

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 $\text{Ba}_2\text{RCu}_3\text{O}_{6+x}$ (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 $\text{Ba}_2\text{RCu}_3\text{O}_{6+x}$, 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 $\text{Ba}_2\text{RCu}_3\text{O}_{6+x}$ 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 $(\text{Ba,Sr})_3\text{RTi}_2\text{O}_{8.5}$, $(\text{Ba,Sr})\text{R}_2\text{CuO}_5$, $(\text{Ba,Sr})\text{Ti}_2\text{O}_4$, and $(\text{Ba,Sr})_2\text{RCu}_3\text{O}_{6+x}$, etc.

Keywords: superconductor-substrate interface, $\text{Ba}_2\text{RCu}_3\text{O}_{6+x}$ - SrTiO_3 , coated conductors

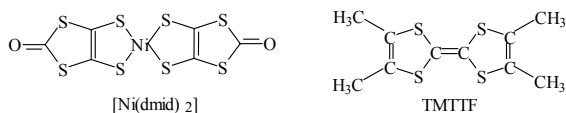
P.11.01.6

Acta Cryst. (2005). A61, C386

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

Oleg Dyachenko^a, Vladimir Starodub^b, Grigori Alexandrov^c, Tatiana Zinenko^b, Anna Kravchenko^b, Alexandr Khotkevich^d, Olga Kazheva^a, ^aDepartment of Substance Structure, Institute of Problems of Chemical Physics, Chernogolovka, Russia. ^bKharkov National University, Kharkov, Ukraine. ^cKurnakov Institute of General and Inorganic Chemistry, Moscow, Russia. ^dVerkin Institute for Low Temperature Physics & Engineering, Kharkov, Ukraine. E-mail: doa@icp.ac.ru

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



A lot of compounds have been obtained containing $[\text{Ni}(\text{dmit})_2]^{n-}$ anion analogous to $[\text{Ni}(\text{dmid})_2]^-$ 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 $[\text{Ni}(\text{dmid})_2]$ 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). A61, C386

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

Ryoko Tazaki^{ab}, Hajime Sagayama^b, Yusuke Wakabayashi^b, Hiroshi Sawa^b, Reizo Kato^c, ^aGraduate school of Science and Technology, Chiba University, ^bPhoton Factory, High Energy Accelerator Research Organization (KEK), ^cRIKEN, Japan. E-mail: rtazaki@post.kek.jp

Molecular conductor (DBr-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 $\text{Cu}^+ \text{Cu}^+ \text{Cu}^{2+}$ 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). A61, C386

Twin Formation in InP Nanowires Epitaxially Grown on Germanium and Silicon

Harry Wondergem, Erik Bakkers, Ruud Balkenende, Marcel Verheijen, *Philips Research, Prof. Holstlaan 4, 5656 AA, Eindhoven, the Netherlands*. E-mail: h.j.wondergem@philips.com

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 $\langle 1.1.1 \rangle$ 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 $\langle 1.1.1 \rangle$ 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). A61, C386-C387

Low Temperature Structural Investigations of the J_1 - J_2 Model System VOMoO₄

Fabienne Duc, Sabine Gonthier, *Centre d'Elaboration de Matériaux et d'Etudes Structurales, Toulouse, France*. E-mail: fduc@cemes.fr

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, $\text{Li}_2\text{VOSiO}_4$ and $\text{Li}_2\text{VOGeO}_4$ [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 VOMoO₄ [6]. VOMoO₄ 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 $\text{Li}_2\text{VOSiO}_4$ and $\text{Li}_2\text{VOGeO}_4$ (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 VOMoO₄ phase. An anomalous evolution of the lattice parameters [7] which could be related to its magnetic properties was clearly revealed.