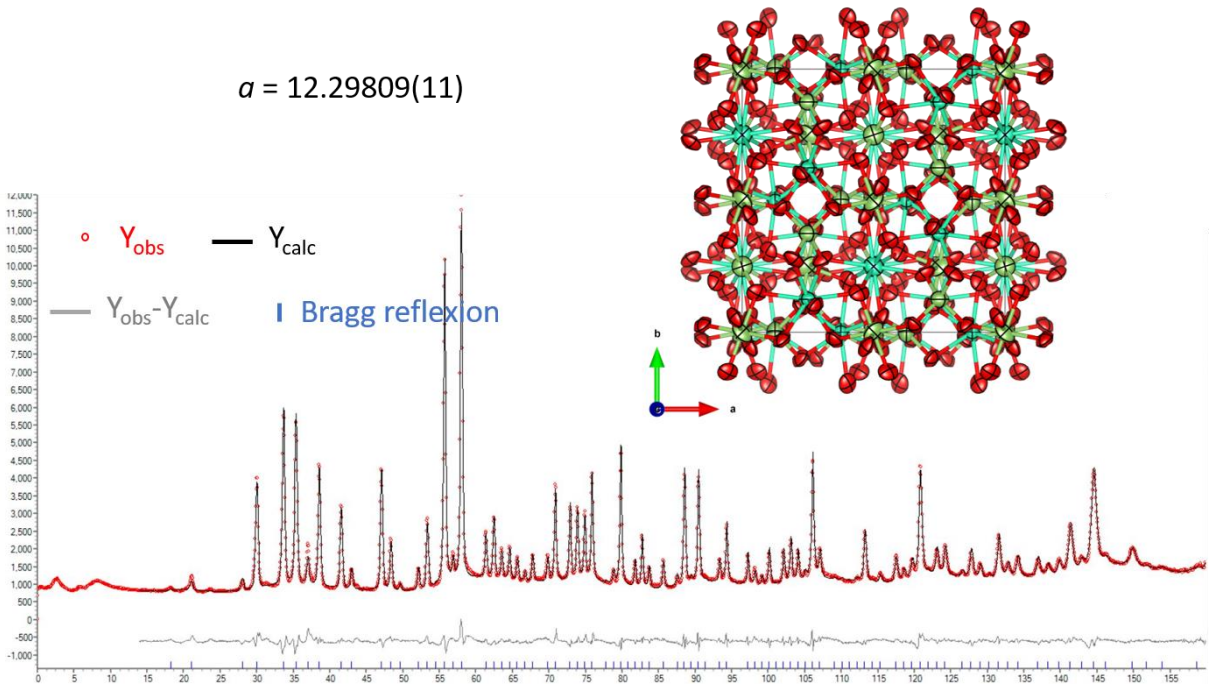
Samples: Lu1.5Ca1.5Ga5O11.25

Instrument	Requested days	Allocated days	From	To
D2B	4	4	15/09/2021	16/09/2021

Abstract:

A3B5O12 garnets are well-known phosphor host materials used for various optical applications such as solid state lasers, scintillators and LED lighting. The flexibility of the structure enables numerous substitutions and large doping contents on both A and B sites of the structure.
In this work, using full crystallization from glass (the glass is synthesised by laser-heated aerodynamic levitation (ADL) technique), we have obtained a new Lu3-xCaxGa5O12-x/2 solid solution. The cationic structure determined by XRD fits well with the garnet structure. However, given that Lu3+ is substituted by Ca2+, the oxygen network must be seriously modified. To our knowledge, there is no report of such substitution in garnet. NMR results show that 80% of the Ga environment is in tetrahedral coordination instead of 60% in the garnet structure. In order to determine the oxygen positions (not seen by XRD given that the scattering factor of Lu is much too strong), high resolution and high flux NPD data are required.
We propose here to measure the Lu1.5Ca1.5Ga5011.25 composition at room temperature on the D2B diffractometer.

First refinement trials have been performed considering a garnet structure such as Lu1.5Ca1.5Ga5011.25 (Lu3Ga5012 structure with substitution of Lu by Ca and oxygen vacancies to compensate). These led to correct fits such as the one presented below.



No obvious modification of the garnet structure has been identified. However, given that Lu3+ is substituted by Ca2+, the oxygen network must be seriously modified.

More investigations are underway to understand the structure of this surprising garnet material.