Structure of $LaSrCuO_{3.5}$

Joke Hadermann[a], N. Creon[b], O. Perez[b], C. Michel[b], M. Hervieu[b],
[a]*EMAT, University of Antwerp, Belgium* [b]*ISMRA-CNRS Caen, France.*
E-mail: joke.hadermann@ua.ac.be

The oxygen deficient $La_{1.07}Sr_{0.93}Cu_{0.92}O_{3.52}$ has been synthesized and the structure has been determined using a combination of transmission electron microscopy, X-ray diffraction and neutron diffraction.

X-ray diffraction showed a basic K_2NiF_4 type structure of a=3.7583(3) Å and c=13.005(3) Å in space group *I4/mmm*. However some reflections remained unexplained. Therefore electron diffraction was performed which showed the presence of an incommensurate modulation and allowed the detemination of the superspacegroup and modulation vectors as *I4/mmm(αα0, α-α0)00mg*, q_1=0.22a* + 0.22b* and q_2=0.22a*-0.22b*. Following these observations neutron diffraction was used to determine the origin of these modulations.

The five-dimensional model obtained using the super space formalism shows oxygen-vacancy ordering, implying three different environments present for the copper in the structure: octahedral, pyramidal and square plane coordination. Significant displacements in the (a,b) plane occur for all atoms, no displacement is observed along the c-axis.

High resolution electron microscopy images support the model.

Keywords: incommensurate structures, copper oxides, structural determination