MS26 P06

Lattice Geometry Change of Nanothin Selenium Crystals with the Growth in Amorphous Films

V.B. Malkov[a], A.V. Malkov[b], O.V. Malkov[b], V.G. Pushin[c], B.V. Shulgin[d] [a]Institute of High-Temperature Electrochemistry, Ural Branch RAS, [b]"ROSNA" Scientific and Production Center, [c]Institute of Metal Physics, Ural Branch RAS, [d]Ural State Technical University.
E-mail: mvb@ihte.uran.ru

Keywords:selenium -1, crystals -2, Riman curvature - 3

The real structure of hexagonal selenium nanothin (100 nm.)crystals growing in amorphous films in the crystallization temperature range of 180÷140°C have been investigated by means of diffraction electron microscopy methods. It is shown that observed diversity of selenium nanothin crystals real structures types [1] is conditioned by diversity of relaxation processes types of non-uniform elastic rotational bending of selenium crystals lattice around c-axis. The classification of selenium nanothin crystals real structures types and the classification of relaxation processes causing their formation have been made.

It is revealed that with the crystal growth in amorphous films at 150÷140°C in the result of continuous non-linear relaxation of selenium crystals non-uniform elastic rotational lattice bending around c-axis the lattice geometry changes from Euclidean geometry to Riman geometry (Fig. 1). Given change of the lattice geometry is accompanied by effect of arc-shaped reflexes erosion on the electrronograms of investigated crystals.
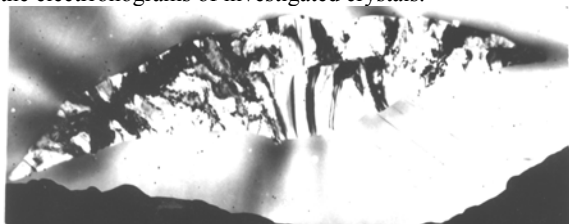

Fig. 1 Nanothin selenium crystal with Riman lattice geometry.

On the base of the consideration of nanothin crystal with rotational lattice bending as 2-d Riman space the equation for Riman curvature determining their lattice have been obtained. The methodic of Riman curvature determining of nanothin crystals lattice was elaborated. The values of Riman curvature of thin selenium crystals growing in amorphous films at crystallization temperatures of 150÷140°C have been obtained. Given values is compared with the values of Riman curvature of the crystal objects lattice which was obtained in the work.

[1] Bolotov I. E., Malkov V. B. *Proc. XI Int. Congr. On Electron Microscopy*. 1986, Japan, Kyoto, V.1., P.92

MS26 P07

Curvature-optimization of silica mesoporous crystals

Keiichi Miyasaka, Osamu Terasaki,
Department of Physical, Inorganic and Structural Chemistry, Stockholm University, Sweden.
E-mail: kei@struc.su.se

Keywords: mesoporous material, curvature, curvature elastic energy

We present self-consistently determined structures of silica mesoporous crystals (MCs) based on the minimization of the curvature elastic energy, along with the investigation of the curvature properties on the isosurface of the 3D electrostatic potential density (EPD) map of such MCs; (i)bicontinuous type: MCM-48 (*Ia3d*) and AMS-10 (*Pn3m*), (ii)cage-type: SBA-06 (*Pm3n*), SBA-12 (*Fm3m*), SBA-16 (*Im3m*) and AMS-8 (*Fd3m*). This way allows us to determine the framework structures of porous solids independently of gas adsorption experiment, which includes the information about the pore volume and the surface area.

A characteristic feature of silica MCs is that the disorder on the atomic scale and the well-defined order on the mesoscopic scale, where mesoscopic pores (2 – 50 nm) are periodically arranged in 2D/3D manner.[1] Direct derivation of such 3D crystal structures have been provided previously on the basis of transmission electron microscopy (TEM) observation and electron crystallography imaging.[2]

Syntheses of silica MCs are generally based on the cooperative self-assembly of surfactants and silica precursors in the presence of water. In the end of the synthesis, the space occupied by surfactants is replaced with pores through the calcination process. Therefore, the structure of silica MCs can be interpreted as the "frozen" version of the mesostructure resulting from surfactants' self-organization. In this regard, it is natural to consider the boundary surface between the silica wall and the pore region to reflect the shape of the self-assembled micelles, in which the curvature elasticity plays a dominant role.[3] We intend to optimize those silica mesostructures by the minimization of the curvature elastic energy that is described in terms of invariants of curvatures, i.e. the mean curvature and the Gaussian curvature. In other words, the level depth of the EPD distribution of such mesostructures derived from TEM observation, is decided heading toward the constant mean curvature surface. The result shows that the bicontinuous structures generally permit homogeneous surfaces. Whereas some caged mesostructures unexpectedly exhibit negative Gaussian curvature distribution on their surfaces.

[1] Kresge, C. T.; Leonowicz, M. E.; Roth, W. J.; Vartuli, J. C.; Beck, J. S. *Nature*, 1992, 359, 710.
[2] Y. Sakamoto, Y.; Kaneda, M.; Terasaki, O.; Zhao, D.; Kim, J.-M.; Stucky, G. D.; Shin, H. J.; Ryoo, R. *Nature*, 2000, 408, 449.
[3] Helfrich, W., *Z. Naturforsch. Teil C*, 1973, 28, 693.