

Experiment title: Structural changes of NaV_2O_5 at pressures up to 30 GPa

Experiment number:
HS809

Beamline:
ID9

Date of Experiment:
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Date of Report:
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Shifts:
9

Local contact(s):
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Report:

The experiments have been very successful. A paper has been written on the crystal structure results for NaV_2O_5 . The paper has been accepted for publication in the Physical Review B - Rapid Communications Section. The abstract is reproduced below.

Structural Properties of NaV_2O_5 under High Pressure

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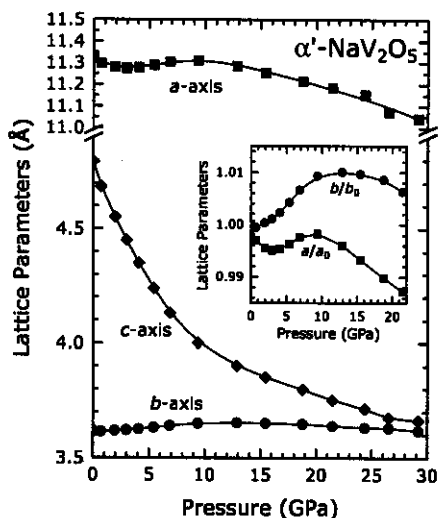
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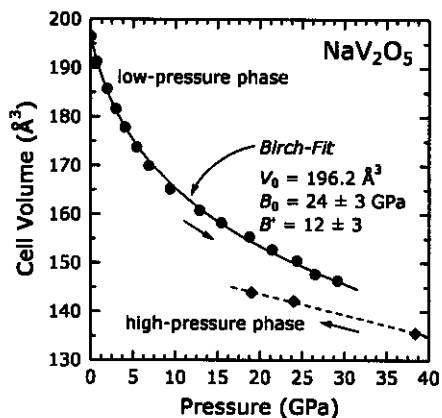
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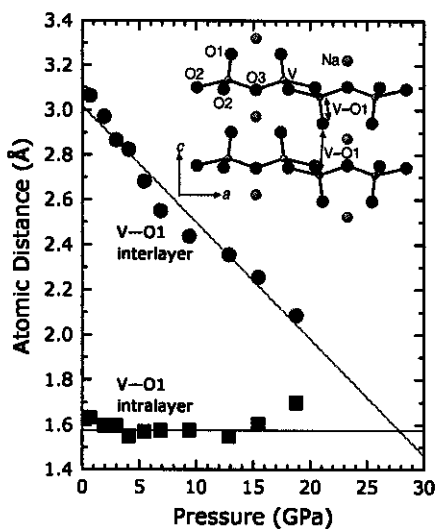
We have investigated the structural properties of NaV_2O_5 under hydrostatic pressure up to 38 GPa at ambient temperature by high-resolution angle-dispersive x-ray powder diffraction. The compression is highly anisotropic with the *c* direction being the soft axis. The pressure dependences of all three axes exhibit pronounced nonlinearities including negative compressibility for the *a* and *b* axis. A reversible structural phase transition towards a pseudotetragonal monoclinic phase starts near 25 GPa and is completed at 35 GPa. Full-profile refinements of the diffraction data provide the internal structural parameters for the low-pressure phase, showing that the structure evolves from a pyramidal towards an octahedral coordination of the vanadium ions.



Lattice parameters of $\alpha - \text{NaV}_2\text{O}_5$ (low-pressure phase) as a function of pressure. Solid lines are guides to the eye. The inset depicts the *relative* changes of a and b .



Unit cell volume of NaV_2O_5 as a function of pressure. The solid line refers to a fitted Birch relation.



Pressure dependence of the intra- and interlayer V-O1 distance.