

LAMOX, the new family of oxide conductors, obtained on the basis of  $\text{La}_2\text{Mo}_2\text{O}_9$  compound with the use of different substitutions is the object for intensive studies. In 2005 year single crystals of the anionic conductor  $\text{La}_2\text{Mo}_2\text{O}_9$  were grown by crystallization from the nonstoichiometric flux [1]. Their polymorphism, domain structure and temperature dependences of conductivity and permittivity were studied [1]. Conductivity of these crystals at 750-600 °C reaches  $10^{-1}$ - $10^{-2}$   $\text{Om}^{-1}\text{sm}^{-1}$ . It was established that in dependence of the cooling rate and of the admixture content, these crystals can exist at the room temperature as stable monoclinic A-phase or metastable cubic B<sub>1</sub>-phase or as their mixture. Obtaining of the most complete and precise structural data about the crystals of cubic metastable B<sub>1</sub>-phase from X-ray experiment was the purpose of the present study. It is important that these studies were done for the first time for single crystals. Cubic cell with  $a=7.158(1)\text{\AA}$ , which was found for the studied single crystal, allowed to index about 84% of measured reflections. While solving the structure (in sp.gr.  $P2_13$ ) it was established that La and Mo atoms are shifted from the threefold axes. Occupation of three positions of La and Mo atoms was found to be equal to 100%. Two of the three independent oxygen positions in this crystal are not fully occupied, have quite large thermal parameters and are located at the short distances from each other. Concluding R-factor for this structure was 2.46%. The work was done with the partial support of the grant RFBR No.07-02-00180, Grant for the Leading Scientific Schools NSh-2192.2008.5 and "Russian Science Support Foundation".

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Keywords: conducting materials, crystal structure analysis, structure-properties relationships

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### Pulse laser deposition of AgInSe<sub>2</sub> films

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High quality  $\text{agInSe}_2$  (AIS) films were grown on Si and glass substrates by the ultra-high-vacuum pulsed laser deposition technique from the AIS target synthesized from high-purity materials. The X-ray diffraction and microscopic studies of the films show that films are textured in (112) direction. The effect of substrate temperature on growth on Si and glass substrates was observed. The substrate temperature appears to influence the properties of films. The films prepared on Si show more crystallinity than on glass showing good lattice matching. Chalcopyrite phase (112) is dominant up to 3000 °C. The optical studies of the films show that the optical band gap is about 1.24 eV, which also show change with change in temperature. This shows that AIS films are very good absorber material for solar cell technology.

Keywords: pulse laser deposition, thin films, optical properties

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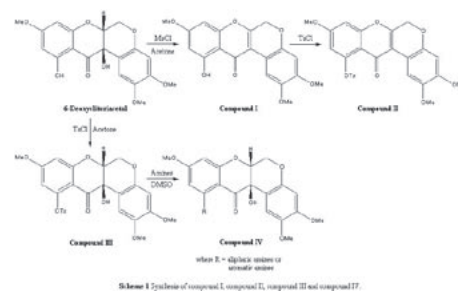
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### Modified 6-deoxyclitoriacetal and their crystal structures as anticancer agents

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6-Deoxyclitoriacetal is a substance extracted from the dried roots of *Stemona collinsae* Craib. It has been known to have a cytotoxic activity against various types of human carcinoma possibly due to by its ability to intercalate with DNA as evidenced *in vitro* assay. In order to enhance its activity, 6-deoxyclitoriacetal was derivatised to contain a functional group with more flexible and can be participated hydrogen bonding with DNA. The derivatives of 6-deoxyclitoriacetal were prepared as shown in scheme 1. In this work, we studied the relationship between crystal structures, hydrogen bonding and cytotoxic activity of 6-deoxyclitoriacetal and its derivatives based on spectroscopic and X-ray crystallographic techniques.



Keywords: 6-deoxyclitoriacetal, hydrogen bonding, cytotoxic activity

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### Using electron microscopy techniques studies in microstructure of NdFeCoAl-(B,C) based alloys

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Magnetic materials on basis of the NdFeAl alloys have been intensively studied because of their interesting physical properties and application potential. The magnetic measurements reveal that the samples exhibit hard-magnetic characteristics quite good at room temperature. However, the relationship between hard magnetic properties and microstructure in these alloys are still not well understood. We present here the results of studies on the microstructure of some NdFeCoAl-(B,C) alloy system by the electron microscopy techniques as TEM, HRTEM, SEM, SAED, EDX and EBSD. Rods and ribbons of the NdFeCoAl-(B,C) alloys were prepared from the pure elements Nd, Fe, Co, Al, B and C by rapid-quenching methods. We used a Philips CM20-FEG TEM and a FEI NovaNanoSEM 200 SEM to characterize the microstructure of these alloys. We found the different crystalline phases in the alloys. In the NdFeCoAlB samples, the tetr.  $\text{Nd}_2(\text{Fe},\text{Co})_{14}\text{B}$  (2:14:1), fcc Nd rich, hcp Nd, alpha-Fe and in the NdFeCoAlC samples, the tetr.

$\text{Nd}_6(\text{Fe},\text{Co},\text{Al})_{14}$  ( $\delta$ ), m phase and hex.  $\text{Nd}_2(\text{Fe},\text{Co})_{15}\text{Al}_2$  (2:15:2) crystalline phases embedded in an amorphous matrix were identified. The grain size of the crystallites is ranging from 3 nm to 250 nm. The 2:14:1 phase is supposed the high coercivities up to 1202 kA/m at room temperature of the NdFeCoAlB alloys. Other antiferromagnetic phases as the 2:15:2,  $\delta$  phase can be played an important role in hard magnetic properties of alloys at low temperature ranges. The amorphous phase with high fraction was found in all of these alloys have also good hard magnetic properties (higher than 3 kOe). In the NdFeCoAlC alloys, we did not find the crystalline phase 2:14:1 but still obtained higher 7 kOe in coercivity.

Keywords: hard magnetic materials, TEM, scanning electron microscopy

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### Negative and low positive thermal expansion behaviour of niobate based ceramics and solid solutions

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Our understanding of the thermal behaviour of the solid state has led to the development of novel materials that encompass many diverse applications. In this regard materials that possess negative and low positive coefficient of thermal expansion are of interest because they have a number of possible engineering, electronic and optical applications. Currently, negative and low positive coefficients of thermal expansion have been observed in several metal oxide, natural mineral and alloy systems [1]. In this study the thermal expansion of several Niobate ( $\text{Nb}_2\text{O}_5$ ) ceramic and solid solution systems were investigated. Currently, negative thermal expansion behaviour has been observed in  $\text{TiO}_2\text{-Nb}_2\text{O}_5$  and  $\text{Nb}_2\text{O}_5$  ceramic and single crystal materials [2]. The materials under investigation in this study include ceramics and solid solutions of the type  $\text{Nb}_2\text{O}_5\text{-AO/AO}_2\text{/A}_2\text{O}_3$  ( $A = \text{Y}, \text{Bi}, \text{Hf}, \text{Zr}, \text{Ti}, \text{Fe}$  and  $\text{Al}$ ). Samples were prepared by standard solid state techniques from the constituent oxides. Sample characterization was performed using variable temperature Powder X-ray Diffraction (VT-PXRD) in conjunction with the Rietveld refinement technique. Several of the materials currently under investigation have been found to exhibit low to moderate thermal expansion over a broad temperature range with evidence of hysteresis between heating and cooling stages. Currently, our focus is on establishing a structural relationship between the different Niobate materials in an attempt to correlate the thermal expansion behaviour exhibited by these materials. Selected results will be presented.

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[2] H. Choosuwana, et al., *J. App. Phys.*, **91** (2002) 5051 - 5054.

Keywords: Rietveld, VT-PXRD, negative thermal Expansion

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### The crystal structure analysis of release factor 3 from sulfate-reducing bacterium

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The translation of an mRNA is terminated when a stop codon is encountered. Since tRNAs do not recognize the stop codons, this event is done by proteins called release factors. Prokaryotes have three release factors, RF1, RF2 and RF3. The class 1 release factors, RF1 and RF2, hydrolyze and release the completed polypeptide from the tRNA at P-site in response to a stop codon. RF1 recognizes the stop codons of UAA and UAG, whereas RF2 does UAA and UGA. RF3 is a class 2 release factor, and it catalyses the removal of release factor RF1 and RF2 from the ribosome in a GTP-dependent manner. We have studied the structure-function relationship of the RF3 found in sulfate-reducing bacterium, *Desulfovibrio vulgaris* Miyazaki F. Here we present the high resolution crystal structure of RF3-GDP complex (Fig.1). Structural comparison with *E. coli* RF3 in the GDP-bound form as well as EF-G-2 and EF-Tu in the GTP-bound forms is also described.

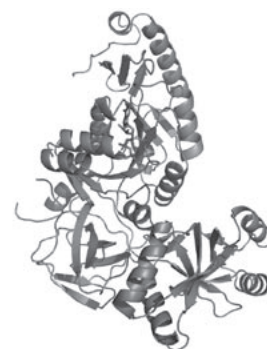


Fig. 1. Crystal Structure of RF3-GDP

Keywords: X-ray crystal structure analysis, translation factors, GTP-binding proteins

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### The structure and photoluminescence of chiral tin and lead inorganic-organic hybrid perovskites

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Inorganic-organic hybrids have been studied extensively in recent times because of the variety of interesting and useful properties associated with this family of compounds. The layered hybrids specifically the 2D  $(\text{RNH}_3)_2\text{MX}_4$  and  $(\text{NH}_3\text{RNH}_3)_2\text{MX}_4$  series, have shown good semi-conduction, photoconductivity, photoluminescent and electroluminescent behaviour [1]. These properties are dominated by the metal halide used [1]. The ability to fine tune these systems, structure and property alike; lies with the choice of the organic moiety. The choice of the organic moiety also influences the symmetry of the crystal. Chiral and polar crystals are of interest because of their inherent Second Harmonic Generation (SHG) nonlinear optical behaviours [2]. We report here the characterization and study of chiral amines in the following hybrid systems: the 2D  $\text{MI}_4((\text{R})\text{-C}_6\text{H}_5\text{C}^*(\text{H})(\text{CH}_3)\text{NH}_3)_2$ ;  $\text{MI}_4((\text{S})\text{-C}_6\text{H}_5\text{C}^*(\text{H})(\text{CH}_3)\text{NH}_3)_2$ ; and  $\text{MI}_4((\pm)\text{-C}_6\text{H}_5\text{CH}(\text{CH}_3)\text{NH}_3)_2$  series where  $\text{M} = \text{Pb}$  and  $\text{Sn}$  (Pb structures [3-4]). The 1D chains of  $\text{MI}_3((\text{R})\text{-C}_6\text{H}_5\text{C}^*(\text{H})(\text{CH}_2\text{CH}_3)\text{NH}_3)$  and  $\text{MI}_3((\text{S})\text{-C}_6\text{H}_5\text{C}^*(\text{H})(\text{CH}_2\text{CH}_3)\text{NH}_3)$  where  $\text{M} = \text{Pb}$  and  $\text{Sn}$ . The photoluminescence of all of the above mentioned structures have displayed unique luminescence shifts from 77-293K of the respective enantiomer and racemic crystals. The luminescence behaviour is rationalized from the subtle structural changes observed following a series of SC-XRD studies done at different temperatures.

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