SESSION 3

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New aspects of Ca doping in 123

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Recent investigations of Ca doped 123 give a quite different picture, contrasting the generally accepted properties:
1) Very accurate oxygen determinations (Ax = + 0.001) of fully oxidized samples show that the oxygen content does not decrease linearly but oscillates stepwise between x = 6.980 and 6.966. up to 17% Ca. The question arises if these oscillations are due to phase transitions.
2) EXAFS measurements of the same samples (Röhler et al. 1999) do not find changes in the pair distribution function of Ca-doped and O-doped 123 up to a radius of 5 A, opening the question if Ca is at all incorporated in the lattice. The decrease of T_c and the data of the average crystallographic structure (Böttger et al. 1996) show of course clearly that this is the case. To solve this discrepancy, Röhler proposed that Ca is dissolved in the 123 lattice as a monodisperse solution i.e. in the form of single Ca-123 unit cells surrounded by Y-123. This cloud of Y-123 cells surrounding completely each Ca-cell is probably shielding the holes introduced by Ca, so that they could remain localized. In this case the observed decrease of T_c would come not from increase of the mobile holes but on the contrary from their decrease, due to the decreasing Y-123 units with Ca doping.
3) NEXAFS investigations (Merz et al. 1998) show that Ca doping introduces holes only in the planes, whereas O-doping both in the plains and chains (apical oxygen). The later seems necessary for changes of T_c. This supports the above idea that Ca-holes are localized and do not contribute to superconductivity.

Keywords: *Ca-doping in 123, oxygen content of Ca-monodisperse solution in 123.*

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Local lattice distortions in $YBa_2Cu_3O_y$ single crystal: phase separation and pseudogap opening

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In our previous work [1], using oriented $YBa_2Cu_3O_y$ thin films grown on $SrTiO_3$ substrate, the in-plane lattice distortions around copper atoms in the CuO_2 plane has been probed by polaized X-ray absorption spectroscopy (XAS). We find that the LTT-like tilting of CuO_5 pyramids occurs below T*, spin- or charge-excitation gap opening temperature. The hole concentration dependence, although limited in Tc range (55-78K), suggested that the onset temperature of lattice distortion which indicates the coexistence of distorted and undistorted domains coincides or at least is lower than T*. The average radial distribution of oxygens around copper atoms in $YBa_2Cu_3O_y$ varies in a similar manner with that of $La_{1.85}Sr_{0.15}CuO_4$ where a charge-lattice stripe is observed [2]. Because of insufficient data quality due to substrate scattering and limited film thickness (100nm), however, a clear relation between the local lattice distortion and pseudogap opening has not been confirmed.
In this paper, the results of polarized XAS for $YBa_2Cu_3O_y$ single crystals [3] will be reported, for which the polarization vector is chosen to be parallel with the c-axis. We find that *the copper-oxygen correlations for optimaly doped samples (Tc=90K) shows a strong distortion exactly at T** (120K), consistent with the previous in-plane experiment but with much larger magnitude. Such a large variation of the oxygen radial distribution function is in agreement with a correlated tilting model [1] where CuO_5 pyramids belonging to separate CuO_2 planes of the unit cell, connected by a rigid O1-Cu1-O1 linkage, tilt with an anti-phase correlation. Results of detailed analysis of polarized XAS, in particular, the hole concentration dependence (Tc=50-90K) will be reported. The results demonstrate that local lattice distortion occurs at T*, indicating that the charge segregation and/or ordering (stripe) appears to be closely related to the change of the Fermi surface as discussed by Kamimura et al. [4].

This work has been conducted as a collaboration with T. Haage, J. Zegenhagen, K. Oka, A.M. Moe, T. Ito, S. Tajima and T. Masui, A. Bianconi and N. L. Saini.

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Dynamic charge inhomogeneities in underdoped cuprates from the atomic pair distribution function

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The possible importance of stripes of charge and spin to the high temperature superconductivity phenomenon is clearly of great current interest. However, when the stripes are not long range ordered they become hard to detect since there is no superlattice in diffraction experiments: they are dynamic and only short-range ordered. It is exactly in this dynamic regime where superconductivity occurs. The charge stripes couple to the lattice producing a modulated structural distortion and therefore a superlattice. When they are short-range ordered, the local distortion must survive even though the superlattice does not. We show that in underdoped but superconducting $La_{2-x}A_xCuO_4$ (A=Sr,Ba,Nd), charge inhomogeneities are evident in the *local atomic structure,* studied using the atomic pair distribution function (PDF) analysis of neutron powder diffraction, consistent with the presence of fluctuating stripes. These disappear in the overdoped regime. The charge inhomogeneities appear with decreasing temperature in the temperature range 60-150 K depending on the sample composition. In Nd codoped samples they appear at 60 K close to the long-range charge ordering temperature. We will discuss evidence for local charge inhomogeneities in a number of different systems.

Keywords*: Pair distribution function, neutron diffraction, local structure, charge stripes, high temperature superconductivity.*

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Quantum chemical studies on the doping mechanism in cuprate superconductors

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Cuprate super-conductors are hole doped by replacement of cations with less charge ions or by introducing vacancies, or by putting excess oxygen atoms. We have simulated the doping process by a quantum chemical calculation on model clusters by changing the charges on the cluster or by removing the counter ions. A detailed analysis on the electronic structure revealed that unpaired electrons, which may give metallic state, are produced on the O pi and the (Cud_{x2-y2} - O sigma) orbitals at doped site. This result is in conformity with a one-dimensional band structure of under doped cuprates recently found by photo-emission spectroscopy. Nature of magnetic excitation will be discussed based on this calculation.

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Pressure effect and specific heat of RBa$_2$Cu$_3$O$_x$ at distinct charge carrier concentrations: possible influence of stripes

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In $YBa_2Cu_3O_x$, distinct features are found in the pressure dependence of the transition temperature, dT_c/dP, and in the jump of the specific heat, $\Delta C/T_c$, at x_S and x_Q: dT_c/dP peaks at x_S and is zero at x_Q, whereas $\Delta C/T_c$ shows a maximum at x_Q and becomes small below x_S. Substituting Nd for Y and doping with Ca leads to a shift of both x_S and x_Q to larger and smaller oxygen contents, respectively, since content and order of oxygen in these compounds are quite different. Using the hole concentration n_h in the CuO_2 planes at x_S and x_Q, which can be calculated from the parabolic $T_c(n_h)$-behavior, the features coalesce at $n_h(x_S) \approx 0.11$ and $n_h(x_Q) \approx 0.18$, irrespective of substitution and doping. Hence, this behavior seems to reflect an intrinsic property of the CuO_2 planes. A charge carrier content of $n_h \approx 0.18$ is usually attributed to the appearance of the pseudogap and $n_h \approx 0.11$ close to 1/8 may express a localization of charge carriers as predicted for stripe correlations. In order to clarify whether the features at $n_h(x_S) \approx 0.11$ and $n_h(x_Q) \approx 0.18$ are connected to stripe formation and the occurrence of the pseudogap, respectively, we additionally investigated the influence of Zn doping on dT_c/dP and found a completely different behavior of $dT_c/dP(n_h)$.

Keywords: *specific heat, pressure effect, charge-carrier concentration, doping.*

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