

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  $Rb_2Li_4(SeO_4)_3 \cdot 2H_2O$**   
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A title rubidium and lithium selenate hydrate has monoclinic symmetry ( $P2_1/c$  space group) and room temperature lattice parameters:  $a = 5.256 \text{ \AA}$ ,  $b = 5.178 \text{ \AA}$ ,  $c = 26.739 \text{ \AA}$ ,  $\beta = 93.11^\circ$ . 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. 1a), additional diffraction effects in the form of long, strongly structuralized streaks, parallel to  $c^*$  and crossing  $a^*b^*$  reciprocal plane at  $h \pm \frac{1}{2}$ ,  $k \pm \frac{1}{2}$ , are observed (Fig. 1b).

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  $2 \times 2 \times 1$  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

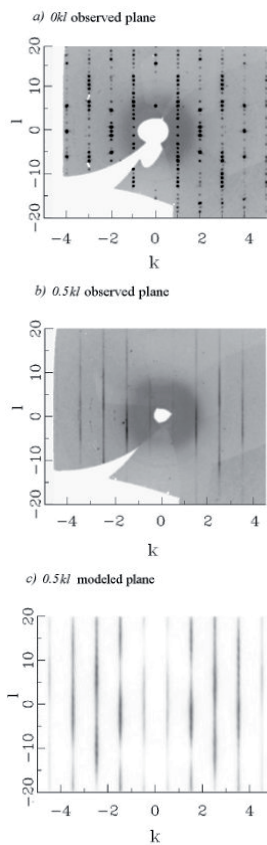


Fig. 1

allowed us to find the best agreement between experimental and calculated diffuse scattering effects for generated sequences of Se-substituting packages (Fig. 1c). 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)**

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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'-biphenylene)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  $PmN$  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**

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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 where there is an ever increasing need for a functional material with sufficient strength at high