ESRF	**Experiment title:** Incommensurate structure in $BaCuSi_2O_6$ under high pressure and low temperature	**Experiment number**: HC 2802
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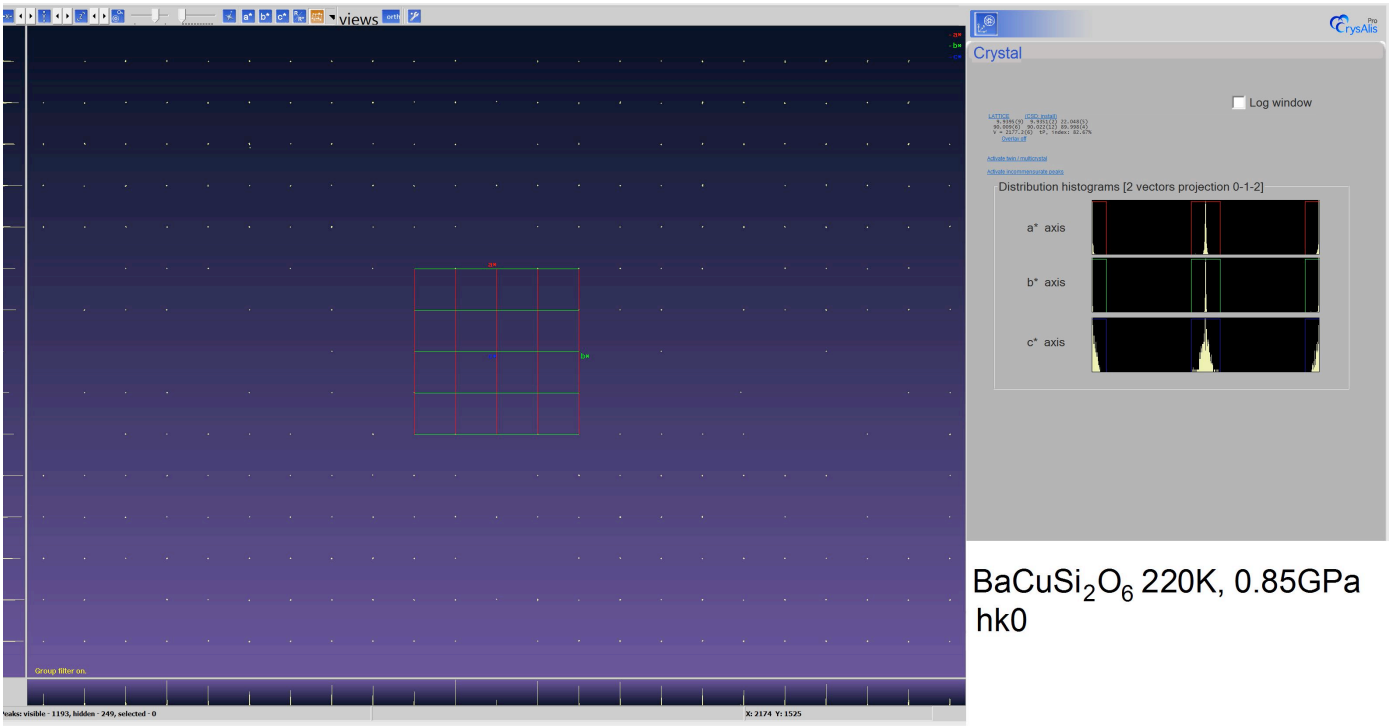
Report:

In our experiment, we have measured the equation of the state and the development of the incommensurate structure modulation in $BaCuSi_2O_{6\pm\delta}$ at high/moderate pressures and at low temperatures. This detailed study by means of single crystal diffraction as a function of temperature and pressure on $BaCuSi_2O_{6\pm\delta}$ single crystal samples elucidated the change of the incommensurable structure depending on temperature and pressure, and revealed a phase transition dependence on pressure. It is verified that the incommensurate modulations are susceptible to the application of external pressure. Furthermore, the phase transition from the tetragonal to the orthorhombic structure is shifted to higher temperature under application of external pressure.

The investigated samples are $BaCuSi_2O_{6\pm\delta}$ single crystals, grown with $LiBO_2$-flux with a size of 35x35x10µm. We used He loaded diamond anvil cells (culet diameter 500 µm). Temperature was controlled by a He flow cryostat. Measurements were performed in a pressure range between 0.5 to 2.5GPa and at temperatures between 60K and 300K. We have used monochrome X-rays of with $\lambda = 0.3738$ Å and collected data in an angular range of -35° and +35°.

The phase transition from tetragonal phase (structure - $I4_1/acd$) to orthorhombic phase (averaged structure – *I*bam at low temperature), is shifted to a higher temperature with increasing external pressure. At 0.85GPa pressure, we determined the phase transition of $BaCuSi_2O_{6\pm\delta}$ between 220K and 200K, which is in clear contrast to ambient pressure, where the phase transition appears between 100K and 80K. In Figure 1, we show the *hk0* reconstructed reciprocal space plane for both temperatures.

a)



b)

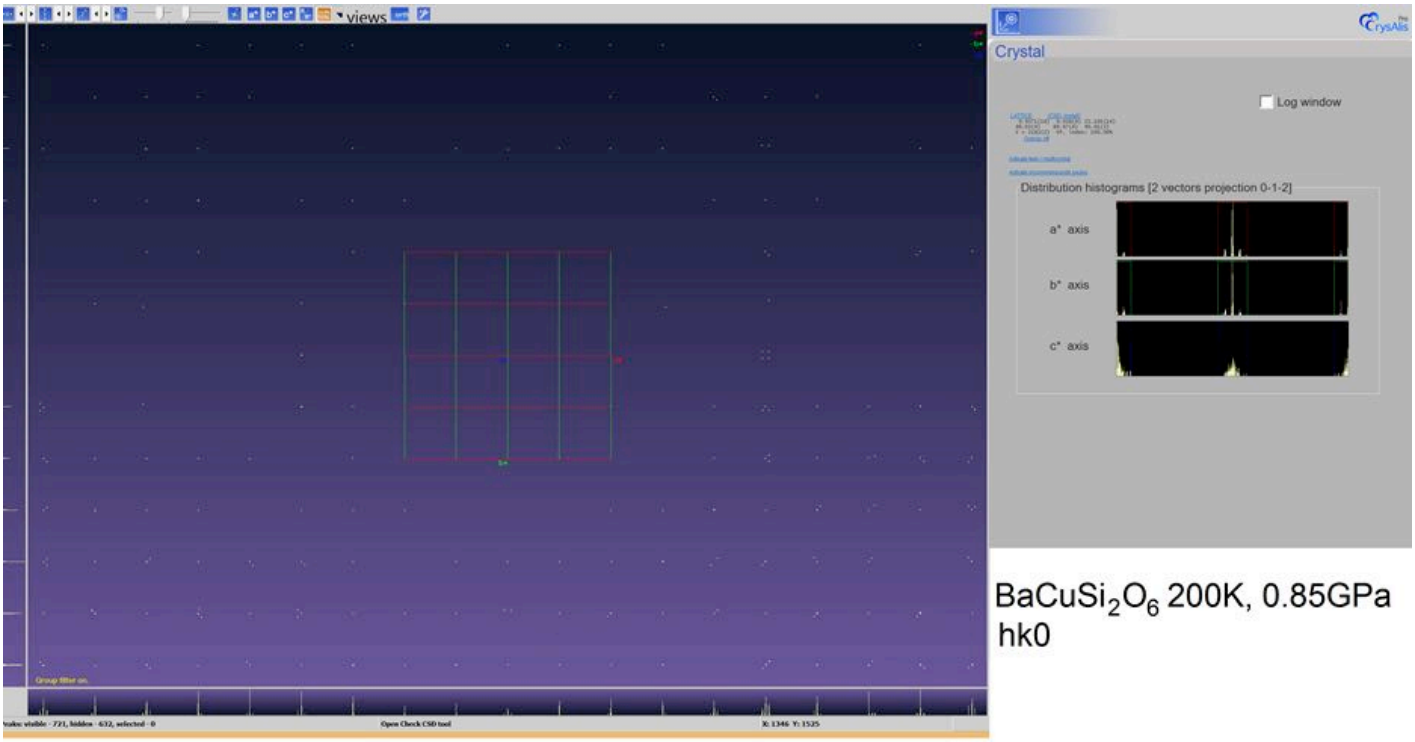


Figure 1: The experimental (*hk0*) reciprocal space plane of $BaCuSi_2O_{6\pm\delta}$ reconstructed from synchrotron x-ray diffraction data (ID27@ESRF) a) at 220K and b) at 200K, which show the phase transition between 220K and 200K.

The pressure dependence of the incommensurate modulation is investigated at a constant temperature of 140K, where we successively increase pressure. A change of the modulation vector is not observed. However, a phase transition to a new phase is observed at P = 2.49GPa and a temperature of 140K. An angular integrated image is shown in Figure 2). The phase transition is not reversible down to 0.85GPa, applying the same temperature 140K. In Figure 2 you can see the comparison of the structure at temperature 140K, using a pressure of 0.85GPa and 1.29GPa.

a)

b)

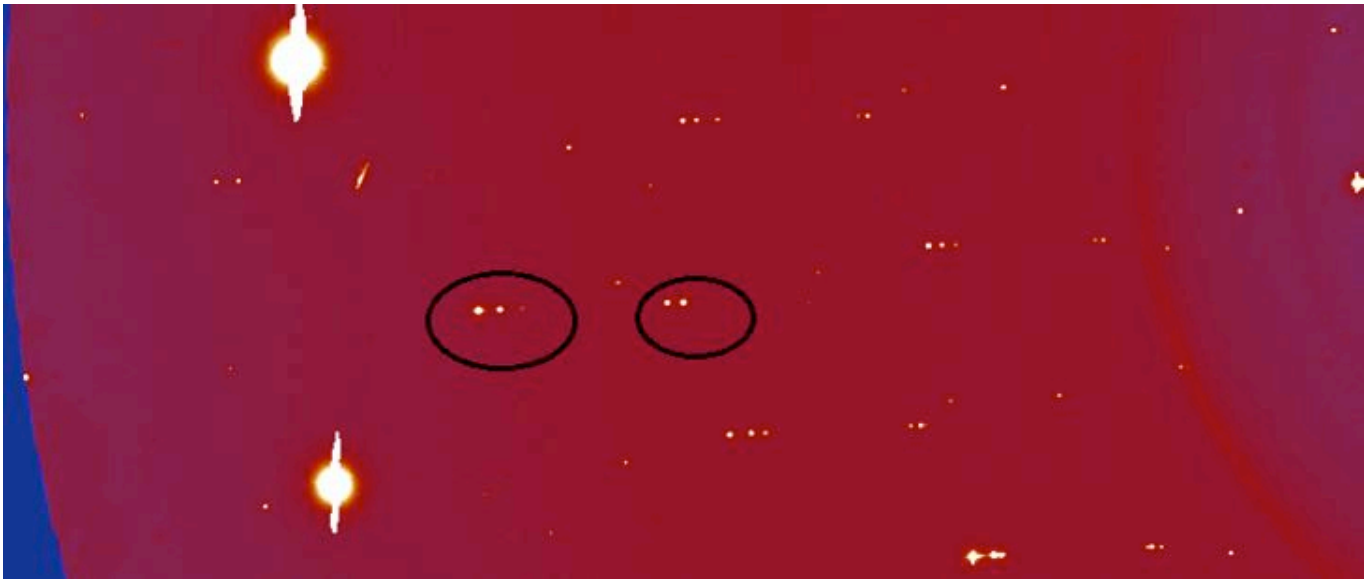


Figure 2: Angular integrated (-35° to 35°) of $BaCuSi_2O_{6\pm\delta}$ at 140K, at a) P = 0.85GPa, b) P = 1.29GPa.

In summary, we have established the equation of the state and gained a detailed knowledge of the incommensurable structure in $BaCuSi_2O_{6\pm\delta}$ at moderate pressures and low temperatures. The results help to understande and solve the solution of the structure at low temperature, which is in progress, and the magnetic interaction of the Cu – dimer system for the experiments under extreme conditions.