EUROPEAN SYNCHROTRON RADIATION FACILITY
INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report

	Experiment title: Incommensurate structure in $BaCuSi_2O_6$ at low temperatures	**Experiment number**: 01-02-1101
Beamline: BM01	**Date of experiment**: from: 17/05/2016 to: 21/05/2016	**Date of report**: 23/05/2016
Shifts: 9	**Local contact(s)**: Dmitry Chernyshov	*Received at ESRF:*

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Report:

The investigation of Han purple - $BaCuSi_2O_6$ and $Ba_{1-x}Sr_xCuSi_2O_6$ single-crystal samples, using synchrotron x-ray diffraction at low temperature, was performed to study the incommensurate structure of the compounds.

High quality single crystal diffraction data were recorded at 4.5K and 300K, additionaly in more detail in the temperature range of 5-140K, whereby the new SNBL helium cryostream between 4.5 and 60K, and a nitrogen cryostream for higher temperatures was used.

We were able to resolve the incommensurate reflections with high resolution and couvering a large volume in reciprocal space. The incommensurate modulation is present in $BaCuSi_2O_6$ grown with a flux and in samples gwon with oxygen partial pressure of 1bar and appears together with the symmetry lowering phase transition. The incommensurate reflections are in the order of 10^4 times weaker than the strongest Bragg peaks.

Representative reciprocal space reconstructions of scattering intensities in the (*hk1*) plane of $BaCuSi_2O_6$ and $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ at 4.5K are shown in Figure 1.

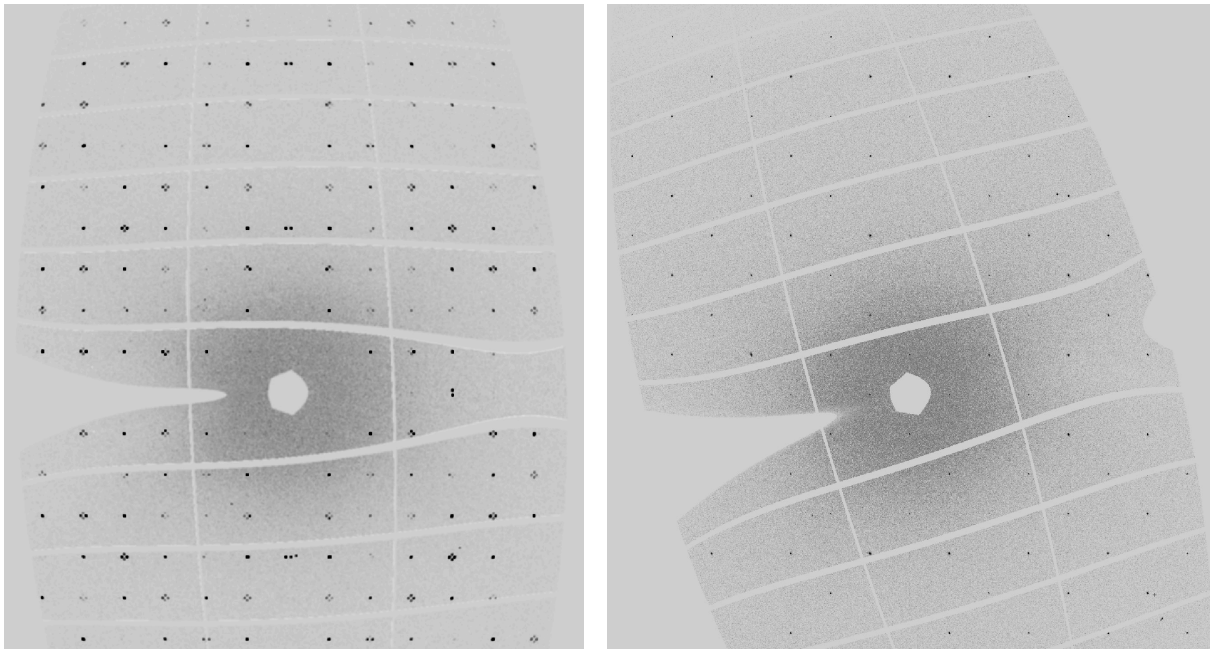
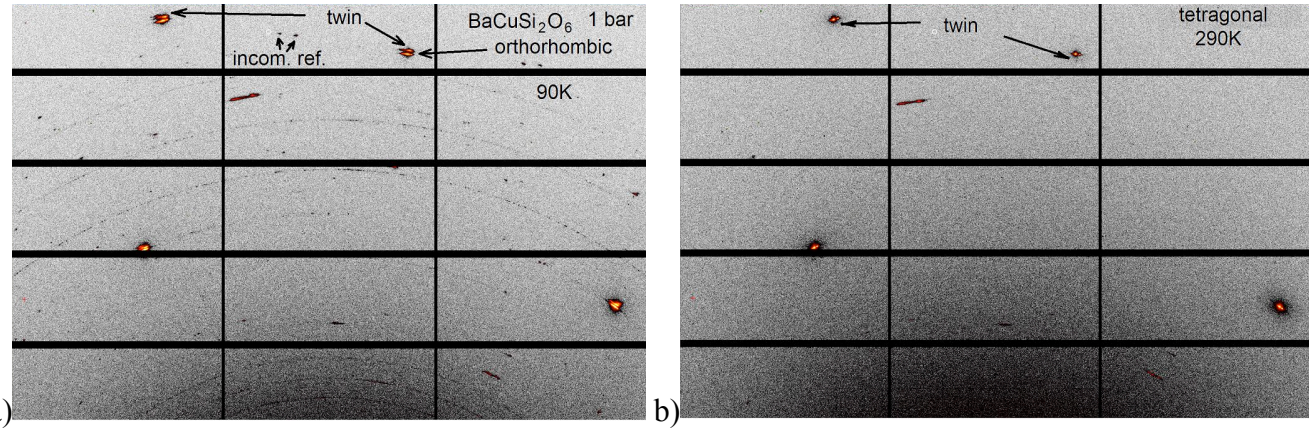


Figure 1. The first experimental (*hk1*) reciprocal space plane of $BaCuSi_2O_6$ (left panel) and $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ at 4.5K (right panel), reconstructed from synchrotron x-ray diffraction data (BM01A@ESRF).

The structural investigation revealed the absence of a the symmetry lowering phase transition and incommensurate modulations in $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ grown with oxygen partial pressure, see Figure 1.
The temperature evolution of the incommensurate structure and the phase transition was determined in more detail and direct comparison of diffraction patterns in the same geometry are shown in Figure 2. The essential features of the phase transition are visible, the orthorhombic splitting disappears together with the incommensurate reflections upon heating.



a) b)

Figure 2: Diffraction of $BaCuSi_2O_6$ grown with oxygen partial pressure 1 bar a) at 90K shows orthorhombic spliting and b) at 290K the symmetry is tetragonal.

The high quality data recorded during this experiment allow for the determination of the incommensurate structure and the temperature dependece of the modulation vectors. Such data analysis is currently in progress.