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, Aobaku, 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 $ScRh_3B_x$ (x = 0~1) 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, betaunsaturated 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 treatmenting with 3,5-dinitrobenzoyl chloride in the presence of a base. We present two ester derivatives [1], $(1R^*, 7R^*, 8R^*)$ -8-methoxy-8-phenylbicyclo[5.1.0]octan-1-yl 3,5-dinitrobenzoate and (1R*,8R*,9R*)-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