

Keywords: fiber texture, strain, Laue symmetry

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Local structure of the tetragonal phase in nanostructured zirconia-based solid solutions

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Zirconia-based ceramics are widely used because of their electrical and mechanical properties. Pure ZrO₂ exhibits 3 polymorphs of monoclinic (m), tetragonal (t) and cubic (c) symmetries. The m phase is stable at room temperature and transforms to the t one at 1170°C during heating, while this phase transforms to the c one at 2370°C. The c phase can be fully stabilized at room temperature by doping with other oxides (Y₂O₃, CaO, CeO₂, etc.). The t phase can not be fully stabilized, but it can be retained, in a metastable condition, in nanopowders and fine-grained ceramics. In previous works, we studied the crystal structure and the local order of ZrO₂-based nanomaterials with compositions close to the t/c phase boundary. EXAFS study showed that the t-to-c transition observed by XRD is only related to a symmetry change of the local order around Zr⁴⁺ cations. We also found that the expected crystallographic model (two oxygen subshells with 4+4 oxygen atoms) does not agree with EXAFS data, while a 5+2 model yields better agreement factors. It is worth to remark that, while the sevenfold coordination of Zr⁴⁺ cations has already been proposed for the c phase and attributed to the presence of oxygen vacancies that are preferentially located around Zr cations, only a few papers reported this coordination for the t phase. In this work, we present an EXAFS study of Zr-O bond in pure or lightly-doped ZrO₂ nanopowders that exhibit the retention of the t phase in metastable condition. The results on Zr-O bond were compared with those obtained by synchrotron radiation XRD analysis in order to establish a model for the local structure around Zr atoms that agrees with the crystal structure accepted for the t phase. The influence of the crystallite size was also investigated.

Keywords: ZrO₂, nanomaterials, EXAFS

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Phase separation inside the CdTe-CdSe type II quantum dots revealed by synchrotron PXRD and SAXS

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Using synchrotron powder X-ray diffraction and small-angle X-ray scattering (SAXS), we have studied the structures of the two CdSe/CdTe and CdTe/CdSe type II quantum dots (QDs), including the crystalline structure, particle shape and size, as well as phase separation of the two components. The X-ray results suggest that the spherical CdTe/CdSe QDs of a size of ~8 nm, synthesized in a two-step procedure with CdTe nanoparticles (4 nm) as nuclides, have a structure of a CdTe-rich core enclosed by a CdSe shell. On the other hand, the spherical CdSe/CdTe QDs of a size of ~9 nm, synthesized in a similar two-step procedure but with CdSe nanoparticles (~3 nm) as nuclides, show mainly one phase structure with a uniform distribution of CdSe and CdTe. The phase separation of the two components CdSe and CdTe inside the two QDs, a decisive factor in the photovoltaic applications, is furthermore examined using anomalous SAXS for a consistent conclusion. For comparison, single phase nanoparticles CdSe and CdTe are also examined. The correlation between the synthesis procedures and the structures of the QDs is discussed.

Keywords: CdTe-CdSe, quantum dots, PXRD and SAXS

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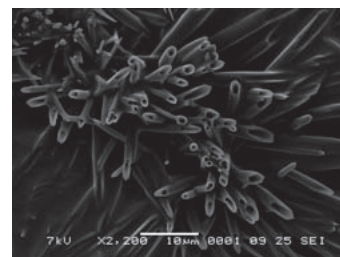
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Teaching an old molecule new tricks: A novel tubular morphology of caffeine

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Crystals of caffeine with a novel tubular morphology have been prepared. Scanning electron microscopy (SEM) images of caffeine crystallised by rapid evaporation from solution show a network of interlinked hollow tubes with hexagonal cross-section and internal diameter of 0.5-5 μm. X-ray powder diffraction (XRPD) analysis demonstrates that these tubular structures are of the metastable, trigonal polymorph of caffeine, form I. The application of transmission electron microscopy (TEM) to the study of this species will be presented and the use of this technique as a tool to study pharmaceutical compounds in general will be discussed.



Keywords: nanotubes, pharmaceuticals, transmission electron microscopy