Doping effect of nano TiO_2 has been the main concern of material scientists in the field of photocatalyst and dye-sensitized solar cell (DSC). The electronic states of doped surface and interface, without regard to the sort of interface including solid/solid and solid/liquid, are very different from the bulk states. For example, Si doping on TiO_2 bulk almost brings minor changes of the main energy level structure near conduction band and valence band. However, when Si is doped on the surface, new doping levels appear in middle position between the conduction band edge and valence band edge. This means that the surface doping of Si will seriously change the electric and optical properties of TiO_2 having high surface area such as nano particle and mesoporous film, although the bulk doping doesn't show any effect.
The doping elements in this calculation involved a series of transient metals, IV family group and some light metals. Here, main discussion will be concentrated on the electric properties in association with DSC.

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Keywords: Electronic state, first principles calculation, Surface doping

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Evolution of Formation of Interblock Boundaries in Nanothin Selenium Crystals. Malkov Vyacheslav[a], Strekalovsky Victor[a], Malkov Andrey[b], Malkov Oleg[b], Puchin Vladimir[c], [a]*Institute of High-Temperature Electrochemistry, Ural Division RAS,* [b]*"ROSNA" Scientific and Production Center,* [c]*Institute of Metal Physics, UD RAS, Ekaterinburg, Russia*
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Transmission electron microscopy methods were used to study the evolution of formation of interblock boundaries in nanothin (80÷100 nm) crystals of hexagonal selenium growing in amorphous films at crystallization temperatures of 180÷120 °C.
The nanothin selenium crystals growing in amorphous films at crystallization temperatures of 180÷160°C were found to form rotational interblock boundaries with the modulus and the sign of the misorientation vector **ω** varying along the boundary (Fig.1a).
It was found that as the crystallization temperature decreased to 150°C, the nanothin selenium crystals formed boundaries, along which not only the modulus and the sign of the misorientation vector **ω** changed [1], but also a variable appeared, in addition to the rotational component, along the boundary of the slope component. (Fig.1b).
Distorted interblock boundaries appeared in the nanothin selenium crystals at a crystallization temperature of 140÷120°C. Along with the aforementioned crystal geometry parameters, the direction of the vector of the normal to the boundary surface changed at the distorted interblock boundaries. The sign of the distortion of the interblock boundary surface always matched the sign of the azimuthal distortion of the lattice in the nanothin selenium crystals (Fig.1c,d). The lattice of the nanothin selenium crystals underwent a rotational distortion generally around three mutually perpendicular directions. A decrease in the crystallization temperature from 180 to 120°C caused an increase in the density of interblock boundaries with variable crystal geometry parameters, which were formed in the nanothin selenium crystals.

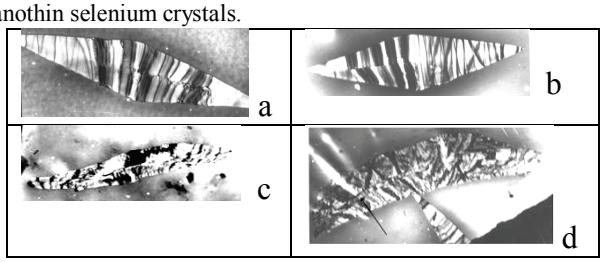

Fig. 1. Broken boundary with varying modulus **ω** (a); boundary with varying parameters of torsion and inclination (b); distorted boundaries and ensembles of boundaries in nanothin selenium crystals (c, d), ×10 000

It has been proposed to develop a model describing the formation of interblock boundaries with variable crystal geometry parameters in nanothin selenium crystals on the basis of concepts underlying relaxation of a nonuniform elastic rotational distortion of the lattice in a nanothin crystal of hexagonal selenium around [001].

[1] Malkov V.B. et al. Acta Cryst A. (2009). A.65. s340-s341

Keywords: selenium-1, crystals-2, boundaries-3

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High Brilliance microfocus beam delivery systems with scatterless collimation for SAXS. Vincent Roger[a], Pierre Panine, Blandine Lantz, Peter HOGHOJ
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Small Angle X-ray Scattering applications require sample illumination with a high brilliance x-ray beam having a well controlled spatial and angular distribution. Indeed high intensity at the sample is required with small beam expansion towards the detector to achieve low values of wave vector. We have developped a X-ray beam delivery system (the GeniX) made of a low power microfocus source and incorporating a unique combination of multilayer optics with innovative scatterless collimation for high performance SAXS in the lab.
The coupling of microfocus source with efficient aspheric multilayer optics (the FOX 3D optics) provides an intense x-ray beam with a well controlled beam propagation. Advantages in term of brightness preservation and range of wave vector reachable in SAXS, both for compact and for long-collimated setups will be reviewed. We will also present the new and innovative scatterless collimation integrated in the GeniX reducing parasitic slit scattering and providing simplified design. Advantages in terms of flux and resolution improvement compared to standard collimation will be detailed.
We will present SAXS data measurements acquired on high Z colloids, and polymer samples with different set-ups (radiation, detectors) illustrating the benefits of the new GeniX configuration.

Keywords: SAXS, High brilliance source, scatterless collimation