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Twinning in the adamantine-like quaternary calcogenide Li_2ZnSnS_4; A crystallographic detective story

Charles H Lake[1], Beth M Leverett[1], Jonathan W Lekse[2], Jennifer A Aitken[2]

[1]Indiana University of Pennsylvania, Chemistry, Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA 15705, Indiana, PA, 15705, USA, [2]Duquesne University, Department of Chemistry and Biochemistry, 600 Forbes Avenue, Mellon Hall 302, Pittsburgh, PA 15282, E-mail：Lake@iup.edu

Li_2ZnSnS_4 is a diamond-like semiconductor (DLS) material which is of interest as a host structure for the creation of potentially interesting magnetic and photovoltaic materials. The crystal structure of the compound was predicted to adopt the wurtz-stannite structure with all atoms possessing tetrahedral geometries. Initial studies indicated that the structure was disordered but, upon closer examination this "disorder" violated many basic chemical principles. The structure was reevaluated and the apparent "disorder" problem was the result of pseudo-merohedral twinning. The twinning masqueraded as "static disorder". The final result was that the crystal crystallized in the non-centrosymmetric space group *P*n which is a subgroup of the predicted *P*mn2_1. The resulting structure was chemically reasonable and the refinement converged with R_{all} = 1.61 %.

Keywords: diamond-like semiconductor, twinning, wurtz-stannite

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Nanoscale structural inhomogeneity at the phase boundary in $Nd_{1-x}Sr_xMnO_3$

Masahiro Nagao[1], Toru Asaka[1], Daisuke Akahoshi[2], Takuro Nagai[1], Toru Hara[1], Koji Kimoto[1], Hideki Kuwahara[2], Yoshio Matsui[1]

[1]National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki, 305-0044, Japan, [2]Sophia University, Tokyo, 102-8554, Japan, E-mail：NAGAO.Masahiro@nims.go.jp

Strongly correlated electron systems are materials with a tremendous amount of application potential for a new electronics. The reason comes from the fact that the physical properties change dramatically by application of external stimuli such as magnetic field, hydrostatic pressure and electric field. The changes arise from a close interplay among spin, charge, and orbital degrees of freedom. Colossal magnetoresistive perovskite manganites, which show a large variety of intriguing phenomena, have made a great contribution to understand the strongly correlated electron systems. The orbital degree of freedom has a critical role to play in the magnetoelectric properties. Moreover, the orbital orderings have an intense effect on the crystal structures through an innate electron-lattice interaction, i.e., Jahn-Teller effect. This indicates the crystal structure analyses can decide the orbital ordering states. Recently, a large magnetoresistance was discovered at the phase boundary of A-type and C-type antiferromagnetic phases in $Nd_{1-x}Sr_xMnO_3$ crystals. We will report that nanoscale structure exists in the orbital ordered phase in the vicinity of the phase boundary, by the combination of transmission electron microscopy and synchrotron X-ray diffraction. The diffraction studies revealed that the nanoscale structure is an orbital disordered state. The electron micrographs show the direct evidence for the presence of the nanoscale structure. This phase is characterized by a nanoscale inhomogeneity but is not a phase separation which has been the much-discussed subject of the colossal magnetoresistance effect.

Keywords: magnetic perovskite materials, magnetic materials, electron microscopy, Lorentz

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Crystal structure and magnetic properties of complex oxides $Mg_{4-x}Ni_xNb_2O_9$, x=0-4

Nadezda V Tarakina[1], Elizaveta A Nikulina[1], Joke Hadermann[2], Dina G Kellerman[1], Alexander P Tyutyunnik[1], Ivan F Berger[1], Vladimir G Zubkov[1], Gustaaf Van Tendeloo[2]

[1]Institute of Solid State Chemistry, Ural Branch of Russian Academy of Sciences, 91 Pervomayskaya str., GSP-145, Ekaterinburg, Sverdlovskaya, 620041, Russia, [2]EMAT, University of Antwerp, Groenenborgerlaan 171, Antwerp, Belgium, E-mail：tarakina@ihim.uran.ru

In the $Mg_{4-x}Ni_xNb_2O_9$ (x=0-4) system two ranges of solid solution have been found. One of the solid solutions has a corundum related structure type (space group *P-3c*1); the second one adopts the II-$Ni_4Nb_2O_9$ structure type (space group *Pbcn*). Two samples, $Mg_3NiNb_2O_9$ and $MgNi_3Nb_2O_9$, from the first and the second range respectively, have been selected for a detailed crystal structure and microstructure investigation. The unit cell constants and atomic positions have been determined and refined using neutron powder diffraction data. Structures of $Mg_3NiNb_2O_9$ and $MgNi_3Nb_2O_9$ can be described as layers of hexagonally close packed oxygen atoms with 2/3 of the octahedral sites occupied by metal atoms. In the case of $Mg_3NiNb_2O_9$, cations fill the octahedral sites forming honey-comb pattern. In the case of $MgNi_3Nb_2O_9$, the metal layer with honey-comb pattern alternates two metal layers with chain pattern. Electron diffraction and high resolution transmission electron microscopy from $MgNi_3Nb_2O_9$ crystals identify the presence of planar defects and the intergrowth of several (structurally related) phases, which appear due to rotational staking faults between chain corundum layers. The extent and frequency of these defects suggest the possibility to obtain new modifications of corundum related compounds. The magnetic susceptibility of $Mg_3NiNb_2O_9$, measured in the temperature range T = 2-300 K, shows no indications of magnetic ordering at low temperatures, while for $MgNi_3Nb_2O_9$ there is a magnetic ordering at temperatures below 45.5K. This work was supported by Belgium Science Policy, by the Council for Grants of the President of the Russian Federation for Support of Young Scientists (grant no. MK 84.2007.3) and for Support of Leading Scientific Schools (grant no. NSh − 1170.2008.3).

Keywords: niobates, neutron powder diffraction, electron microscopy

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RXMS study of non-collinear spin structure of $BaFe_{10}CoTiO_{19}$

Maki Okube[1], Seiji Ohsawa[1], Satoshi Sasaki[1], Takeshi Toyoda[2], Takeharu Mori[3]

[1]Tokyo Institute of Technology, Materials and Structures Laboratory, 4259, Nagatuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8503, Japan, [2]Industrial Research Institute of Ishikawa, Kuratsuki 2-1, Kanazawa 920-8203, Japan, [3]Photon Factory, Institute of Materials Structure Science, KEK, Oho 1-1, Tsukuba 305-0801, Japan, E-mail：makisan@lipro.msl.