	Experiment title: XAFS Study of Superconducting PrBa ₂ Cu ₃ O _{7-x}	Experiment number: HE 838
Beamline: BM 29	Date of experiment: from: 10-May 2000 to: 17-May 2000	Date of report: 30-Aug.-2000
Shifts: 21	Local contact(s): Dr. Bowron	<i>Received at ESRF:</i>
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Report: We have measured as a function of temperature (25 - 300 K) the Pr and Ba *K*-EXAFS from several polycrystalline samples of PrBa₂Cu₃O_{7-x}, $x \approx 7$, (Pr-123) synthesized by the modified polymeric precursors (MPP) method [1,2]. Two batches of Pr₆O₁₁ were scanned for reference purposes. Some of these Pr-123 (MPP) samples, for example # PBCO-II, have been found to exhibit unusual physical properties compared with Pr-123 samples from the standard preparation routes: a tetragonal unit cell with $a = 3.9057 \text{ \AA}$, a strongly elongated c - axis of 11.8035 \AA , and most interestingly below 90 K a diamagnetic deviation of about 8% from a modified Curie-Weiss law $\chi = \chi_0 + C/(T+\theta)$, where $\theta = -4.5 \text{ K}$, and the Curie constant $C = 0.5274 \text{ emu K/mol}$ [1]. A similarly small Curie constant is also extracted from the susceptibility data of Zou et al. [3] showing superconductivity in a piece of a single crystal grown by the traveling-solvent floating-zone method (TSFZ). It is suggested that the lanthanide site in this material is not fully occupied by Pr, but at half by nonmagnetic Ba [4]. The large ionic size of Ba partially substituting Pr by would give a natural explanation of the elongated c - axis, too.

Our analysis of the local atomic structure (using FEFF6) from both, the Pr -, and Ba - EXAFS of sample PBCO-II yields no evidence for significant structural deviations from the nominal 123 - structure. Neither evidence is found for Pr/Ba anti-site disorder, nor evidence

for partial substitution of Pr by Ba. These findings corroborate the Rietveld refinements of the x-ray diffraction data [1] showing only 2% of a BaCuO₂ impurity. We have also extracted the T -dependence of the average plane dimpling (spacing of the Cu₂ and O_{2,3} planes) from the well resolved multiple scattering signals at $R = 5 \text{ \AA}$ and 6.2 \AA [6]. We find the average dimpling in PBCO-II to be 0.25 \AA , and independent on temperature as recently observed in slightly underdoped Y-123 [6], $x = 6.81$. The individual out-of-plane displacements of Cu₂ and O_{2,3} in PBCO-II however behave very differently from those in superconducting Y-123 [6]. While the temperature dependency of the Cu₂ and O_{2,3} out-of-plane displacements in Y-123 tends to saturate for $T < 120 \text{ K}$, it exhibits a nearly quadratic increase in Pr-123 (MPP, PBCO-II). The detailed analysis of the data is in progress.

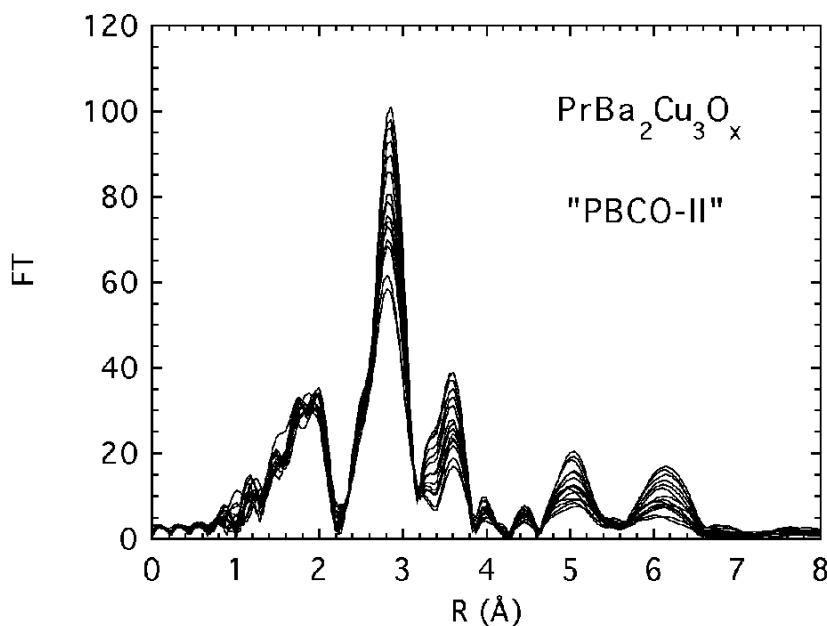


Fig. 1 Fouriertransform spectra of the Pr K - EXAFS ($k = 2.2 - 16.2 \text{ \AA}^{-1}$) in Pr-123 (PBCO - II. MPP) from $T = 35$ to 280 K . The spectra correspond within about 5% to those calculated from the nominal crystallographic structure of Pr-123. No evidence is found for Pr/Ba anti-site disorder. Pr only occupies the lanthanide site.

High energy EXAFS around 42 KeV can be reliably scanned at BM 29 using the (311) cut of the monochromator crystals. Although the absorption contrast of the interference function, and hence the S/N is reduced by almost a factor of two compared with the Y-EXAFS of Y-123, high quality data are obtained up $k = 22 \text{ \AA}^{-1}$. The effects of beam harmonis however are still important, and special care is necessary to suppress them.

Literature:

- [1] P.N. Lisboa Filho, PhD-Thesis, Universidade Federal de São Carlos-UFSCar (1999).
- [2] F.M. Araujo-Moreira, P.N. Lisboa Filho, S.M. Zanetti, E.R. Leite, W.A. Ortiz, *Physica* **B284**, 1034 (2000).
- [4] Z. Zou, J. Ye, K. Oka, Y. Nishihara, *Phys. Rev. Lett.* **80**, 1074 (1998).
- [5] V.N. Narozhny, S.L.Drechsler, *Phys. Rev. Lett.* **82**, 461 (1999), comment to Ref. 4.
- [6] J. Röhler, S. Link, K. Conder, E. Kaldis, *J. Phys, Chem. Sol.* **59**, 1925 (1998).