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

$NdSr_2Cu_2NbO_8$ is a perovskite type compound isostructural with $LaBa_2Cu_2NbO_8$ which contains a CuO_2-La-CuO_2 sandwich as well as NbO_6 octahedra. The structure is therefore analogous to a $YBa_2Cu_3O_{7-\delta}$ structure in which the linear Cu-O chains have been replaced by NbO_6 octahedra. $NdSr_2Cu_2NbO_8$ was prepared by firing stochiometric mixtures of Nd_2O_3, $SrCO_3$, CuO and Nb_2O_5 in air at 1070°C for 16 hours. Attempts to introduce superconductivity in $NdSr_2Cu_2NbO_8$ by substitution of Ca for Nd was unsuccesful.

The structure of $NdSr_2Cu_2NbO_8$ was studied by time of flight neutron powder diffraction. Rietveld refinements were performed in space groups P4/mmm, P4/mbm and I4/mcm. The NbO_6 octahedra are corner shared in the a,b plane and initial refinements showed that the octahedra are displaced from ideal corner sharing in such a way that neighbouring octahedra are rotated in opposite directions around the c-axis. No superlattice reflections were observed and the final refinement was therefore performed in space group P4/mmm with oxygen in the NbO layers statistically distributed over the 4n (x 1/2 0) positions.The rotation angle around the c-axis for the NbO_6 octahedra was found to be 14.4°. Although no super lattice peaks were found in the neutron data, electron diffraction indicates that the structure locally has P4/mbm symmetry. Bond lengths and bond valency sums for $NdSr_2Cu_2NbO_8$ will be compared with the corresponding quantities for high temperature superconducting cuprates.

PS-10.01.18 SUDDEN DISAPPEARENCE OF THREE-DIMENSIONAL MAGNETIC ORDERING IN Gd_2CuO_4

T. Chattopadhyay and P.J. Brown, Institut Laue-Langevin, 156X, 38042 Grenoble Cedex, France
B. Roessli, Labor für Neutronenstreuung, ETH Zürich, CH-5232 Villigen PSI, Switzerland

We have studied the magnetic ordering of Gd_2CuO_4 by neutron diffraction on isotope (^{158}Gd) enriched single crystals. Below T = 6.4 K Gd magnetic moments order antiferromagnetically with the wave vector **k** = (0,0,0). Ferromagnetic Gd layers parallel to a-b plane are antiferromagnetically stacked along [001]. Cu^{2+} ions in Gd_2CuO_4 orders at T_N = 285 K to a La_2NiO_4 type antiferromagnetic structure with the propagation vector **k** = (½,½,0). Fig. 1 illustrates the magnetic structure of Gd_2CuO_4 at 1.5 K. We have investigated the temperature dependence of the intensity of a few magnetic reflections from room temperature down to 1.5 K. The intensity of ½,½,1 magnetic reflection (Fig. 2) increases continuously with decreasing temperature up to 45 K below which it starts to decrease and shows a minimum at about 20 K. There is a further sharp anomaly at about 7 K at which the intensity of the reflection becomes practically zero. These neutron results are in agreement with the temperature variation of the magnetic susceptiblity which also shows anomalies at 7 and 20 K. Search for magnetic reflection at Q = (½,½,0), (½,½,2) and (½,½,3) and other incommensurate positions at 7 K did not reveal any magnetic intensity. These results indicate that at this temperature three dimensional ordering of the Cu sublattice disappears. Low temperature anomalies in the temperature variation of the intensity of ½,½,1 reflection obviously result from the interaction of the Cu and Gd sublattices which order with different and incomatible wave vectors. Above the ordering temperature of Gd sublattice the antiferromagnetic CuO_2 planes polarize antiferromagnetic gadolinium planes. But as the ordering temperature of Gd sublattice is approached, ferromagnetic exchange interaction becomes dominant in the Gd planes. At 7 K presumably due to this frustration effect the copper sublattice loses its three dimensional order. We

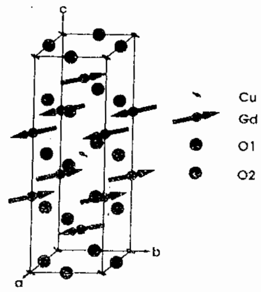

Figure 1: Magnetic structure of Gd_2CuO_4.

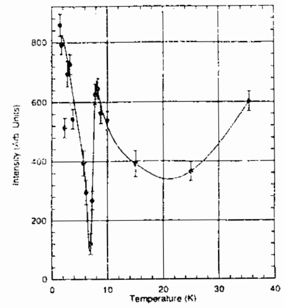

Figure 2: Temperature variation of $\frac{1}{2}\frac{1}{2}1$ reflection.

believe that two dimensional ordering of the CuO_2 must still persist due to very strong exchange coupling but the three-dimensional ordering vanishes in a narrow temperature range just above the Gd ordering temperature. As the temperature is further lowered, the copper sublattice recovers its three dimensional ordering because the antiferromagnetically stacked ferromagnetic planes now have resultant zero field on copper. To our knowledge this type of frustration induced disappearence of magnetic ordering is quite unique and has not been observed in any other magnetic system.

PS-10.01.19 STRUCTURAL FLUCTUATIONS IN METALLIC SODIUM.

By H. Abe, K. Ohshima, S. Hoshino, T. Suzuki and K. Kakurai*, Institute of Applied Physics, University of Tsukuba, Japan, *Institute for Solid State Physics, The University of Tokyo, Japan.

Metallic sodium undergoes martensitic phase transformation from bcc to 9R structure at 37 K (Ms). We have performed neutron elastic and inelastic scattering experiments from metallic sodium to understand detailed structural informations over a temperature range of 10 to 300 K. The spherical single crystal was prepared in liquid paraffin above the melting point (97°C) and gradully cooled down to room temperature. The size of the specimen was 18 mm in diameter and the mosaic spread was 20'. The data were collected with the use of a triple-axis spectrometer at the beam line 5G of JRR-3M, JAERI. Phonon dispersion curves from 200 K to Ms were measured along high symmetry directions. There were no peculiar temperature changes for TA1[110] branch. The temperature dependence of integrated intensity and full width at half maximum (FWHM) was obtained from the (110)bcc Bragg reflection. They have increased drastically at Ms due to the structural change which took place after an incubation time of the order of few hours. We also observed peculiar Huang scattering around the Bragg reflection. Above As (70-80 K), both the integrated intensity and FWHM were decreased where Huang scattering disappeared. It is thought that these phenomena are important to understand the phase transformation in metallic sodium.

