MS21-P3 **Structure modulation and charge ordering in selfdoped $M_x CuO_2$ crystals** <u>Ognjen Milat</u>, Kreso Salamon, Tomislav Ivek, Tomislav Vuletić, Silvia Tomić *Institute of Physics, Zagreb, Croatia*
e-mail: <u>milat@ifs.hr</u>

An electron diffraction study of a number of rare earth cuprates $M_x CuO_2$, is presented (for M_x = Ca$_{.83}$, Sr$_{.73}$, Ba$_{.67}$, [Sr/Ca$_2$Cu$_2$O$_3$]$_{.70}$). These cuprates belong to class of composite crystals consisting of two subsystems [1]: „CuO$_2$-chains" and „M$_x$". These subsystems are interpenetrated, mutually modulated, and usually incommensurate along the chain direction. The lattices of these subsystems have common ***a*** and ***b*** parameters while the ratio of parameters along chains ***c_M/c_{Ch}*** varies with 1/x. For M_x = [(Ca/Sr)$_2$Cu$_2$O$_3$]$_{0.7}$, it is the case of "chain-ladder" compound: (Sr/Ca)$_{14}$Cu$_{24}$O$_{41}$. It is well known because of exotic interaction, ordering and dynamics of electron holes and spins within either of the two constituting subsystems [2],[3]. Various level of self doping (also related to nonstoichiometry x) affects Cu-valency to vary in the range from +2.66 for Ba$_{.67}$CuO$_2$ to +2.30 for Ca$_{.85}$CuO$_2$, and even to +3.0 in NaCuO$_2$, and +2.0 in Li$_2$CuO$_2$. In the case of [(Sr/Ca)$_2$Cu$_2$O$_3$]$_{.70}$CuO$_2$, the average Cu valency is +2.25, but for all excess charge distributed in the CuO$_2$-chains, the Cu valency should be: +2.6 on „chains" (+2.0 on „ladders"). In addition Cu^{+2} carries spin ˝ while Cu^{+3} is nonmagnetic. La for Sr substitution strongly affects crarge distribution and spin depletion in CuO$_2$-chains resulting with no excess charge in La$_6$Ca$_8$Cu$_{24}$O$_{41}$. On the other hand, our electron diffraction study of „chain-ladder" compounds reveals that it is only the amplitude of displacive modulation of basic crystal structure that is slightly affected by charge and spin ordering [4].

[1]   Milat O., Van Tendeloo G., Amelinckx S., Mebhod M., Deltour R. (1992), *Acta. Cryst.*, **A48**, 618-625.
[2]   T. Ivek, T. Vuletić, B. Korin-Hamzić, O. Milat, and S. Tomić, at all (2008) Phys. Rev. **B78**, 205105.
[3]   T. Vuletić, B. Korin-Hamzić, T. Ivek, S. Tomić, B. Gorshunov, M. Dressel, J. Akimitzu (2006), Phys. Rep. **428**, 169-258.
[4]   O. Milat, K. Salamon, S. Tomić, T. Vuletić, T. Ivek (2011) Proceedings of the 10th MCM2011, Urbino, Italy, September 4-9th, 2011, ed. E. Falcieri, SISM 2011, pp 41

Keywords: composite crystal, electron diffraction, charge ordering

---

MS21-P4 **Standard and non-standard settings of superspace groups.** <u>Sander van Smaalen</u>,[a] Harold T. Stokes[b] and Branton J. Campbell,[b] [a]*Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany,* [b]*Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA*
E-mail: <u>smash@@uni-bayreuth.de</u>

Tables of $(3+d)$-dimensional [$(3+d)$D] superspace groups have recently been generated by us for d = 1, 2, 3 [1]. The table for d = 1 is in agreement with previous tabulations of (3+1)D superspace groups [2]. The tables for d = 2 and 3 define for the first time a standard setting for each superspace group. The tables are available as the online data repository SSG(3+d)D at http://stokes.byu.edu/ssg.html [3]. Part of SSG(3+d)D is a utility, 'findssg,' which returns the standard setting of a superspace group for any user-given superspace group, along with the transformation between the two settings.

The relation between two settings of a superspace group can be described by an appropriate transformation of the external-space lattice vectors (the basic-structure unit cell) along with a transformation of the internal-space lattice vectors (new modulation wave vectors are linear combinations of the old modulation wave vectors plus 3D reciprocal lattice vectors). Here we introduce the nomenclature of $(3+d)$D superspace groups and explain the unique four-part number assigned to each group. We discuss the need for non-standard settings in some cases and the desirability of employing standard settings of superspace groups in other cases [4]. These features are illustrated by the analysis of the symmetries of a series of compounds, comparing published and standard settings and the transformations between them. A compilation is provided of standard settings of superspace groups of compounds with two- and three-dimensional modulations. The problem of settings of superspace groups is discussed for incommensurate composite crystals and for chiral superspace groups.

[1]   Stokes, H.T., Campbell, B.J. & van Smaalen, S. (2011). Acta Crystallogr. A **67**, 45-55.
[2]   van Smaalen S. (2007): Incommensurate Crystallography (Oxford University Press, Oxford).
[3]   Stokes, H.T., Campbell, B.J. and van Smaalen, S. (2011). SSG(3+d)D at http://stokes.byu.edu/ssg.html Provo, Utah, USA.
[4]   van Smaalen, S., Stokes, H.T., Campbell, B.J. (2012). In preparation.

Keywords: superspace groups; aperiodic crystals; incommensurate crystals