ESRF	**Experiment title:** Hydrostatic pressure induced lattice distortions and possible phase separation in the $YBa_2Cu_4O_8$ (Y124) superconductor	**Experiment number**: CRG SNBL-BM01A 01-02-778
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Report:

We have measured high quality fully refineable angular-dispersive synchrotron powder diffraction patterns under high hydrostatic pressure (up to ~**14GPa** a with a ~ 0.5GPa step) of the **$YBa_2Cu_4O_8$ (Y124)** superconductor which is a model compound for the under-doped high T_c superconducting cuprates. In order to compare the pressure-induced lattice distortions on other related cuprates, we have also collected corresponding patterns of the optimally doped **$YBa_2Cu_3O_y$ (Y123)** superconductor (which has a very similar structure to Y124), the non-superconducting isostructural to Y123 **$PrBa_2Cu_3O_y$ (Pr123)** system, and the parent compound **$La_{2-x}Sr_xCuO_4$ (x=0.0, 0.15)**. The data have been collected both on pressure increase and on decompression using a diamond anvil cell and a 4:1 methanol- ethanol mixture as a pressure medium. 2D diffraction images have been recorded with a wavelenght λ= 0.7117Å using a MAR345 image plate detector and have been converted to 2θ patterns after correcting for distortions and refining the detector distance using a LaB_6 standard by fit-2d.[1] The intensity-*vs* 2θ patterns have been analyzed with the Rietveld method using Fullprof.[2]

The purpose of the experiments was to study lattice distortions and possible pressure-induced phase separation effects such as were previously anticipated by micro-Raman studies in the **Y123** and **Y124** compounds.[3,4] In these measurements it was observed that the Raman spectral modifications upon application of an external pressure, follow closely the pressure dependence of the superconducting transition temperature of the corresponding compounds.[3,4] Those changes can be attributed to charge transfer from the chains to the planes, its redistribution between the Cu-O plane ions, and the separation into phases. To this context we were planning to investigate slight structural modifications and lattice distortions that correlate with pressure modifications of T_c in order to contribute to our understanding of the high temperature superconductivity mechanism.

Structural high pressure studies in these compounds previously reported to our measurements were limited either to low pressures (up to 0.6GPa)[5] or by the low resolution of the energy dispersive diffraction method used in the experiments.[6] The corresponding structural studies of the Y124 compound as a function of pressure gave only marginal evidence that the changes of the lattice parameters and bond lengths follow the non-linear pressure depencence observed for T_c above 4GPa.[7,8]

Our measurements of high quality synchrotron powder diffraction patterns with a dense sampling over an extended pressure range (a ~ 0.5GPa pressure step up to ~14GPa) have revealed a clear deviation of the structural parameters from the expected equation of state that correlates with phase separation effects.

The results for the **Y123** compound have been published in our paper :

Pressure-induced phase separation in the Y123 superconductor

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Abstract – We study the hydrostatic pressure dependence of the Y123 lattice by synchrotron angle-dispersive powder diffraction up to 12.7GPa in order to detect any lattice instabilities or phase separation observed by Raman measurements. In the pressure range (3.7GPa<p<10GPa) mainly the c-axis (and to a smaller extend the a-, b-axis) undergoes a clear deviation from the expected equation of state. Upon the pressure release the data follow the anticipated dependence showing a strong hysteresis. At the pressure of ~3.7GPa new peaks appear in the diffraction patterns, which can be attributed to another apparently coherent phase that exhibits enhanced disorder and texture effects. The intensity of the new peaks decreases with increasing pressure and upon pressure release they disappear for p<3.9GPa. The in-plane Cu-O_{pl} bonds, the Cu2- Cu1 distance and the fractional coordinate of Ba atom along the c-axis of the Y123 phase show modifications at characteristic pressures in complete agreement with the Raman measurements under pressure, strongly indicating a pressure-induced lattice instability and phase separation.

Similar structural features, which correlate with Raman spectra modifications (measured in parallel in the laboratory of NTUA) have been obtained for the other cuprates under investigation. Fig. 1 shows the appearance of new lines for *p*>3.5GPa in the diffraction pattern of the hydrostatically compressed **Y124**. The pattern analysis indicates a similar lattice distortion as in the case of the Y123. A paper comparing the pressure-induced lattice instabilities in Y124 and the other studied compounds is under preparation.

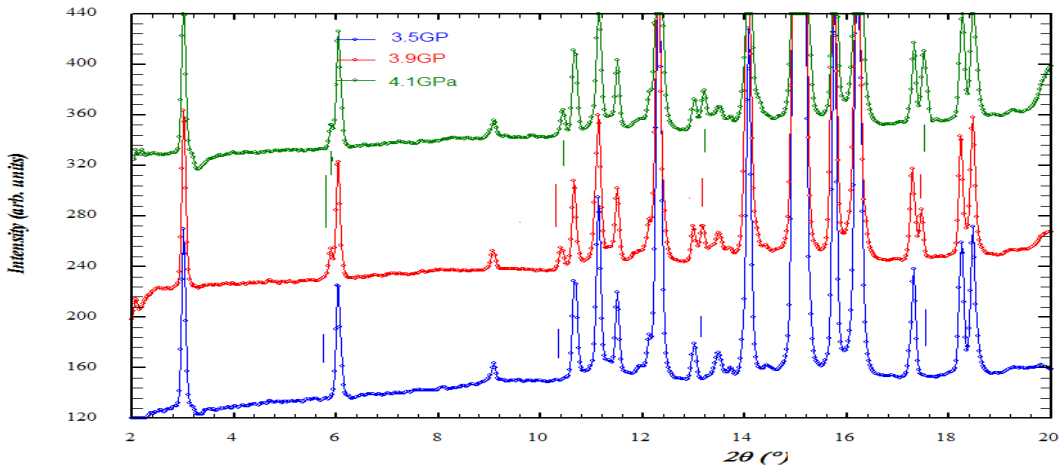

Fig.1 XRD patterns (λ=0.7117Å) of the Y124 compound at 3.5, 3.9 and 4.1GPa.

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