

$\text{Nd}_6(\text{Fe},\text{Co},\text{Al})_{14}$ (δ), 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, δ 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

P08.14.120

Acta Cryst. (2008). A64, C455

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

Roy P Forbes^{1,2}, David G Billing^{1,2}

¹University of the Witwatersrand, Chemistry, Private Bag 3 PO Wits, Johannesburg, Gauteng, 2050, South Africa, ²DST/NRF Centre of Excellence in Strong Materials, E-mail: roy.forbes@students.wits.ac.za

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 (Nb_2O_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 Nb_2O_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 = Y, Bi, Hf, Zr, Ti, Fe and 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.

[1] R. Rustum, et al., *Ann. Rev. Mat. Sci.*, **19** (1989) 59 - 81.

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

Keywords: Rietveld, VT-PXRD, negative thermal Expansion

P08.14.121

Acta Cryst. (2008). A64, C455

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

Kiyohito Kihira¹, Shuko Numata², Masaya Kitamura², Shinichi Terawaki¹, Yasuhito Shomura¹, Hirofumi Komori¹, Naoki Shibata¹, Yoshiki Higuchi¹

¹University of Hyogo, Graduate School of Life Science, 3-2-1, Koto,

Kamigori-cho, Ako-gun, Hyogo, 678-1297, Japan, ²Osaka City University, 3-3-138 Sugimoto Sumiyoshi-ku, Osaka-shi, Osaka, 558-8585, Japan, E-mail: rl06r004@stkt.u-hyogo.ac.jp

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.

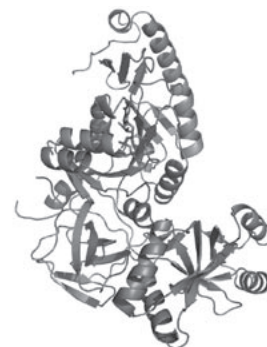


Fig. 1. Crystal Structure of RF3-GDP

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

P08.14.122

Acta Cryst. (2008). A64, C455-456

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

Robert S Black, David G Billing

University of the Witwatersrand, Chemistry, Private Bag 3 PO Wits, Johannesburg, Gauteng, 2050, South Africa, E-mail: Robert.Black@students.wits.ac.za

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 M = Pb and 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 M = Pb and 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.

[1] Mitzi D.B., *Progress in Inorganic Chemistry* 1999, **48**, 1-121

[2] Mercier N., Barres A., Giffard M., Rau I., Kajzar F., Sahraoui B.

Angew. Chem. Int. Ed. 2006, **45**, 2100-2103

[3] Billing D.G., Lemmerer A. *CrystEngComm*, 2006, **8**, 686-695

[4] Billing D.G., *Acta Cryst.* 2002. **E58**, m669-m671

Keywords: inorganic-organic hybrids, photoluminescence, nanocomposites

P08.14.123

Acta Cryst. (2008). **A64**, C456

Boron ordering in CeRh₃B_x and ScRh₃B_x alloys

Kunio Yubuta, Akiko Nomura, Nakajima Kazuo, Shishido Toetsu
Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai, Miyagi, 980-8577, Japan, E-mail: yubuta@imr.tohoku.ac.jp

A large number of simple and complex perovskite oxides have been performed due to the interesting features of superconductor, insulator-metallic transition, ion conduction characteristics, dielectric properties. We synthesized perovskite-type boride CeRh₃B_x and ScRh₃B_x ($x = 0\sim 1$) and measured various physical and chemical properties. On the basis of the powder X-ray diffraction, although the lattice constant changes almost linearly with B content, it could be found no drastic transitions of the crystal structures, i.e., CeRh₃B_x and ScRh₃B_x exists in a wide range of boron concentration with the space group *Pm-3m*. On the other hand, the observed electron diffraction patterns of CeRh₃B_{0.5} and ScRh₃B_{0.5} show the appearance of 1/2 1/2 1/2-type superlattice reflections and fine satellite reflections around all reflections in which anomalous drop of hardness was observed in both system. The new ordered structures producing the superlattice reflections belong to a tetragonal system, space group *I4/mmm*. The observed high-resolution images taken with diffraction patterns showing the satellite reflections along the [011] direction show a domain structure, and a lattice modulation and some edge dislocations have been observed at boundaries between the domains. Conclusively, ordering of B atoms and followed by the appearance of the long-ranged modulated structure could lead to the anomalous behavior of hardness in CeRh₃B_x and ScRh₃B_x alloys.

Keywords: borides, ordering, TEM characterization

P08.14.124

Acta Cryst. (2008). **A64**, C456

The effect of extension axis orientation on the localized plasticity in FCC single crystals

Svetlana A. Barannikova, Lev B. Zuev
Institute of Strength Physics & Materials Science SB RAS, Strength Physics Laboratory, 2/1 Akademicheskii Ave., Tomsk, Tomsk Oblast, 634021, Russia, E-mail: bsa@ispms.tsc.ru

The present paper is aimed at refining the concept of macroscopic self-organization of plastic flow variation, which is based on the assumption that the localization behavior of plastic deformation is related to the conventional parameters of the processes of form changing of material in a stress-strain state. The investigations were performed for FCC single crystals of gamma-Fe alloys. The choice of material is motivated by its capability to deform by different mechanisms (glide or twinning); moreover, the shape of the deformation curve obtained for the test specimens is determined by extension axis orientation. The investigation of plastic deformation macrolocalization was performed by the method of double-exposure speckle photography. It is found that active localized plasticity nuclei would emerge and evolve on the macro-scale level over the entire

flow process. It should be noted that this phenomenon has not been earlier observed for materials deforming by twinning. These nuclei can be regarded as meso-scale defects responsible for plastic flow development on the macro-scale level. Their salient feature is that the spatial distributions of elongation, shear and rotation increments within a nucleus are interrelated. Each active localization nucleus corresponds with a set of shears or deformation twins over the glide plane of the acting glide or twinning system, which have maximal Schmidt factor values. A new two-component plastic flow model is proposed, which is appropriate for addressing the distinctive features of plastic flow localization in solids which cannot be explicitly interpreted in the framework of conventional approaches.

Keywords: crystal geometry, deformation behaviour, *in-situ* experiments

P08.14.125

Acta Cryst. (2008). **A64**, C456

Structural studies of a new series of ester derivatives in cyclopropanol chemistry

Laura Torre-Fernandez¹, Santiago Garcia-Granda¹, Marcos G Suero²
¹University of Oviedo, Physical and Analytical Chemistry, Julian Claveria, 8, Oviedo, Asturias, 33006, Spain, ²Organic and Inorganic Chemistry, University of Oviedo, Julian Claveria, 8, Oviedo, Asturias, 33006, Spain, E-mail: ltf@fq.uniovi.es

Cyclopropanol was first synthesized in 1942. The development of cyclopropanol chemistry in the past decades has been quite fruitful, and these compounds occupied their own niche in synthetic practice as useful intermediates in organic synthesis and as substances which are capable of possessing important kind of biological activity. A range of synthetic approaches to this class of compounds exist and involve Simmons-Smith-type cyclopropanation of enolates with SmI₂ - CH₂I₂, cross coupling reactions between alpha,beta-unsaturated ketones and aldehydes with CrCl₂ and cyclopropanation of carboxylic esters with ethylmagnesium bromide and titanium(IV) isopropoxide. A new method for the synthesis of cyclopropanol through the cyclopropanation of lithium ketone enolates with Fischer carbene complex is presented. Different derivatives can be obtained by changing the initial bicyclic cyclopropanols which are going to be treatment with 3,5-dinitrobenzoyl chloride in the presence of a base. We present two ester derivatives [1], (1*R**,7*R**,8*R**)-8-methoxy-8-phenylbicyclo[5.1.0]octan-1-yl 3,5-dinitrobenzoate and (1*R**,8*R**,9*R**)-9-methoxy-9-phenylbicyclo[6.1.0]nonan-1-yl 3,5-dinitrobenzoate, which are the first members of a new family of compounds. The members of this family present similar crystallographic characteristics. They crystallize in the same space group with similar unit cell. They also present similar hydrogen interactions. In this work we present the new synthesis method and the X ray study of these both compounds, including its electron density topological features [2].

[1] Barluenga, J.; Suero, M. G.; Perez-Sanchez, I.; Florez, J. J. *Am. Chem. Soc.* (2008), **130**, 2708-2709. [2] Menendez-Velazquez, A.; Garcia-Granda, S. *J. Appl. Cryst.* (2003), **36**, 193-205.

Keywords: organic compounds, topological aspects of structure, crystallographic structure