m14.p08

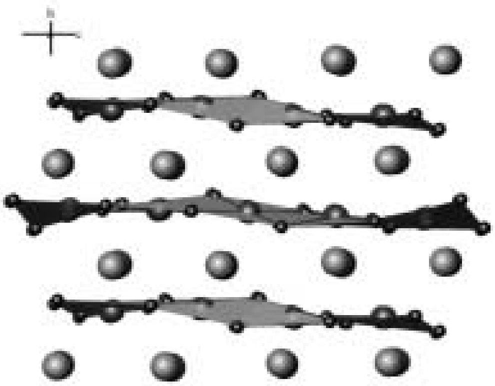
Neutron structure investigation of $Ca_2Y_2Cu_5O_{10}$

Jörg Thar[a], Ralf Müller [b], Stefan Mattauch[c], Bernd Büchner[c], Georg Roth[a]

[a]Institute of Crystallography, RWTH Aachen University, Germany. [b]Carl Zeiss SMT AG, Germany. [c]Institute of solid state research, FZ Jülich, Germany. [d]Institute of solid state research, IFW Dresden, Germany.E-mail: thar@xtal.rwth-aachen.de

Keywords: neutron and X-ray diffraction, composite structures, float zone growth

$Ca_2Y_2Cu_5O_{10}$, a calcium yttrium cuprate, is the yttrium rich end member of a homologous series of compounds with composition $(Ca_{1-x}Y_x)_4Cu_5O_{10}$ ($0 \leq x \leq 0.5$) [1]. According to the chemical formula the formal charge of copper can be varied between +2 and +2.4. The structure is incommensurate and related to the structure of $NaCuO_2$ [2]. In both case the central structural elements are one dimensional Cu-O chains. According to the x-ray experiments we found a Ca/Y disorder. Instead of having 5 Na and 5 Cu positions in the quintupled supercell in the case of $NaCuO_2$ there are 4 Ca/Y and 5 Cu positions in the supercell of $Ca_2Y_2Cu_5O_{10}$. Therefore Ca/Y positions and Cu-O chains have to be rearranged and distorted. Single crystals were grown in an optical floating zone furnace and were examined by single crystal diffraction experiments (x-ray and neutron scattering). Structure refinement was done with Shelxl-97 [3] (supercell: $P2_1/c$, a=5.4730(10)Å, b=6.1801(10)Å, c=14.081(2)Å, β=104.550(14)°, z=2) and 3+1dimensional with Jana2000 [4]. As a result of the neutron experiment we got the cell metrics of both composite parts and the associated q vectors. One can describe one composite part as $P2_1/c(\alpha 0 \lambda)00$ (a=5.474(5)Å, b=6.181(9)Å, c=2.,818(7)Å, β=104.87(15)°), the other one as $P2_1/m(\alpha 0 \lambda)0s$ (a=5.458(5)Å, b=6.181(9)Å, c=3.523(9)Å, β=104.24(15)°). The associated q vectors are (-0.0177 0 0.8) and (0.0221 0 1.25). On the poster a detailed description of the contents of the composite parts, positions of the atoms and distortion of the Cu-O chain will be given.



[1] Davies, P. K.; Caignol, E.; King, T. *J. Am. Ceram. Soc.*, 1991, 569-573.
[2] Davies, P. K. *J. Sol. Stat. Chem.*, 1991, 365-387.
[3] Sheldrick, G. M. *Shelxl-97*, 1997, Universersity of Göttingen, Germany.
[4] Petricek, V.; Dusek, M.; Palatinus, L. *Jana2000*, 2000, Institute of Physics, Praha, Czech Republic.

m14.p09

On the symmetry of magnetic structures in terms of the fibre bundles

Jerzy Warczewski, Pawel Gusin

University of Silesia, Institute of Physics, ul. Uniwersytecka 4, PL-40007 Katowice, Poland. e-mail: warcz@us.edu.pl, pgusin@us.edu.pl

Keywords: fibre bundles, symmetry of magnetic structures, aperiodic structures

To describe symmetry of magnetic structures in terms of the fibre bundles one needs in general two 3-dimensional spaces, namely $\mathbf{R_3}$ and a vector space $\mathbf{V_3}$. One needs also a corresponding relationship between these two spaces. It is well-known that the fibre bundles as a generalization of the Cartesian product of two given spaces present the most general way to relate them. As a result of such a relationship one obtains a 6-dimensional space $\mathbf{E_6}$. This space has the structure of a **fibre bundle** with $\mathbf{R_3}$ as a **base space** and with $\mathbf{V_3}$ as a **fibre**. In such a case $\mathbf{R_3}$ is the position space of the magnetic structure, while $\mathbf{V_3}$ is spanned by the orthogonal unit vectors $\mathbf{e_1}$, $\mathbf{e_2}$, $\mathbf{e_3}$ and makes the space of the magnetization vector. In the simplest case of a trivial bundle the space $\mathbf{E_6}$ presents the Cartesian product of the $\mathbf{R_3}$ and $\mathbf{V_3}$. In this formalism a magnetic structure can be represented as a certain subspace **S** of $\mathbf{E_6}$. In terms of the fibre bundles the subspace **S** is called the **section of $\mathbf{E_6}$**. Thus a certain symmetry group of **S** determines the corresponding magnetic symmetry group. Therefore the problem of formulating the different magnetic symmetry groups consists in searching the corresponding symmetry groups of **S**. Every such a symmetry group has to conserve a given structure defined by the magnetization vector. Moreover a magnetic symmetry group in this approach makes the **structure group of the bundle $\mathbf{E_6}$.** For the illustration of the above approach a ferromagnetic, an antiferromagnetic, both different spiral magnetic structures and spin waves as well as fan structures have been considered (see also [1] where the different magnetic structures have been found by the authors to be related with the values of certain topological invariants). This approach can serve for the determination of all the other magnetic symmetry groups as well as for the determination of the symmetry groups of all the other aperiodic structures, like the modulated nonmagnetic structures, quasicrystals etc. On the other hand this approach can be treated as a kind of the generalization of the wreath groups method by Litvin [2, 3].

[1] P. Gusin, J. Warczewski, JMMM, Vol. 281/2-3 (2004) 178-187
[2] D. Litvin, Phys. Rev. B, Vol. 21, Number 8, (1980) 3184-3192
[3] D. Litvin, Physica 101A (1980) 339-350