

**PS10.04.33 5D SUPERSTRUCTURE MODEL OF DECAGONAL Al-Ni-Co QUASICRYSTALS.** Akiji Yamamoto, Steffen Weber\*, National Inst. Res. Inorg. Mat. Namiki 1, Tsukuba, 305 Japan, \*Institute of Applied Physics, University of Tsukuba, Tsukuba, 305, Japan, An Pang Tsai, Institute for Materials Research, Tohoku University, Sendai, 980 Japan

A superstructure has been found in decagonal Al-Ni-Co quasicrystals (Edagawa, Ichihara, Suzuki and Takeuchi, *Phil. Mag. Lett.*, 66 (1992) 707). This has a unit cell volume 5 times larger than that of the normal phase. We proposed a model for this superstructure (Hiraga, Sun and Yamamoto, *Mat. Trans. JIM*, 35 (1994) 657) based on HRTEM images, where the clusters are arranged at vertices of a Penrose pattern with edges of about 20 Å (3D model). In this paper, we construct the corresponding 5D model of such a superstructure by the section method. In cluster models, we consider small occupation domains which generate the cluster centers. In the present case, these are 4 pentagons situated at  $(i, i, i, z)/5$  ( $i=1, 2, 3, 4$ ) in the 5D decagonal lattice. Atoms around the centers can be obtained by shifting these domains along the external space. It can be shown that all atom positions in the 3D model can be obtained from the occupation domains around 20 points in the 5D unit cell of the superstructure. Its space group is  $P10_5/mcm$ . Their site symmetry is  $2/m$ . This means that two of them are independent. Each independent occupation domain consists of several small ones as mentioned above and has an irregular shape with the symmetry of  $2/m$ . Thus the 5D model is quite different from 5D structures of known decagonal quasicrystals. It is however remarkable that the number of independent sites is two and many other positions are related to them by symmetry operations. This model gives reasonable point density and chemical composition.

## Materials V

### High T<sub>c</sub> Superconducting Materials

**MS10.05.01 HIGH T<sub>c</sub> SUPERCONDUCTORS AND RELATED OXIDES : HIGH PRESSURE PHASES.** Mikio Takano, Institute for Chemical Research, Kyoto University.

High T<sub>c</sub> cupric oxide superconductors and related quantum antiferromagnets prepared at high pressures of 6GPa typically will be reviewed.

The use of high pressure generally leads us to new phases through pressure-induced changes in structure and/or chemical composition of ambient pressure phases and also through stabilization of novel compositions and structures. All these cases can be seen for cupric oxides.

Superconductors prepared at high pressure are featured by the multiplicity of the 2D CuO<sub>2</sub> sheets (e.g. (Sr, Nd)CuO<sub>2</sub> and CuBa<sub>2</sub>Ca<sub>3</sub>Cu<sub>6</sub>O<sub>14</sub>), inclusion of 2D CuO<sub>2</sub> sheets capped with halogen atoms (e.g. (Ca, Na)CuO<sub>2</sub>Cl<sub>2</sub> and Sr<sub>2</sub>Ca<sub>2</sub>Cu<sub>3</sub>O<sub>8</sub>F<sub>2</sub>), etc. Many other new phases will be prepared in near future.

The speaker's group is now more involved in a research of spin-ladder compounds. SrCu<sub>2</sub>O<sub>3</sub> and LaCuO<sub>2.5</sub> prepared at 3-6GPa contain two-leg ladders, the legs and the rungs of which are CuO chains and Cu-O-Cu bonds, respectively. The electronic ground state of SrCu<sub>2</sub>O<sub>3</sub> has been found to be a singlet spin liquid, which is separated from the first excited magnetic state by a wide "spin gap" of 420 K. On the other hand, interladder interactions cause long range magnetic ordering in the latter oxide, though the ordering is easily destroyed by the substitution of Sr<sup>2+</sup> for La<sup>3+</sup>. Novel physics of quantum spin ladders is progressing fast.

**MS10.05.02 UNUSUAL LAYERED METAL OXIDES** Susan M. Kauzlarich, Department of Chemistry, University of California, Davis, California 95616

There are a relatively small number of transition metal pnictide oxides compounds that have been reported to date. Of these types of compounds, the Sr<sub>2</sub>Mn<sub>3</sub>As<sub>2</sub>O<sub>2</sub> structure type has the unique feature of independent metal oxide and metal pnictide layers which form a

1:1 intergrowth. The structure and properties of compounds which crystallize in this structure-type will be presented along with new results in this area.

**MS10.05.03 LAYERED CUPRATES.** Kenneth Poeppelmeier, Department of Chemistry and Science and Technology Center for Superconductivity, Northwestern University, Evanston, Illinois 60208

Layered copper-oxide superconductors exhibit the highest critical transition temperatures of any materials. Yet all the known double perovskites A'A''B'B''O<sub>6</sub> containing copper have a random or rock salt distribution of the B cations with the exception of the unique layered arrangement found in La<sub>2</sub>CuSnO<sub>6</sub>.<sup>1</sup> Only the layered arrangement contains the CuO<sub>2</sub><sup>2-</sup> planes which are necessary for high-temperature superconductivity. The occurrence of layered or two-dimensional structures increases markedly when vacancies are introduced on the oxygen sublattice. Similarities among oxygen-deficient structures, especially those with two-dimensional solid-state features, will be discussed.<sup>2</sup> Combined conductivity and thermopower analysis will be presented to elucidate the unique internal chemistry, defect structure, and conduction parameters associated with the quadruple perovskites La<sub>2</sub>Ba<sub>2</sub>Cu<sub>2</sub>Sn<sub>2</sub>O<sub>11</sub>, La<sub>2</sub>Ba<sub>2</sub>Cu<sub>2</sub>Ti<sub>2</sub>O<sub>11</sub> and LaYBa<sub>2</sub>Cu<sub>2</sub>Ti<sub>2</sub>O<sub>11</sub>.<sup>3,4</sup> The similarities of layered Cu-Sn and Cu-Ti perovskites to high-T<sub>c</sub> cuprates will be presented.

1. M. T. Anderson, K. R. Poeppelmeier, S. A. Gramsch, and J. K. Burdett, *J. Solid State Chem.*, **102**, 164 (1993).

2. M. T. Anderson, J. T. Vaughey, and K. R. Poeppelmeier, *Chem. Mater.*, **5**, 151 (1993).

3. P. A. Salvador, L. Shen, T. O. Mason, K. B. Greenwood and K. R. Poeppelmeier, *J. Solid State Chem.*, **119**, 80 (1995).

4. K. B. Greenwood, G. M. Sarjeant, K. R. Poeppelmeier, P. A. Salvador, T. O. Mason, B. Dabrowski, K. Rogacki, and Z. Chen, *Chem. Mater.*, **7**, 1355 (1995).

**MS10.05.04 Hg-BASED SUPERCONDUCTING Cu MIXED OXIDES.** E. V. Antipov<sup>1</sup>, S. N. Putilin<sup>1</sup>, E. M. Kopnin<sup>1</sup>, V. A. Alyoshin<sup>1</sup>, A. M. Balagurov<sup>2</sup>, S. M. Loureiro<sup>3</sup>, J. J. Capponi<sup>3</sup>, M. Marezio<sup>4</sup>. <sup>1</sup>Dpt. of Chemistry, Moscow State University, Moscow 119899 Russia; <sup>2</sup>Lab. of Neutron Physics, JINR, Dubna, Russia; <sup>3</sup>Lab. de Cristallographie CNRS, BP 166, 38042 Grenoble France; <sup>4</sup>MASPEC, Parma, Italy

The arrangement of the (CuO<sub>2</sub>) layers in the HgBa<sub>2</sub>Ca<sub>n-1</sub>Cu<sub>n</sub>O<sub>2n+2+δ</sub> structures is supposed to be optimal for the existence of superconductivity at high temperatures. The structure investigation of these compounds is important for understanding the superconductivity phenomenon among layered Cu mixed oxides.

The six members of the series were isolated and characterized. The third member (Hg-1223) undergoes superconducting transition at the highest T<sub>c</sub>, while the other members exhibit lower superconducting transition temperatures due to several reasons such as underdoping of the higher members and alterations of the in-plane and apical Cu-O bond lengths.

The neutron powder refinement was made for monophasic HgBa<sub>2</sub>CuO<sub>4+δ</sub> samples prepared in sealed tubes with different extra oxygen content (δ=0.055, 0.12 and 0.18) and T<sub>c</sub> (71K, 98K and 83K, respectively). No substitution on the Hg site and additional extra oxygen except the one in the middle of the mesh in the Hg-layer was found. The dependence of T<sub>c</sub> vs. δ will be discussed.

The substitutions of Hg and O atoms in the (HgO<sub>8</sub>) layer of the HgBa<sub>2</sub>CuO<sub>4+δ</sub> structure by carbonate (sulphate) group and fluorine, respectively, were studied. The different geometry or formal valence of substituents causes different variations of the structure and properties of the Hg-1201 superconductor.

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