

**Experiment title:**Compressibility and phase transition in lanthanide copper oxides Nd_2CuO_4 and LaNdCuO_4 **Experiment number:**
HS-124**Beamline:**

ID09

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9

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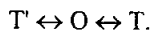
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Report:

The pressure evolution of Nd_2CuO_4 (tetragonal T' type) has been studied at room temperature from 1 atm. to 36 GPa in a membrane-type DAC with nitrogen as pressure transmitting medium. From the results of the data analysis several pressure domains have been determined, which involve the following reversible phase transitions :



Due to kinetic problems, these domains are significantly shifted from one another at increasing and decreasing pressure.

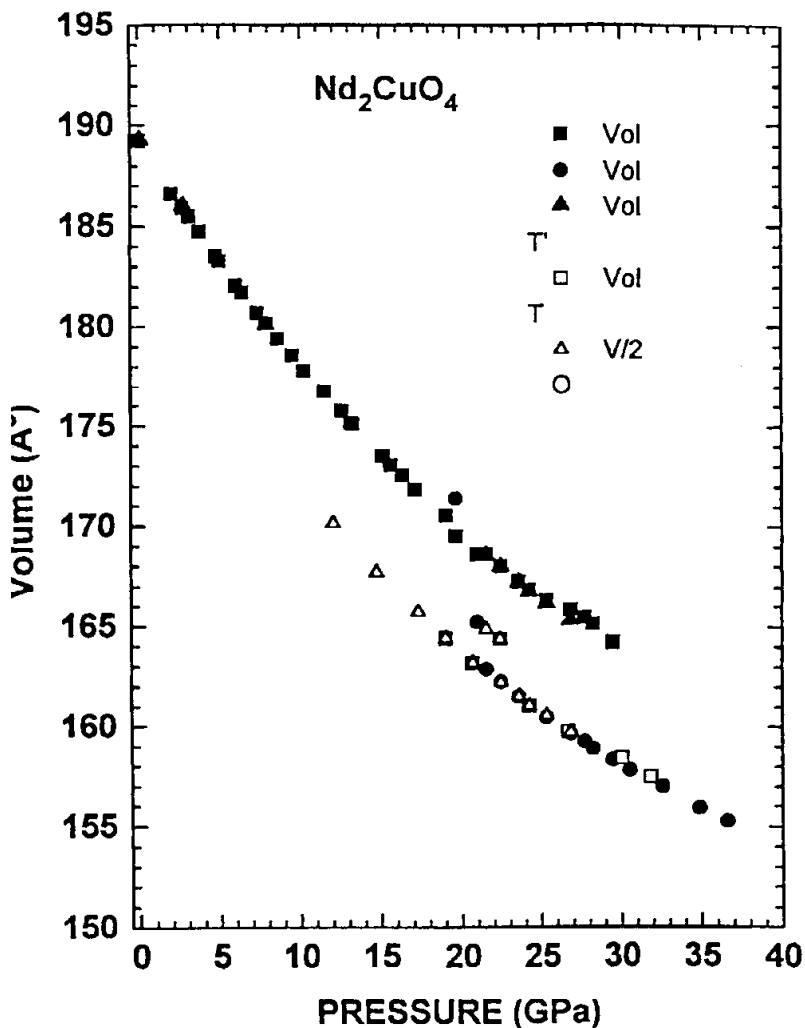
At increasing pressure the T' form of the structure is maintained up to 20 GPa and the decrease of the c/a ratio from 3.086 at 1 atm. to about 3.00 at 20 GPa shows that the compressibility is anisotropic. In the pressure range 21-30 GPa, new diffraction lines appear, which involve the gradual transformation into the T form (normal K_2NiF_4 -type structure), with the possible formation of some amounts of the O form (orthorhombically distorted K_2NiF_4) between 21 and 24 GPa. Above 30 and up to 36 GPa, the highest pressure attained the single T form is observed.

At decreasing pressure the T form is maintained down to 19 GPa. In the pressure range 19-12 GPa a gradual splitting of some lines indicate a clear and progressive distortion into the orthorhombic O form. Finally, the T' low pressure form is restored below 8 GPa.

From the refinement by the Rietveld method of the XRD data, very accurate values of the pressure evolution of the unit-cell parameters and volume of the T', 0 and T forms of Nd_2CuO_4 have been determined, as well as the interatomic distances in T' and T forms (Fig.).

These results will be published in details in a near future.

During the allocated shifts, we had not time to study the pressure evolution of the other compound, LaNdCuO_4 , because of problems of hydrostaticity in the first two runs of Nd_2CuO_4 when a mixture of methanol and ethanol was used as pressure transmitting medium.



FIGURE

Pressure evolution at increasing and decreasing pressure of the unit-cell volume of the T' (tetragonal Nd_2CuO_4 -type), 0 (orthorhombically distorted K_2NiF_4 -type) and T (normal K_2NiF_4 -type) forms of Nd_2CuO_4 .