[1] Paz F.A.A., Klinowski J., *J. Solid. State Chem*, 2004, **177**, 3423. [2] Paz F. A.A., Shi F.-N., Klinowski J., Rocha J., Trindade T., *Eur. J. Inorg. Chem*, 2004, **13**, 2759. [3] Paz F.A.A., Shi F.-N., Klinowski J., Rocha J., Trindade T., *submitted.*

Keywords: coordination polymers, frameworks, materials

P.11.15.9

Acta Cryst. (2005). A**61**, C404

Structure Fingerprints of Ordered Mesoporous Silica

Marcia C. A. Fantini[a], Luis Silva[b], Jivaldo Matos[b], Lucildes Mercuri[c], [a]*Instituto de Física, Universidade de São Paulo.* [b]*Instituto de Química, Universidade de São Paulo .*[c]*UNICSUL, São Paulo, Brazil.* E-mail: mfantini@if.usp.br

Mesoporous materials present structural complexity, that together with the small volume of ordered domains, make it difficult the precise assignment of their structure. The combination of many different characterization techniques, like X-ray diffraction (XRD) or scattering (SAXS), transmission electron microscopy (TEM) and electron diffraction (ED) are necessary to properly determine the mesoporous structure. The use of different templates, like block copolymers (PEO-PPO-PEO; PEO-PBO-PEO) and methyl-ammonium compounds (CTAB), gives hexagonal and cubic silica structures having different pore's diameter and wall thickness. In this work, the optimized synthesis of hexagonal *P6$_3$/mmc* SBA-15 and MCM-41 and, cage-like cubic *Fm3m* FDU-1 and *Im3m* SBA-16 are described. The samples were prepared with commercial TEOS and Cab-O-Sil silicon sources. The as-synthesized and calcined (at 540^{o}C) powders were analyzed by SAXS, TEM and N_2 gas adsorption, allowing a precise determination of the different material's structure, by the recognition of typical results.

The cubic structures present larger lattice parameter; the FDU-1 has a ~20 nm and, SBA-16 has a ~14 nm. The hexagonal SBA-15 and MCM-41 have a ~ 5 nm. Besides the analysis of the diffraction peaks, information on the non-ordered pores and micropores in the silica walls were also obtained from the SAXS data. The extent of pore's shrinkage effect, due to the calcination process, was also analyzed.

Keywords: porous solids, silicon oxides, small-angle diffraction

P.11.15.10

Acta Cryst. (2005). A**61**, C404

Design of Porous Bilayer Compounds Containing 1D Channels

Kjell Ove Kongshaug, Helmer Fjellvåg, *Department of Chemistry, University of Oslo, Oslo, Norway.* E-mail: k.o.kongshaug@kjemi.uio.no

In the concept of reticular synthesis of porous metal-organic framework (MOF) structures [1], the inorganic secondary building units (SBU) described most often consist of a limited number of metal centres. However, larger structural motifs may also lead to porous MOF structures. In particular, Kitagawa et al. [2] have shown how 2D layered structural motifs can be pillared into 3D porous structures.

Recently, Wu et al. [3] reported a novel MOF structure based around infinite 2D layers of tetrahedral Zn and 5-aminoisophthalic acid (aip) ligands showing a dense triangular topology. By introduction of 4,4-bipyridine, 1,2-di(4-pyridyl)ethylene, 1,2-di(4-pyridyl)ethane and 1,3-di(4-pyridyl)propane, respectively, into mixtures of dimethylformamide and water with $Zn(NO_3)_2$ and aip, we are able to synthesize a series of isostructural pillared bilayer compounds built around these triangular Zn(aip) layers. In all four compounds, the pillars are creating spaces inside the bilayers resulting in 1D channels with dimensions of 3.5x6.7 Å^2. Inside these channels there are water molecules that can be removed upon heating to 150^{o}C. The structural integrity of the compounds is maintained after removal of the water molecules, resulting in porous structures with estimated free volumes in the range of 20.7 to 25.5% of the unit cell volumes.

[1] Yaghi O.M., O'Keeffe M., Ockwig N.W., Chae H.K., Eddaoudi M., Kim J., *Nature*, 2003, **423**, 705. [2] Kitagawa S., Kitaura R., Noro S., *Angew. Chem. Int. Ed.*, 2004, **43**, 2334. [3] Wu C.D., Lu C.Z., Yang W.B., Zhuang H.H., Huang J.S., *Inorg. Chem.*, 2002, **41**, 3302.

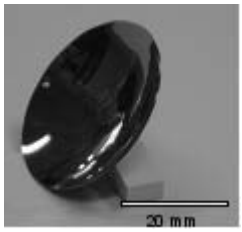
Keywords: single-crystal structure determination, coordination polymers, porous materials

P.11.16.1

Acta Cryst. (2005). A**61**, C404

Si Crystal Mirrors prepared by Plastic Deformation for Solar Cell Systems

Kazuo Nakajima[a], Kozo,Fujiwara[a], Wugen Pan[a], Hiroshi Okuda[b], [a]*Institute for Materials Research, Tohoku University.* [b]*International Innovation Center, Kyoto University.* E-mail: nakajimk@imr.tohoku.ac.jp



No one has ever intentionally undertaken to obtain shaped Si crystal wafers by plastic deformation. If plastically deformed Si crystals could be freely obtained, new applications based on various creative concepts could be actively developed in a wide range of fields. In this paper, we report on the successful plastic deformation of Si crystal wafers for the preparation of wafers with various shapes. A Si wafer was set Fig. 1 A Si crystal mirror between dies and pressed at high temperatures.

One application of shaped wafers is as well-shaped concaveSi crystal lenses or mirrors [1,2] as shown in Fig. 1. The lattice plane of such a crystal lens has a curvature exactly along the surface.

A new solar cell system is proposed and demonstrated with the concave Si crystal mirror used as both a solar cell and a focused mirror. The effective number of total photons is the sum of photons from both the mirror solar cell and the small cell set at the focused spot, and it determines the efficiency of the entire system. The total conversion efficiency of the present system using the focused solar beam increases to 12.2 % comparing with the conversion efficiency of 9.2 % only for the concave Si mirror solar cell. This system can make effectively use of the reflected photons from solar cells.

[1] Nakajima K., Fujiwara K., Pan W., Okuda H., *Nature Materials*, 2005, **4**, 47. [2] Nakajima K., Fujiwara K., Pan W., *Appl. Phys. Lett.*, 2004, **85**, 5896.

Keywords: deformation, silicon crystals, solar cells

P.11.16.2

Acta Cryst. (2005). A**61**, C404

Low Temperature Anomaly of Plasticity and a Local Arrangement in Pb-In Alloys

Vitalyi V. Pustovalov, I.S. Braude, N.V. Isaev, V.D. Natsik, S.E. Shumilin, V.S. Fomenko, B.I. Verkin, *Institute for Low Temperature Physics and Engineering NAS of Ukraine, 47, Ave. Lenin, Kharkov, 61103, Ukraine.* E-mail: pustovalov@ilt.kharkov.ua

The temperature dependencies of the yield stress and the strain rate sensitivity of flow stress for Pb-1; 5; 10 and 20 at. % In single crystals were studied by tension in the temperature range 0,5 - 295 K. For Pb-1;5 and 10 at. % In the dislocation-impurity interaction parameters estimated from the experimental data were found typical for thermally activated depinning of dislocations from solute atoms at deformation temperatures 30 – 140 K. The anomaly of plasticity in these alloys below 30 K is consistent with the inertial unzipping of dislocations from impurity atoms. However, a further increase in indium concentration up to 20 at. % it was found affect the experimental dependencies, contradicting the above conclusions. The estimated plasticity parameters of concentrated alloy are seems to be atypical for the case of impurity atom as an effective barrier for mobile dislocations. For understanding this contradictions the Cowley's local order parameters α was estimated from the diffuse X-ray scattering measurements. The expected positive values of α indicate that clustering takes place in this system.. For Pb-1 at. % In alloy α= 0, but as the indium concentration increase the clustering becomes more dominant. The interaction of clusters with mobile dislocations leads to modify the mechanisms of low temperature plasticity and can explain the experimental data for concentrated alloy.

Keywords: low temperature, plasticity, local order