Conference abstracts

10-Physical and Chemical Properties of Materials in Relation to Structure (Superconductors, Fullerenes, etc)

PS-10.01.14 SUPERCONDUCTIVITY AT 94 K IN A NEW Hg-BASED CUPRATE, HgBa2Cu3Ox by S. N. Putilin1, 2, E. V. Antipov1, O. Chmaissi2, and M. Maréchal3, 4, 1Chemical Department, Moscow State University, 119899, Russia, 2National Institute of Standards and Technology, Gaithersburg, Maryland, 20899, USA, 3Laboratoire de Cristallographie CNRS-UMR, BP 166, 38042 Grenoble cedex 09, France, 4AT&T Bell Labor. Hrs, Murray Hill, NJ 07974, USA.

A new high-Tc superconductor, HgBa2Cu3Ox, has been synthesized and characterized by X-ray powder diffraction, EDS analysis, scanning electron microscopy, a.c. magnetic susceptibility and electric resistivity. The latter measurements revealed a transition into a large diamagnetic state at 94 K and a drop of resistivity at the same temperature, indicating that HgBa2Cu3Ox is the first Hg-based cuprate superconductor. The estimated susceptibility signal corresponds to more than 50% of ideal diamagnetism, indicating bulk superconductivity.

The samples were prepared by solid state reaction between stoichiometric mixtures of BaCu2O4·5H2O and HgO in sealed silica tubes heated up to about 800°C during 5 h and then cooled slowly in the furnace.

The composition of this phase was confirmed by EDS analysis. The average metal ratio found for 8 measurements was Hg:Ba:Cu = 38.1(4):74.2(2):(2) with the standard deviations between parentheses. Besides Hg, Ba, Cu and O, no other element was detected on the spectra.

The X-ray powder pattern was indexed in a space group P4/mmm with the following lattice parameters: a = 3.879(5) Å, c = 9.509(5) Å. This tetragonal compound is the first member of the homologous series Hg2Ba2Cu3Ox (n = 1). The another member of this family HgBa2Cu2O6 was synthesized earlier (Putilin et al., Mat. Res. Bull., 1991, 26, 1299-1307). The value of the c-cell parameter for the different members of this homologous series can be calculated with a formula a = 9.5 + 3.7n (1) similar to that for the Tl2Ba2CuO4 compound.

The structure of Hg-1201 was refined by Rietveld analysis of powder X-ray data. The structural arrangement of Hg-1201 is illustrated by the layer sequence (CuO2)(BaO)(HgO)Cu(O)(BaO)(CuO2). It is quite similar to that of Tl2Ba2CuO4, except for the oxygen stoichiometry of the HgO and TiO layers. For the former, 5 is very small and this depletion is possible because the cumbellin coordination is appropriate for the Hg6+ cations. For the latter, the TiO6 layer is only slightly oxygen depleted, which creates the appropriate coordination for the thallium cations, either a distorted octahedron or a five-coordinate polyhedron. This different behavior for attaining the optimal hole concentration is due to the different chemical properties of the Ti3+ and Hg6+ cations.

PS-10.01.15 MAGNETIC ORDER IN THE PHOSPHIDES H2Fe12P17, Nd2Co3P17, and Ho2Co12P17. By M. Rehboi, B. Uhrdaff, T. von Hofh, and W. Jelschko, Institut Lasse-Langevin, Grenoble (France) and Anorganisch-Chemisches Institut, Universität Münster (Germany).

Magnetic susceptibility measurements with a Faraday balance show that the magnetic moments of the Co atoms of these hexagonal ZrF6-Fe12P17-type phosphides order ferromagnetically at 140 K and 152 K for Nd2Co3P17 and Ho2Co12P17, respectively, while the Fe atoms of Ho2Fe12P17 are essentially nonmagnetized (M. Rehboi and W. Jelschko, J. Phys. Chem. Solids, 1989, 50, 53-569). Our magnetization measurements of single crystals with a SQUID magnetometer and our neutron powder diffraction data show that the three Co sites with tetragonal phosphorus environments carry magnetic moments of approximately 0.2 μB, while the Co site with square-pyramidal phosphorus coordination has a moment of 0.9 μB. The hexagonal c-axis is the easy axis of magnetization for both Co compounds. The magnetic moments of the Nd atoms in Nd2Co12P17 order antiparallel to the Co moments. In contrast, in Ho2Co12P17 the Ho moments are aligned parallel to the Co moments. The magnetic order of the lanthanoid moments sets in gradually below about 60 K and thus seems to be induced by the ferromagnetic cobalt sublattice. The magnetic moments obtained from the refinements of the 2 K neutron diffraction data are 1.8 μB and 7.4 μB for the Nd and Ho atoms, respectively. They are thus smaller than the theoretical values of 3.27 μB and 10.0 μB, indicating considerable deviations from the full order for this temperature.

In Ho2Fe12P17 the Ho moments order ferromagnetically at the Curie temperature Tc = 3.3 K. The refinement of the neutron diffraction data suggests, that only one half of the Ho moments is aligned nearly parallel to the c-axis with a magnetic moment μH ≈ 7.5 μB/Ho. This value is smaller than the theoretical one of μH ≈ 10.0 μB most likely because of crystal field effects.

PS-10.01.16 CORRELATION BETWEEN TWEED TWINNING, AND FLUX PENTRATION IN YBa2Cu3Mn1-xOy. By W. W. Schmalz*, Y. R. Cho, E. Brecht, and H. Fuchs, Fachbereich Materialwissenschaft, Technische Hochschule Darmstadt, Germany.

The decrease of the orthorhombicity with increasing x in substituted YBa2Cu3Mn1-xOy (M=Mn, Co, or Al), leads to a decrease in lamellar spacing between the (110) twin walls when x approaches 0.02. The phase change to macroscopically tetragonal symmetry (x > 0.03) occurs when the twin wall spacing gets approximately equal to or smaller than the thickness of the twin walls (30-50Å). In the macroscopically tetragonal material, the (110) and (110) twin orientations interpenetrate, resulting in a cross-hatched tweed microstructure. From AC susceptibility measurements we found, that in the lamellar regime (0 ≤ x ≤ 0.03), the intergrain flux pinning force density is proportional to the spacing between twin walls, while the current remains almost constant. In the tweed regime, the pinning force density is independent of the twin wall current. Hence the twin walls are not only ineffective for flux pinning but they rather act as channels for penetration of the intergrain magnetic flux into the grains. Flux line motion in any direction is facilitated by the cross-hatched network formed by the interpenetrating (1 1 0) / (1 1 0) "twin walls" in the tweed microstructure for x > 0.03.

PS-10.01.17 ON THE STRUCTURE OF Nd3SrCu4NbO8. By L.-E. Jørgensen and N.O. Hornshøj, Department of Chemistry, University of Aarhus, DK-8000 Århus C, Denmark.