Nd₆(Fe,Co,Al)₁₄ (delta), m phase and hex. Nd₆(Fe,Co)₁₄Al₁₄ (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

P08.14.120

**Negative and low positive thermal expansion behaviour of niobate based ceramics and solids**

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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 possesses 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 (Nb₂O₅) ceramic and solid solution systems were investigated. Currently, negative thermal expansion behaviour has been observed in TiO₂-Nb₂O₅ and Nb₂O₅ ceramic and single crystal materials [2]. The materials under investigation in this study include ceramics and solid solutions of the type Nb₂O₅-AO/ AO₂/A₂O₃ (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.


Keywords: Rietveld, VT-PXRD, negative thermal Expansion

**P08.14.121**

**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.

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

**P08.14.122**

**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 (RNH₃)₂MX₄) and (NH₃)RNH₃))₂)MX₄) 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 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 ML((R),H₃)(H₃CH₂NH₃))₂); ML((Ci-Si H₃C(H₂CH₂NH₃))₂); ML((Ci-Si H₃C(H₂CH₂NH₃))₂); and ML((Ci-Si H₃C(H₂CH₂NH₃))₂); where M = Pb and Sn (Pb structures [3-4]). The 1D chains of ML((R),H₃)(H₂CH₂NH₃))₂); ML((Ci-Si H₃C(H₂CH₂NH₃))₂); and ML((Ci-Si H₃C(H₂CH₂NH₃))₂); 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.

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 CeRh$_3$B$_x$ and ScRh$_3$B$_x$ (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., CeRh$_3$B$_x$ and ScRh$_3$B$_x$ exists in a wide range of boron concentration with the space group Pm-3m. On the other hand, the observed electron 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 1/2 1/2-type superlattice reflections and fine satellite reflections around all reflections in which anomalous drop of hardness was observed in both systems. The new ordered structures producing the superlattice reflections belong to a tetragonal system, space group I4/mmm. The observed high-resolution images taken with electron 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 CeRh$_3$B$_x$ and ScRh$_3$B$_x$. alloys.

Keywords: borides, ordering, TEM characterization

**P08.14.123**


**Boron ordering in CeRh$_3$B$_x$ and ScRh$_3$B$_x$ alloys**

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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 CeRh$_3$B$_x$ and ScRh$_3$B$_x$ (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., CeRh$_3$B$_x$ and ScRh$_3$B$_x$ exists in a wide range of boron concentration with the space group Pm-3m. On the other hand, the observed electron 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 CeRh$_3$B$_x$ and ScRh$_3$B$_x$. alloys.

Keywords: borides, ordering, TEM characterization

**P08.14.124**


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

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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: organic compounds, topological aspects of structure, crystallographic structure