EXAFS Study of Oxygen Distortions in Gd2CuO4 as Function of Temperature and Pressure

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Abstract: We studied the temperature and pressure dependence of the oxygen distortion in the Cu-O planes of the Gd_2CuO_4 T'-phase, employing the Gd-L_{III} EXAFS.

1. INTRODUCTION:

Superconductivity and structural properties are closely related in the so-called 2-1-4 systems of tetragonal La_2CuO_4 (T-phase) or Nd_2CuO_4 (T'-phase) type. In the n-doped T'-phase series, $RE_{2-x}M_xCuO_4$ with RE = Nd, Sm, Eu and M = Ce, Th, superconductivity is observed, but not in the corresponding Gd-system. A possible reason for the absence of superconductivity is the distortion of the oxygen positions in the Cu-O planes, as evidenced by XRD studies [1], by Gd-155 Mössbauer effect [1,2] and by neutron scattering [3]. Here we studied in T'-phase Gd_2CuO_4 the temperature (18 K - 300 K) and pressure (up to 4 GPa) dependence of the oxygen distortion in the Cu-O planes employing the Gd-L_{III} and Cu-K EXAFS [4].

2. EXPERIMENTAL DETAILS, RESULTS AND DISCUSSION:

The measurements were performed at the EXAFS-II beamline at HASYLAB (DESY, Hamburg) employing a Si(111) double crystal monochromator and a focussing Au mirror. The high-pressure studies were performed with a diamond-anvil cell and in-situ pressure determination employing the ruby fluorescence [4]. We found that the Gd-L_{III} EXAFS is more sensitive than the Cu-K EXAFS to detect changes of the O(1) positions [5]. Due to the rather complex surrounding of Gd in the Gd_2CuO_4 structure (Fig. 1), multishell analyses of three Gd-O, one Gd-Cu and one Gd-Gd distance, including also all multiple scattering paths up to 4.8 Å, were employed using the FEFF 5.05 program [6].

Fig. 2a exhibits the multishell fits of the backtransformed Gd-L_{III} $\chi(k)$ spectra at various temperatures and pressures. These fits are very sensitive to the O(1) positions; only a splitting in two distances Gd-O(1)' and Gd-O(1)" yielded excellent fits. From the two Gd-O(1) distances shown in Fig. 2b one derives a distortion of the O(1) positions in the a-b plane from the tetragonal structure, which agrees perfectly with results of a recent neutron scattering study of Gd_2CuO_4 at 300 K [3]. Our EXAFS results demonstrate that the oxygen distortion is practical temperature independent, and therefore not connected with the magnetic ordering in the Cu-O(1) planes around 270 K. On the contrary, the distortion decreases strongly with pressure as shown in Fig. 2b. From an extrapolation one may conclude that the O(1) distortion disappears around 7 GPa and may even speculate that superconductivity is observed at such pressures in n-doped Gd_2CuO_4. We finally want to mention that the analysis of the second cumulants of the Gd-L_{III} and Cu-K EXAFS reveals a detailed picture of the anisotropic in-plane vibrations of the O(1) oxygens.

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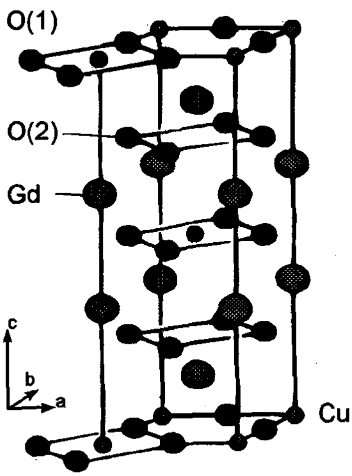

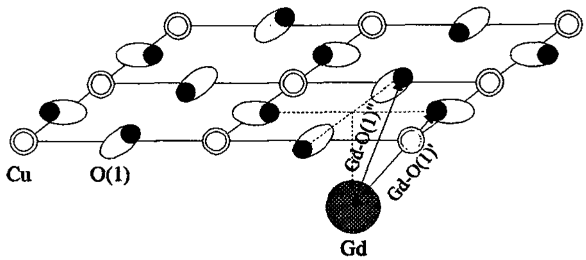

Fig. 1 (left) Structure of Gd_2CuO_4 and (right) Cu-O plane and oxygen distortion (from Ref. 1).

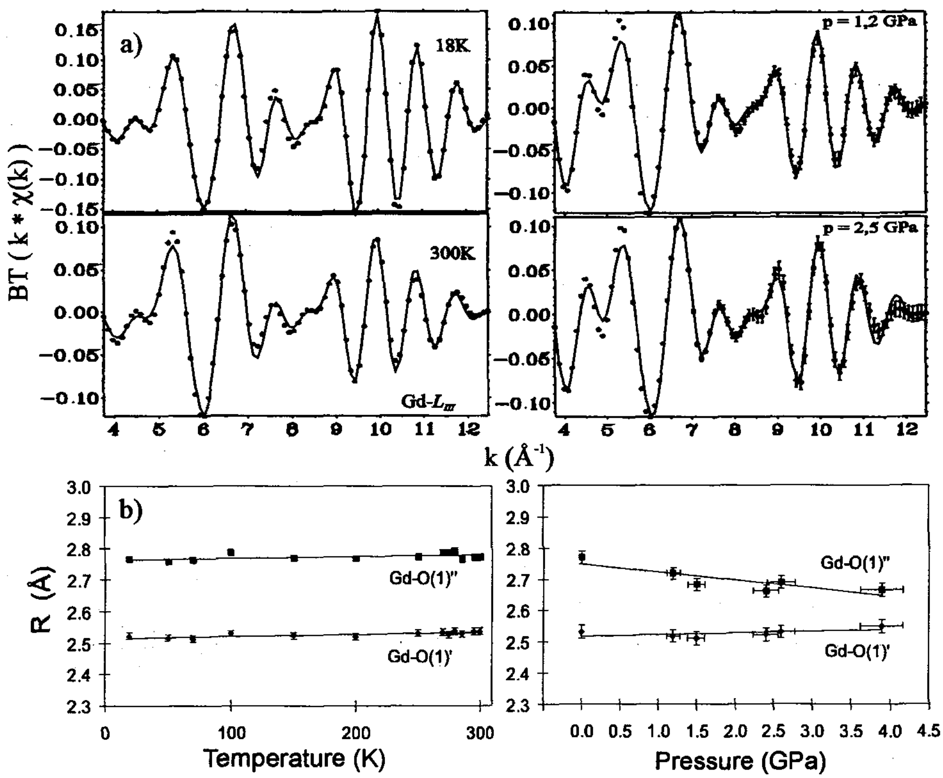

Fig. 2(a) (upper part): Backtransformed $\chi(k)$ spectra of Gd_2CuO_4 at various temperatures at ambient pressure (left) and at various pressures at room temperature (right). **2(b)** (lower part): Temperature (left) and pressure (right) dependence of the Gd-O(1)' and Gd-O(1)" distances, reflecting the oxygen distortion in the Cu-O(1) plane.