lamellar stacks), the thickness of the crystalline lamellae and that of the amorphous layers, l_c and l_a respectively ($L = l_c + l_a$) [3]. Results reveal that PET lamellae in the ultra-thin layers exhibit larger L values than those within the PET control material due to the occurrence of larger amorphous regions between lamellar crystals. In addition, finite-size effects are found to delay the crystallization process. However, the final crystal lamellar structure is similar for both, nanolayered and bulk material.

Room temperature WAXS measurements of the crystallized multilayered materials reveal uniaxial symmetry and indicate that edge-on lamellae are also generated upon crystallization. The simulation of uniaxially oriented patterns with the help of the CLEARER2 software package [4] reveals that the *c*-axis of the edge-on lamellae lies parallel to the layer surfaces. It is proposed that two lamellar populations develop: edge-on lamellae appear close to the interphases while flat-on lamellae are preferentially located in the layer core.

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Keywords: polymer, SAXS, confinement

MS30.P21

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Modeling of X-ray diffuse scattering in $Rb_2Li_4(SeO_4)_3{\cdot}2H_2O$

Dorota Komornicka, Marek Wołcyrz, Adam Pietraszko, *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław (Poland).* E-mail: D.Komornicka@int.pan.wroc.pl

A title rubidium and lithium selenate hydrate has monoclinic symmetry ($P2_1/c$ space group) and room temperature lattice parameters: a = 5.256 Å, b = 5.178 Å, c = 26.739 Å, β = 93.11°. Its structure consists of four planar packages perpendicular to *c*-axis. Selenium tetrahedra are present in each of the four packages but in the two of them Se positions are occupied partially (SOF = 0.5) together with accompanying oxygens forming two alternative tetrahedra [1]. As a result, beside the Bragg reflections coming from the average structure unit cell (Fig. 1*a*), additional diffraction effects in the form of long, strongly structuralized streaks, parallel to c^* and crossing a^*b^* reciprocal plane at $h\pm½$, $k\pm½$, are observed (Fig. 1*b*).

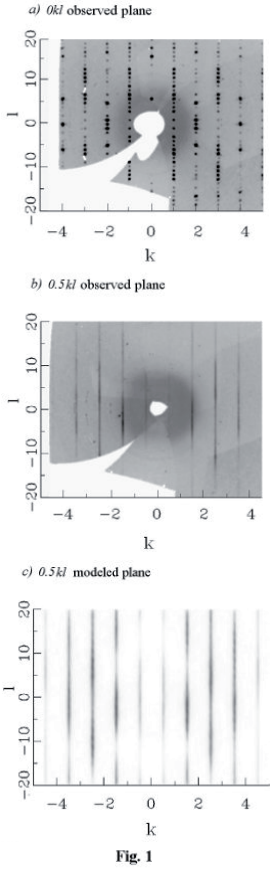

Fig. 1

It appeared that the origin of observed diffuse streaks is the different arrangement of selenium atoms in the partially occupied packages, locally fulfilling conditions for *C*-centering in the 2×2×1 superstructure cell. Characteristic structuralizations of the diffuse streaks is caused by a switching of SeO_4 tetrahedra forming oxygens into two alternative positions.

Preliminary model hunting and followed Monte Carlo simulations allowed us to find the best agreement between experimental and calculated diffuse scattering effects for generated sequences of Se-substituting packages (Fig. 1*c*). Different types of selenium planar domains and ways of multi-plane packaging were also tested and verified.

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Keywords: diffuse_scattering, disorder, selenate_hydrate

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Mesomorphic phase in oriented poly(pentamethylene 2,6-naphthalate)

Hyun Hoon Song,[a] Thi Cuc Do,[a] Hye-Jin Jeon,[a] Kohji Tashiro,[b] [a]*Department of Advanced Materials, Hannam University, Daejeon, S. Korea.* [b]*Toyota Technological Institute, (Japan).* E-mail: songhh@hnu.kr

The thermotropic liquid crystalline (LC) behavior of polymers with rigid mesogenic units interconnected through flexible spacers has been extensively over the past two decades. In the main-chain LC polymer flexible spacers are constrained by the mesogenic units to which they are linked, thus to have some orientational order. Among these polymers poly(alkylene 4,4'-bibenzoate)s whose mesophase existence and transition behavior have been intensively studied. These BB-*n* polyesters invariably form smectic mesophase when *n* varies from 3 to 9. Polyester based on 2,6-naphthalene dicarboxylic acid, poly(*m*-methylene 2,6-naphthalate) is another example of LC polymer that possibly show mesophase. In this family, as was noted in BB-n family, the macroscopic thermal and mechanical properties exhibit odd-even fluctuations as the number of methylene group in P*m*N increases. However, the existence of mesophase in these polymers is relatively rare and has been reported only in PEN and PBN. In this report, we present the mesophase structure in poly(pentamethylene 2,6-naphthalate) (PPN).

Keywords: WAXS, polymer, orientation

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Crystal structures of high-entropy alloys of high melting temperature

Soumyadipta Maiti, Walter Steurer, *Department of Materials, Laboratory of Crystallography, ETH Zurich (Switzerland).* E-mail: smaiti@mat.ethz.ch

In the recent years importance is being given to high-entropy alloys (HEA) where the alloy consists of multiple elements in high proportion (5-35 atomic %) for their many interesting properties [1]. Higher number of constituent elements increases the configurational entropy of the system, which influences the short-range ordering and coloring-problem. A lot of studies have been done in the alloys with Al and other transition metal elements. The most common of the base system has been Al-Co-Cr-Fe-Ni with other few metals. In this study we have focused on system containing high melting temperature refractory metals like W, Mo, Nb, Ta and V. The refractory HEA has potential application in the aerospace industry were there is an ever increasing need for a functional material with sufficient strength at high

temperature. There exists little scientific literature on this system and hence there is scope to develop this field. It has been found from the existing studies that an equiatomic refractory alloy has broadly a BCC structure with some compositional variation in the as-cast structure. In many cases ordering phenomena was not evident from X-Ray powder diffraction data, but was found through HRTEM electron diffraction in Al-Co-Cr-Fe-Ni HEA.

As the above-mentioned refractory materials have melting point of nearly 3000°C, the equiatomic WMoNbTa alloy was prepared through arc melting in argon atmosphere. The starting metal powders all had purity above 99.95 percent. First a 5-gram pellet was made from the well-mixed powders by hydraulic press. Later the pellet was melted under arc five times each for 2 minutes. Each time the sample was melted, it was turned upside down for even better mixing of elements. This was probably a better method than a previous report where metal chips and powder were melted together in the arc-melting furnace, which might remove some small chips when the arc strikes the mixture. After this the samples were wrapped into tantalum foils and sealed inside tantalum ampules. The inside of the ampule had Argon atmosphere and it was annealed at 1800°C for a week. The grain size distribution provides us with 50 micron grains that could be studied for diffuse scattering experiments.

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Keywords: high-entropy_alloy, coloring_problem, refractory_ alloy

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Structural analysis of metal nano-particles prepared by leaching

Reiko Murao,[a] Kazumasa Sugiyama,[a] Satoshi Kameoka,[b] An-Pang Tsai,[b] [a]*Institute for Materials Research, Tohoku University, Sendai (Japan).* [b]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai (Japan).* E-mail: r_murao@imr.tohoku.ac.jp

Catalytic fine particles can be obtained by the leaching of a variety of alloy powders using alkali or acid solutions [1]. During the leaching process, the structure of a parent alloy sample is decomposed and the X-ray diffraction pattern of resultant fine particles is usually very broad and diffuse. These features could be generally attributed to the small size of crystallite and the highly disordered structure [2]. To clarify structural features of such fine particles, the analysis of atomic pair distribution function (PDF), calculated from the total X-ray scattering measured by high-energy X-ray source, is suggested to be one of effective methods. However, high resolution PDF is not enough to discuss the structure around a specific element in the case of multi-component alloy system. In this context, the anomalous X-ray scattering (AXS) method [3] is a powerful tool to provide environmental structural information around a target element, not only in nearest neighbor but also in middle range region. Present paper demonstrates some examples of structural analysis for fine particles by anomalous X-ray scattering.

Structures of Raney Ru(Ni) fine particles prepared from $Al_{13}(Ru,Ni)_4$ alloy powder by alkali-leaching (NaOH) were investigated by the high-energy X-ray scattering and AXS measurement at the Ni-*K* absorption edge. Ordinary PDF for Raney Ru indicates atomic correlation similar to that for *fcc*-Ru. However, a correlation peak at about 0.2 nm, which could not be described by the atomic arrangement in the *fcc*-typed structure, is developed as a function of the Ni content. Additionally this interesting correlation could be clearly observed in the environmental PDF around Ni. These experimental results support the partial oxidation of Ni so as to realize the Ni-O pair in the observed PDFs. In middle range region of the environmental PDF, Ni-Ni(Ru) pairs with respect to the *hcp*-typed structure could be identified. These results suggest that the atomic rearrangement of Ni toward *hcp*-typed structure together with the partial oxidization was realized during the leaching process.

Structure of Pt/Cu fine particles prepared from a Cu_3Pt alloy powder by acid-leaching (HNO_3) was also studied by anomalous X-ray scattering. The ICP analysis indicates the Pt/Cu ratio of the obtained fine particles is about 85/15. Although the overall features observed in PDF is rather similar to that of *fcc*-Pt, the environmental RDF around Pt shows a correlation of the Pt-O pair at around 0.2 nm. Therefore, partial oxidation of Pt in the fine Pt/Cu alloy particles is readily suggested.

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Keywords: high-enrgy X-ray scattering, anomarous X-ray scattering, nanocrystal

MS30.P25

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Low–temperature plasticity of magnezium alloy AZ31 with different microstructure

V.V. Pustovalov,[a] Y. Estrin,[b] P.A. Zabrodin,[a] I.S. Braude,[a] T.V.Grigorova,[a] N.V.Isaev,[a] V.S.Fomenko,[a] S.E.Shumilin,[a] [a]*Institute for Low Temperature Physics and Engineering, Ave Lenin 47, Kharkov 61103, (Ukraine).* [b]*APC Center of Exelence for Design in Light Metals, Department of Materials Engineering Monash University, Clayton, Vic.(Australia)* E-mail: pustovalov@ilt.kharkov.ua

The feature of plastic deformation of magnesium alloy AZ-31 by tension in the temperature range 4.2-295 K are examined depending on microstructure after sqeeze casting (SC) and severe plastic deformation (SPD) via hot rolling and equal channel angular pressing. The SPD processing results in decrease of grain size and formation of a texture for basal dislocation glide. The microstructure of the samples for tension that were cut from the initial SC and SPD materials were also monitored by X-ray diffraction. The ratio of the integrated intensities of the (10.0), (00.2) and (10.1) reflections along and perpendicular to the sample axis are ~1.1 and 1.4 for SC and SPD samples, respectively. The integrated intensity of the (00.2) reflection for a sample from the SPD material is greater by an order of magnitude than for a sample from the initial SC material. These ratios of the integrated intensities indicate that the flat sample for tension retained the texture of the initial material, and its longitudinal axis coincides with the direction of rolling and pressing. The coherent scattering regions for SC and SPD derived from the Hall plots for the basal plane are 150 and 0.2 μm, respectively. These estimates, as is customary in these cases, are lower than the average grain size obtained by transmission microscopy, but the relative change in the coherent scattering region in the SC and SPD samples correlates with significant reduction in the grain size owing to rolling and pressing of the material. It is found that in the temperature range 4.2-25 K the plastic deformation becomes unstable (serrated) with stress jumps in the SPD alloy greater than in the SC one. The temperature dependence of yield stress of this alloy is typical of thermally activation unpinning of dislocations from short range obstacles. Correlation of yield stresses for SPD and SC samples at given temperature is explained by hardening due to refinement of grain size and owing to favorable texture. The work hardening coefficient to alloy decreases a grain size but the ductility (strain to fracture) increases due to texture. The strain rate sensitivity of flow stress at T≤100 K does not