ESRF	**Experiment title:** In-situ high pressure x-ray diffraction and Rietveld refinement of $MgSiO_3$ analog material $NaMgF_3$	**Experiment number**: HS-2780
Beamline: ID-27	**Date of experiment**: from: 9th June 2005 to: 11th June 2005	**Date of report**: 27th Feb. 2006
Shifts: 9	**Local contact(s)**: Wilson Crichton	*Received at ESRF:*

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Report:

This experiment was very sucessful and the beamline contacts were very helpful. Data we collected during this experiment has allowed us to perform in-situ Rietveld refinement on perovskite and post-perovskite phases of $NaMgF_3$ and we have been able to:

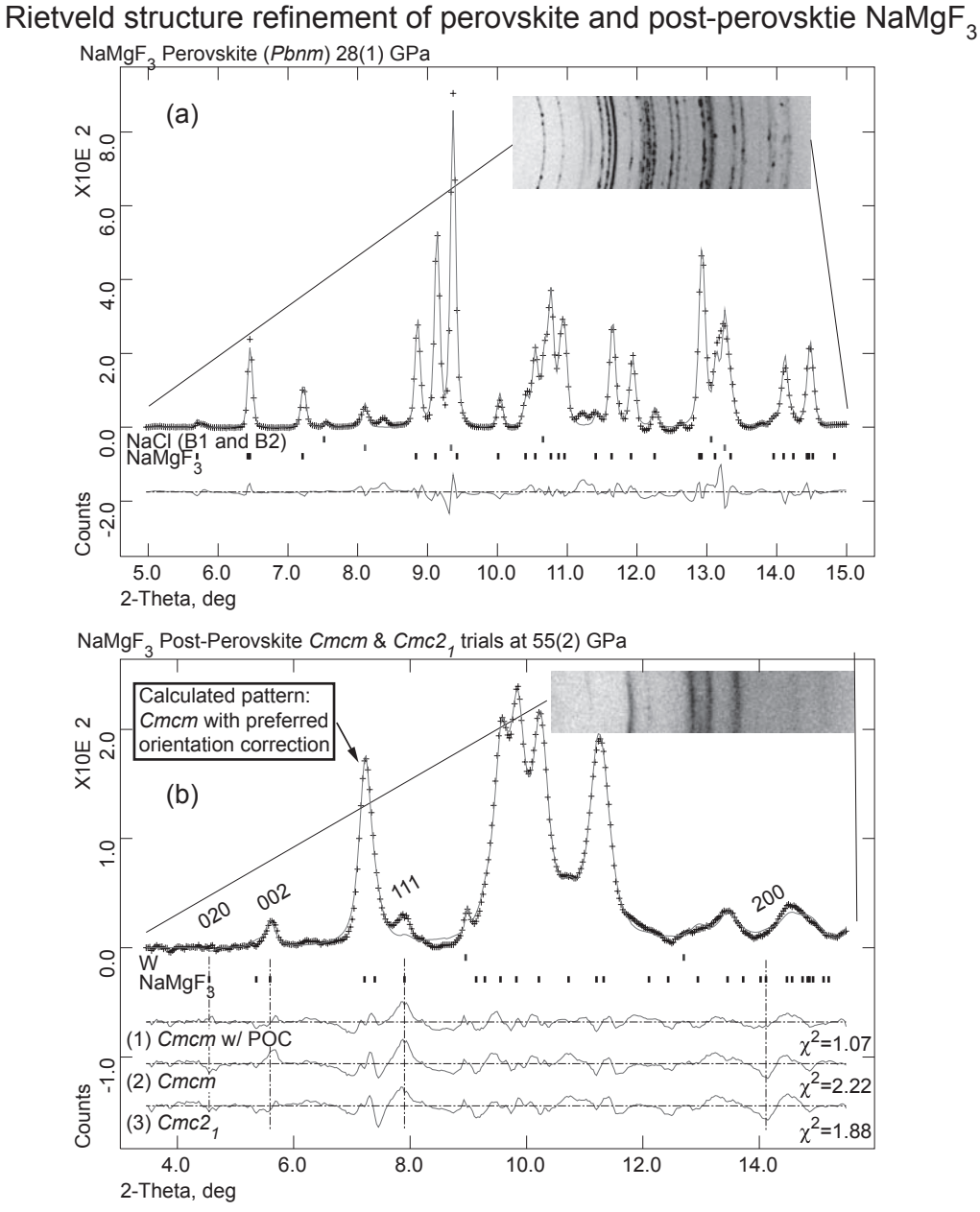
1) Identify the MgF_6 octahedra tilting angles and V_A/V_B ratio in the critical high pressure structure of $NaMgF_3$.
2) Test the strength and validity of the *Cmcm* structure model of post-perovskite $NaMgF_3$.

These results will soon be submitted to either Geophysical Research Letters or a journal highlighting Rietveld structure refinement.

Abstract

Recent work finds perovskite structured Neighborite ($NaMgF_3$) transforms to a post-perovskite phase between 28 and 30 GPa. Using monochromatic x-radiation within the diamond anvil cell, we perform Rietveld structure analysis on data from the critical perovskite as well as the post-perovskite structure of

$NaMgF_3$. We find the V_A/V_B ratio of $NaMgF_3$ spans from 5 in the high temperature cubic perovskite phase to 4 in the critical perovskite phase, matching the V_A/V_B value in post-perovskite $NaMgF_3$. By exploring Rietveld structure models of post-perovskite $NaMgF_3$, we find evidence to support the true structure of $NaMgF_3$ may exist as *Cmc2₁* a non-isomorphic subgroup of *Cmcm*, the space group describing the structure of $CaIrO_3$.



In-situ high pressure Rietveld structure modeling of (a) NaMgF3 perovskite and (b) post-perovskite NaMgF3. Portions of the raw two-dimensional data are inset in each plot to show sample texture. Difference curves of Rietveld structure models are plotted below the calculated (solid) and observed (dotted) background-subtracted x-ray diffraction patterns; (b) in descending order: (1) *Cmcm* with 4th order spherical harmonic preferred orientation correction (POC), (2) *Cmcm* without POC, (3) *Cmc2₁* without POC.
The volume calculated (a) for NaCl at 28(1) GPa is 119.1(1) $Å^3$ for B1 (Z=4) and 28.5(1) $Å^3$ for the B2 phase (Z=1).