Oxygen superstructures throughout the phase diagram of \((Y, Ca)Ba_2Cu_3O_{6+x}\)

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In order to understand the origin of the diffuse scattering which is observed in the \(YBa_2Cu_3O_{6+x}\) compounds, we have investigated \((Y, Ca)Ba_2Cu_3O_{6+x}\) compounds with different charge carrier concentrations ranging from underdoped to overdoped compounds, as well as at the \(YBa_2Cu_3O_8\) compound, which is naturally underdoped and does not sustain oxygen defects. Starting point was the optimally doped \(YBa_2Cu_3O_{6.92}\), where diffuse scattering was observed at 1/4 positions, corresponding to a new 'ortho-IV'-phase.

The experiments were conducted at BW5 using high-energy x-rays of a photon energy of 100keV. The samples were mounted in a Displex cryostat capable of reaching temperatures up to 500K. As monochromator, a Si-Ge gradient crystal was used so that maximum flux was obtained.

In Fig. 1a, b, scans along \((h, 0, 5.5)\) for an underdoped \(YBa_2Cu_3O_{6+x}\)-compound with \(T_C = 67\)K is compared with the same scan for the optimally doped compound \(YBa_2Cu_3O_{6.92}\) \((T_C = 92.7)K\), as well as the \(Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.95}\) compound. The reflections of the optimally doped ortho-IV compounds are much broader than the ones of the underdoped, ortho-III compound, indicating a shorter correlation length. In Fig. 1c, \(l\)-scans at \(T=10K\) and room temperature are compared. Mesh scans of \(YBa_2Cu_3O_{6.92}\) and \(Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.95}\) samples were collected. In Fig. 3 and Fig. 4 reciprocal space maps of \(Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.95}\) are shown for the \((h, k, 5.5)\)-plane and the \((h, 0, l)\)-plane. They are identical to the ones of \(YBa_2Cu_3O_{6.92}\), as already suggested by Fig.1b. Both samples have the same oxygen content but \(Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.95}\) is strongly overdoped due to the Ca substitution, whereas \(YBa_2Cu_3O_{6.92}\) is optimally doped. This means, the charge carrier concentration in the CuO\(_2\)-planes is strongly increased for \(Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.95}\) compared to the optimally doped sample. Any diffuse features related to electronic stripe formation in the CuO\(_2\)-planes should be sensitively dependent on the charge carrier concentration. Thus, since in both samples diffuse reflections at identical positions in reciprocal space are observed, we can draw the conclusion, that the diffuse superlattice reflections originate from oxygen vacancy ordering and subsequent lattice distortions and are not related to stripes. This is supported by the fact that for the \(YBa_2Cu_3O_8\) compound no superlattice reflections were found.

In addition, the temperature dependences of the ortho-V, ortho-III and ortho-IV peaks were investigated. The integrated intensities are shown in Figs. 2a-c. Whereas for the ortho-V and ortho-III samples scans along \(h\) were performed, as shown in the insets, the integrated intensity of the optimally doped sample was obtained from \(l\)-scans over the diffuse peaks, as shown in Fig. 1c. This allows the most reliable subtraction of the background. These temperature dependences further confirm that all features originate in oxygen ordering rather than charge instabilities in the CuO\(_2\) layers. Independent of the doping level, the superstructures persist well above room temperature, with no anomalies observed at the superconducting transition temperature or other temperatures associated with the onset of electronic instabilities. The intensity variation observed in Ref. [1] is clearly outside the statistical variation of the data of Fig. 2a. Rather, the intensity of the diffuse features is reduced smoothly upon heating and vanishes around 400-450 K. Prior work in samples with \(0.5 \leq x \leq 0.8\) has shown that in this temperature range, oxygen order is obliterated due to progressively rapid oxygen diffusion [2].

References

Figure 1: (a) Scans along \((h, 0, 2.5)\) for the ortho-III phase \((x \sim 0.75)\), (b) \((h, 0, 5.6)\) scan for both YBa\(_2\)Cu\(_3\)O\(_{6.92}\) (●) and Y\(_{0.8}\)Ca\(_{0.2}\)Ba\(_2\)Cu\(_3\)O\(_{6.95}\) (○) (c) \(l\)-scans of YBa\(_2\)Cu\(_3\)O\(_{6.92}\) at both T=10K and T=300K along \((4.25, 0, l)\). The insets in a) and b) show the ortho-III and ortho-IV patterns.

Figure 2: Temperature dependences of the integrated intensity of (a) the \((4.4, 0, 2.5)/(4.6, 0, 2.5)\) reflections in YBa\(_2\)Cu\(_3\)O\(_{6.65}\), (b) the \((4.33, 0, 2.5)/(4.66, 0, 2.5)\) reflections in YBa\(_2\)Cu\(_3\)O\(_{6.75}\) and c) the \((5.25, 0, 5.6)\) reflections in YBa\(_2\)Cu\(_3\)O\(_{6.92}\). The insets in (a) and (b) show the respective Q-scan at low temperature.

Figure 3: Contour plot of the diffuse intensity in the \((h, k, 5.5)\)-plane of Y\(_{0.8}\)Ca\(_{0.2}\)Ba\(_2\)Cu\(_3\)O\(_{6.95}\). The main Bragg reflections are masked.

Figure 4: Contour plot of the diffuse intensity in the \((h, 0, l)\) scattering plane of Y\(_{0.8}\)Ca\(_{0.2}\)Ba\(_2\)Cu\(_3\)O\(_{6.95}\).