MS14. Mineralogical crystallography: Nature as a source of inspiration for new materials

Chairs: Nikolai Eremin, Rossella Arletti

MS14-O1 High pressure synthesis and structural studies of zeolite/polymer nanocomposites

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Zeolites represent an important family of porous materials based on corner sharing TO_4 (T=Al, Si) tetrahedra. The microporous nature of these materials allows insertion of a great variety of guest atoms, ions or molecules giving rise to a large number of technological applications in catalysis, molecular sieves and ion-exchange materials. Polymerization of simple organic molecules under high pressure in the subnanometric pores of pure SiO_2 zeolites can be used to produce novel nanocomposite materials, which can be recovered at ambient P and have remarkable mechanical, electrical or optical properties. Polymerization of ethylene in silicalite results in a nanocomposite with isolated chains of non-conducting polyethylene strongly confined in the pores based on single crystal x-ray diffraction data. Compared to the initial silicalite, the nanocomposite is much less compressible and has a positive rather than a negative thermal expansion coefficient. In order to target novel electrical and optical properties, isolated chains of conducting polymers can also be prepared in the pores of zeolite hosts at high pressure, such as polyacetylene, which was polymerized under pressure in the pores of the 1-D zeolite ZSM-22. The structure of this nanocomposite was determined by synchrotron x-ray powder diffraction data with complete pore filling corresponding to one planar polymer chain confined in each pore with a zig-zag configuration in the *yz* plane. This very strong confinement can be expected to strongly modify the electrical properties of polyacetylene. In this nanocomposite, our theoretical calculations indicate that the electronic density of states of polyacetylene exhibit van Hove singularities related to quantum 1D confinement, which could lead to future technological applications. This new material is susceptible to have applications in nanoelectronics, nanophotonics and energy and light harvesting. A second completely novel nanocomposite was prepared by the polymerization of carbon monoxide CO in silicalite. The polymer chains could be readily located on Fourier difference maps and the structure refinement shows that the isolated single polymer chains exhibit orientational and translational disorder. These polymer chains are, however, more stoichiometric and less branched than bulk polymers obtained by high pressure polymerization of this simple system. The polyCO/zeolite composite could be an interesting energetic material.

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