

## Experiment Report Form

**The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.**

Once completed, the report should be submitted electronically to the User Office via the User Portal:

<https://www.esrf.fr/misapps/SMISWebClient/protected/welcome.do>

### ***Reports supporting requests for additional beam time***

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

### ***Reports on experiments relating to long term projects***

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

### ***Published papers***

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

### **Deadlines for submission of Experimental Reports**

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

### **Instructions for preparing your Report**

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.



**Experiment title:** Crystal structure of new high-pressure phase of multiferroic langasite family crystals

**Experiment number:**  
HC-3383

**Beamline:**  
ID27

**Date of experiment:**  
from: 01.11.2017 to: 04.11.2017

**Date of report:**  
28.02.2018

**Shifts:**  
9

**Local contact(s):**  
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*Received at ESRF:*

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## Report:

During the experiment we investigated crystal structures of new high-pressure multiferroics  $A_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  ( $A = \text{Ba}, \text{Sr}$ ) up to 35 GPa by synchrotron single-crystal X-ray diffraction (SXRD) technique. In the results of structural studies we determined crystal structures of two high-pressure modifications of  $\text{Ba}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  at 3 and 17 GPa (Fig.1).

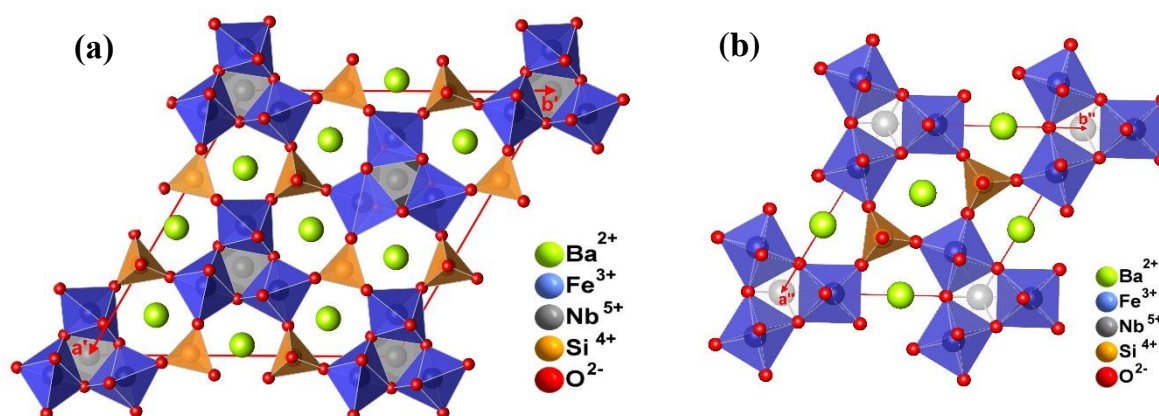


Fig.1 The crystal structures of new high-pressure phases  $\text{Ba}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  in the projection to the plane  $ab$ : (a)  $P = 3\text{-}17$  GPa (at  $P = 5.5$  GPa  $a' = b' = 14.46\text{\AA}$ ,  $c' = 5.14\text{\AA}$ , sp.gr.  $P3$ ,  $V = 930.5(1)\text{\AA}^3$ ,  $Z = 3$ ), (b)  $P = 17.5\text{-}30$  GPa (the parameters of the unit cell at  $P = 29.5$  GPa:  $a'' = 8.733(1)\text{\AA}$ ,  $c'' = 3.688(1)\text{\AA}$ ,  $V = 243.64(7)\text{\AA}^3$ ,  $Z = 1$ ).

The important achievement is the structural explanation of the Neel temperature growth (almost 3 times) under pressure 17.5 GPa due to the change in the coordination environment of  $\text{Fe}^{3+}$  cations, formation of additional Fe-O-Fe bonds and consequently a strong increase in the value of the spin superexchange interactions between  $\text{Fe}^{3+}$  cations.

Single crystal x-ray analysis of  $\text{Sr}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  revealed monotonic decrease of structural parameters up to 35 GPa. The difference of high-pressure behavior of two similar langasites  $\text{Ba}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  and  $\text{Sr}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  will allow us explain nature of multiferroic properties in the langasite family crystals (Fig.2).

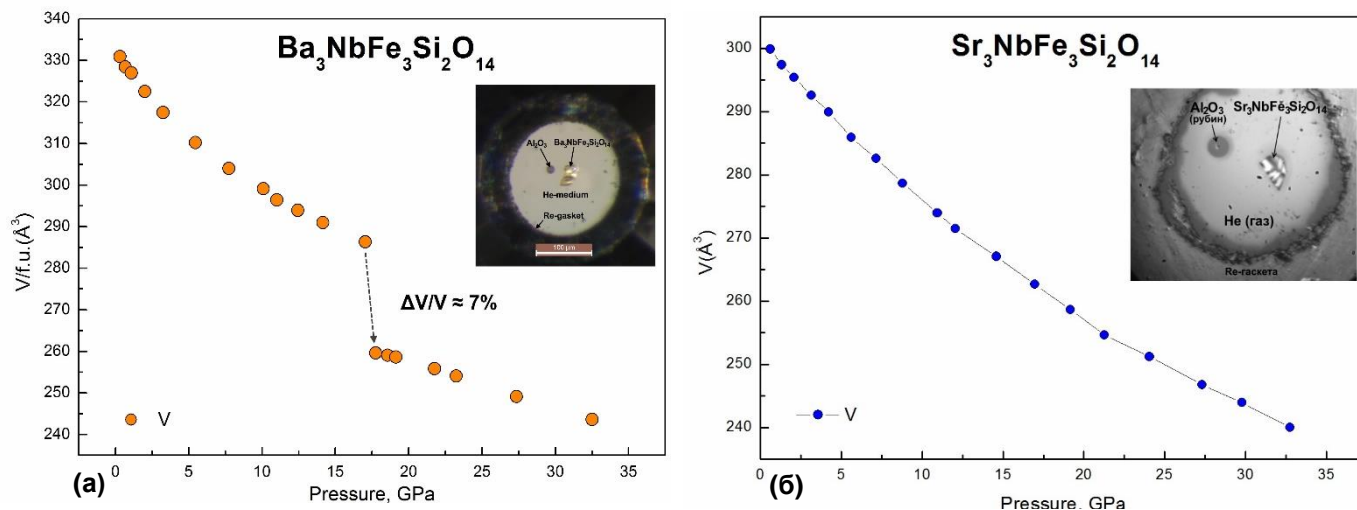


Fig.2 Volume-pressure dependences for  $\text{Ba}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  (left) and  $\text{Sr}_3\text{NbFe}_3\text{Si}_2\text{O}_{14}$  (right)