implement these applications, the availability of low-cost, long-length, and high performance superconductor wire/tape and cable is critical. Preparation of these wires/tapes involve deposition of $Ba_2RCu_3O_{6+x}$ (R-213, R=lanthanides and Y) films on biaxially-textured buffer/substrates. Two promising processes for preparing buffer/substrates are the Ion Beam Assisted Deposition (IBAD) and the Rolling Assisted Biaxially Textured Substrates Buffer (RABiTS). For a given combination of buffer layers that has been found to promote epitaxial growth of $Ba_2RCu_3O_{6+x}$, there may be unavoidable reactions at the interface between layers. Understanding of interfacial reactions of R-213 phase with the buffer layers will provide information about how to avoid and/or control the formation of second phases. Crystallographic and phase equilibrium data will assist analysis of coated conductor interfaces. This paper describes the crystal chemistry and crystallography of the multi-component systems representing the interaction of $Ba_2RCu_3O_{6+x}$ with the al, $SrTiO_3$ buffer. X-ray and neutron Rietveld refinements were employed for structural studies. Examples of phases that will be discussed include $(Ba,Sr)_3RTi_2O_{8.5}$, $(Ba,Sr)R_2CuO_5$, $(Ba,Sr)Ti_2O_4$, and $(Ba,Sr)_2RCu_3O_{6+x}$, etc.

Keywords: superconductor-substrate interface, $Ba_2RCu_3O_{6+x}$-$SrTiO_3$, coated conductors

P.11.01.6

Acta Cryst. (2005). A**61**, C386

New Molecular Conductors based on [Ni(dmid)$_2$] with TMTTF, TTF and ET as Cations

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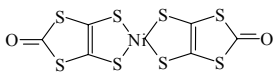
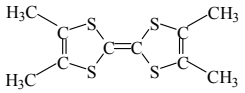
New molecular conductors based on rare π-electron acceptor [Ni(dmid)$_2$] with TMTTF, TTF and ET as cations were synthesized. Investigation of conducting properties revealed that they all are semiconductors. X-ray study of TMTTF[Ni(dmid)$_2$] was carried out.



[Ni(dmid) 2]



TMTTF

A lot of compounds have been obtained containing $[Ni(dmit)_2]^{n-}$ anion analogous to $[Ni(dmid)_2]^-$ anion, where O atom is substituted with S one. Among them are salts with organic π-donors ET, TTF, EDT etc. Some of those salts happened to be superconductors [1-2].

The new semiconducting TMTTF[Ni(dmid)$_2$] salt has a layered structure where cations and anions form mixed regular stacks.

[1] Cassoux P., Valade L., Kobayashi H., Kobayashi A., Clark R., Underhill A., *Coord. Chem. Rev*., 1991, **110**, 115. [2] Tajima H., Inokuchi M., Kobayashi A., Ohta T., Kato R., Kobayashi H., Kuroda H., *Chem.Lett*., 1993, 1235.

Keywords: organic semiconductors, structure-properties relationships, X-ray analysis

P.11.01.7

Acta Cryst. (2005). A**61**, C386

Novel Style of Structure Determination for π-d System by Synchrotron X-ray Diffraction

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Molecular conductor $(DBr\text{-}DCNQI)_2Cu$ undergoes a novel metal-insulator transition at 160K caused by π-d electron interaction, due to the simultaneous appearance of charge order in Cu ions [1] and the CDW in DCNQI molecules in the insulator phase. This phase transition is understood as a unique type of electronic instability caused by cooperation of the Peierls and Mott instabilities. However, the actual three-dimensional (3D) arrangement of these orderings has not been revealed.

In order to obtain the electron distribution in the unit cell by means of synchrotron x-ray measurements, the spatial relation between the charge ordering and the CDW was examined. The charge ordering in the Cu sites as Cu^+ Cu^+ Cu^{2+} along the stacking axis was observed by utilizing the anomalous scattering technique, consistent with previous studies. As for the CDW pattern on DCNQI columns, single crystal structure analysis was conducted.

As a result of these two x-ray experiments' combination, we successfully obtained the 3D pattern, which is different from the structure previously observed. We discuss the implementation to the mechanism.

[1] Hiraki K., Kobayashi Y., Nakamura T., Takahashi T., Aonuma S., Sawa H., Kato R., Kobayashi H., *J. Phys. Soc. Jpn.*, 1995, **62**, 1470.

Keywords: CDW, synchrotron X-ray radiation, structure analysis

P.11.01.8

Acta Cryst. (2005). A**61**, C386

Twin Formation in InP Nanowires Epitaxially Grown on Germanium and Silicon

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Semi conducting nanowires are promising for the integration of III-V based functionalities with Silicon technology. In this work the hetero-epitaxial growth of Indium Phosphide (InP) wires on Germanium and Silicon with a <1.1.1> orientation is discussed. Gold-mediated VLS growth of these wires was performed using either MOCVD or laser ablation. The epitaxial relation between wire and substrate was studied using SEM, cross-sectional TEM and X-Ray Diffraction.

On both Germanium and Silicon substrates, perfect epitaxy of InP was observed, despite the large lattice mismatch of 4% and 8%, respectively. The formation of a series of additional InP orientations was observed with X-Ray Diffraction pole figure measurements. All observed orientations could be ascribed to the presence of rotation twins in the <1.1.1> growth directions and at the substrate wire interface. The presence of some and absence of other orientations could be explained by the occurrence of multiple twinning at the initial stage of wire growth.

Keywords: twinning, iii-v semiconductors, nanowires

P.11.01.9

Acta Cryst. (2005). A**61**, C386-C387

Low Temperature Structural Investigations of the J_1-J_2 Model System $VOMoO_4$

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Frustrated magnets based on transition metal oxides have become subjects of many theoretical and experimental studies in the last ten years [1, 2]. One of the most widely studied model systems is the so-called J_1-J_2 model, i.e. the spin-1/2 Heisenberg antiferromagnet on a square lattice with competing nearest (J_1) and next-nearest (J_2) neighbor antiferromagnetic interactions. Thanks to their structure, Li_2VOSiO_4 and Li_2VOGeO_4 [3] are shown to be the first prototypes of this frustrated two-dimensional system [4, 5] and have enabled to check experimentally several theoretical predictions in the region of the phase diagram in which $J_1 \approx J_2$. This work has been extended these last two years to the closely related system $VOMoO_4$ [6]. $VOMoO_4$ crystallizes in the tetragonal space group $P4/n$ with 2 formula units per cell, the spin-1/2 V^{4+} ions forming a network of VO_5 square pyramids, sharing corners with MoO_4 tetrahedra. The main difference with respect to Li_2VOSiO_4 and Li_2VOGeO_4 (space group $P4/nmm$) is the absence of Li to separate the layers of XVO_5 (X = Si, Ge or Mo).

This contribution will give an overview of recent results obtained by low temperature x-ray and neutron diffraction on the $VOMoO_4$ phase. An anomalous evolution of the lattice parameters [7] which could be related to its magnetic properties was clearly revealed.

[1] Chandra P., et al., *Phys. Rev. Lett*., 1990, **64**, 88. [2] Capriotti L., *Int. J. of Mod. Phys.* B, 2001, **15**, 1799. [3] Millet P., et al., *Mater. Res. Bull.*, 1998, **33**, 1339. [4] Melzi R., et al., *Phys. Rev. Lett.*, 2000, **85**, 1318. [5] Melzi R., et al., *Phys. Rev.* B, 2001, **64**, 024409. [6] Eick H. A., et al., *Acta Chem. Scand.*, 1966, **20**, 722. [7] Bombardi A., et al., *Phys. Rev. Lett*., 2005, *submitted*.
Keywords: lattice anomalies, square lattice, frustration

P.11.01.10

Acta Cryst. (2005). A**61**, C387

Comparison and Analysis of the Samples with Same Synthesis of Bi-Sr-Ca-Cu-O, Prepared by Different Ways of Heating

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For the study of superconducting materials, produced by different ways of heating, five mixtures with proportions 2:2:2:3 of Bi_2O_3, $SrCO_3$, $CaCO_3$, CuO were prepared. The four of them were heated, directly, at 860°, 870°, 880° and 890° C, individually, while the last one, gradually, at the same temperatures. All the samples were heated in free atmosphere, for 48h.

The crystalline phases, created in the eight cases, were studied by XRD measurements and characterized, using the PDF2 database. Further, the Powder Profile Analysis (Rietveld's method) was used for the crystallographic study of the samples. The phase $Bi_2CaSr_2Cu_2O_8$, with space group Amaa and mean unit cell parameters a=5.4028, b=5.3923 c=30.6559 [1], was the main phase for all the samples, with a percentage greater than 80%. Some other phases with percentage 5-15% for the different samples were defined, say the Bi_2SrCuO_5, with structure analogous of Dy_2BaCuO_5 [2] (Pnma space group and mean unit cell parameters a=12.2020, b=5.6732, c=7.1357).

Results of the samples synthesis for each of the processes were discussed.

[1] Petricek V., Gao Y., Lee P., Coppens P., *Powder Diffraction*, 1994, **9**, 28-37. [2] Salinas-Sanchez A., Garcia-Munoz J.L., Rodriguez-Carvajal J., Saez-Puche R., Martinez J.L., *J. of Solid State Chemistry*, 1992, **100**, 201-211.
Keywords: superconductors, crystal structure, Rietveld's method

P.11.01.11

Acta Cryst. (2005). A**61**, C387

Crystallographic Study of Superconducting series $Nd_{1+x}Ba_{2-x}Cu_3O_y$ (x=0.0,0.2,0.4,0.6), Prepared at 850°C and 860°C

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The structural properties of superconducting series $Nd_{1+x}Ba_{2-x}Cu_3O_y$ (x=0.0, 0.2, 0.4, 0.6), prepared at 850°C and 860°C, were studied. For this aim, four powder mixtures with suitable proportions of Nd_2O_3, BaO and CuO were prepared and heated at temperature 850° and next the produced samples were reheated at 860°C, in free atmosphere for 48h, in both cases. The creation and the evolution of the phases, as a function of the quantity x, was studied by analysis of XRD measurements. The phase characterization was realized with a suitable program, using the PDF2 data-base. Farther, the Powder Profile Analysis (Rietveld's method) was used for the phase structure refinement and the exact determination of the phase percentages. Four crystal phases, $NdBa_2Cu_3O_7$ [1], Nd_2BaCuO_5 [2], $BaCuO_2$ [3] and CuO [4], were defined for the samples prepared at 850°C, while only the first three of these were defined for the samples prepared at 860°C. The creation and percentages of the crystal phases in the samples were discussed, as a function of the temperature and the quantity x.

[1] Lundqvist P., Rapp O., Tellgren R., Bryntse I., *B-Condensed Matter*, 1997, **56**, 2824. [2] Schiffler S., Mueller-Buschbaum H., *Monatshefte fuer Chemie und verwandte Teile anderer Wissenschaften*, 1986, **117**, 465. [3] Kipka R., Mueller-Buschbaum H., *Zeitschrift fuer Naturforschung*, Teil B., *Anorganische Chemie*, *Organische Chemie*, 1977, **32**, 121. [4] Asbrink S., Norrby L.J., *Acta Cryst. B*, 1970, **26**, 8.
Keywords: superconductors, crystal structure, Rietveld's method

P.11.01.12

Acta Cryst. (2005). A**61**, C387

Crystallographic Study of Samples Produced from Mixtures $La_{1+x}Ba_{2-x}Cu_3O_y$ (x=0.0, 0.2, 0.4, 0.6), Heated at 850°C and 860°C

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Four powder mixtures with suitable proportions of La_2O_3, BaO and CuO according to general type $La_{1+x}Ba_{2-x}Cu_3O_y$ (x=0.0, 0.2, 0.4, 0.6), were prepared and heated at temperature 850° and next the produced samples were reheated at 860°C, in free atmosphere for 48h, in both cases.

The creation and the evolution of the phases, as a function of the quantity x, was studied by analysis of XRD measurements. The phase characterization was realized with a suitable program, using the PDF2 data-base. Farther, the Powder Profile Analysis (Rietveld's method) was used for the phase structure refinement and the exact determination of the phase percentages.

Three crystal phases (the superconducting $La_{1.76}Ba_{0.24}CuO_4$ [1] and $LaBa_2Cu_3O_7$ [2], and the non superconducting $BaCuO_2$ [3]), were defined for all the samples. The creation and percentages of the crystal phases in the samples were discussed, as a function of the temperature and the quantity x.

[1] Katano S., Fernandez-Baca J.A., Funahashi S., Mori N., Ueda Y., Koga K., *Physica C*, 1993, **214**, 64. [2] Skakle J.M.S., West A.R., *Physica C*, 1994, **227**, 336. [3] Kipka R., Mueller-Buschbaum H., *Zeitschrift fuer Naturforschung*, Teil B., Anorganische Chemie, Organische Chemie, 1977, **32**, 121.
Keywords: superconductors, crystal structure, Rietveld's method

P.11.03.1

Acta Cryst. (2005). A**61**, C387

Growth and Structural Investigations on lead-doped $NdMnO_3$ Single Crystals

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Single crystals of $Nd_{(1-x)}Pb_{(x)}MnO_3$ with different dopant concentrations were grown by high temperature solution growth technique using PbO-PbF_2 flux [1]. Electron diffraction patterns showed the presence of superlattice structure x =0.25 and above The structure of $Nd_{(1-x)}Pb_{(x)}MnO_3$ crystals were determined by single crystal x-ray diffraction for two different x values using a Bruker AXS Smart Apex CCD diffractomenter with MoKα radiation . Positional co-ordinates of Nd and Mn atoms were obtained by SHELXS97 and refined by SHELXL97. Substitution of Pb at Nd site results in structural change from tetragonal (x=0.25) to cubic (x=0.38) lattice. The lattice parameters of tetragonal and cubic unit cells are a = b = 7.725(1)Å, c= 3.884(1) Å and a= b= c= 7.737(2) Å respectively. While the unit cell volume of tetragonal structure (*P4/mmm*) is comparable to that of parent $NdMnO_3$, the volume of cubic unit cell (*Pm3m*) is doubled. The static distortion of MnO_6 octahedra is maximum for parent orthorhombic $NdMnO_3$ (x = 0). The mismatch between different Mn - O bond lengths of $Nd_{1-x}Pb_xMnO_3$ is much less at x = 0.25 and 0.38. The MnO_6 octahedral distortion and inter octahedral tilt are removed progressively with higher doping. Changes in transport properties as a function of temperature at different doping levels are in accordance with the structural changes.

[1] Ghosh N., Elizabeth S., Bhat H.L., Subanna G.N., Sahana M., *Journal of Magnetism and Magnetic Materials*, 2003, **256**, 286-292.
Keywords: crystal growth, crystal structure, magnetic materials

P.11.03.2

Acta Cryst. (2005). A**61**, C387-C388

Atomic Image of Diluted Magnetic Semiconductor $Zn_{1-x}Mn_xTe$ Obtained by X-ray Fluorescence Holography

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