

X-RAY LINE BROADENING STUDY OF TETRAGONAL ZIRCONIA NANOPOWDERS SYNTHESIZED BY GEL-COMBUSTION

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Tetragonal zirconia ceramics have excellent electrical and mechanical properties. However, the physical mechanisms involved in the stabilization of the metastable tetragonal phase at room temperature are not well known yet. This phase can be retained in ceramic specimens provided that the grain size is smaller than a critical value (about 1 micron). In the case of powders, it has been established that the crystallite size must be nanometric (the surface free energy has a very important role), but the influence of stresses and defects are not fully understood. The aim of this work was to study the stability of yttria or ceria-doped tetragonal zirconia nanopowders synthesized by different gel-combustion routes. These methods are based on the gelling of a nitrate solution of the desired metals and some organic fuel (glycine, citric acid, etc.) followed by an intense combustion due to the exothermal redox reaction between nitrate ions and the fuel. The powders were characterized by X-ray diffraction applying the Rietveld method. A conjunct analysis of crystallite size and microstrain was carried out employing the multiple-line integral breadth method and assuming Lorentzian and Gaussian components for both effects. The crystallite size profile presented both components, being the Lorentzian the most important. On the contrary, the microstrain profile had a negligible Gaussian component, which is an interesting result since it is generally represented by a Gaussian function. It was also found that both, crystallite size and microstrains, affect the stability of the tetragonal phase.

Keywords: LINE BROADENING NANOPOWDERS TETRAGONAL ZIRCONIA

NOVEL METAL HALIDE STRUCTURES IN HYBRID ORGANIC/INORGANIC SYSTEMS

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The crystal structures of a series of Cd(II), Pb(II) and Cu(I) halides salts are reported and the role of hydrogen bonding in stabilizing unusual coordination networks in hybrid organic/inorganic salts will be discussed. The structures of (MEDA)_nCd₄Cl₁₀·xH₂O, (MEDA)_nCd₃Br₈·xH₂O and (Et₂NH₂)₃Pb₃X₉·xH₂O all contain extended arrays based on edge-shared octahedra [MEDA = (CH₃NH₂C₂H₄NH₃)²⁺, X = Br, I]. The presence of the organic cations leads to decimation of the CdX₂ parent structures to yield novel low dimensional lattices. The first Cd compound contains simple [Cd₄Cl₁₀]_n²ⁿ⁻ ribbons cut from the parent structure. In contrast, the Pb salts contain [Pb₃X₉]_n³ⁿ⁻ columns that are polytypes of such simple ribbons, with the polytypic nature forced by the N-H...X hydrogen bonding. The Cd/Br salt contains a novel layer structure obtained by perforation and reconstruction of the parent CdX₂ structure.

The structures of the (CHA)₁₀Pb₇X₂₄ salts (X = Br, I) contains another novel layer structure composed of ribbons of corner-shared octahedra connected by columns of face-shared octahedra, while the (CHA)₂PbX₄ salts have simple layer perovskite structures [CHA⁺ = cyclohexylammonium].

Finally, the compounds (MEDA)_nCu₂Br₄ and (EEDA)_nCu₂Br₄ have layered structures composed of chains of face-shared tetrahedral linked by a tight N-H...Br network

TOPOLOGICAL ANALYSIS OF DEFECTS IN GAN EPITAXIAL FILMS

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High quality thin films of GaN are required for microelectronic and optoelectronic devices. In current methods for the epitaxial growth of these films, such as metal-organic chemical vapour deposition and molecular beam epitaxy, substrates of alumina, silicon carbide or silicon substrates are used. Because the lattice parameters and/or spacegroups of these materials are different from the overlying GaN films, the formation of interfacial and bulk defects is promoted. The topological properties of such defects can be predicted a priori using symmetry theory; their diversity and character depend on the extent of symmetry-breaking accompanying the formation of a bicrystal. Also, when experimental observations of defects have been obtained by techniques such as transmission electron microscopy, circuit-mapping methods can be used a posteriori to characterise linear and planar defects. These crystallographic tools will be illustrated by reference to predicted and experimentally observed defects in epitaxial GaN films.

QUANTITATIVE DETERMINATION OF THE MINERALOGICAL CONSTITUTION OF A BRAZILIAN SOIL

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Samples of Dark-Red Latosol from Ponta Grossa, PR, Brazil, were collected from horizons HA (less than 13cm deep), HB (13 to 29 cm deep and HC (89 to 116cm deep). The textural analysis revealed respectively 45, 47 and 52% clay, 13, 15 and 14% silt and 42,38 and 34% sand. The samples of each horizon were fractionated in 4 particle sizes: coarse sand (from 53 micrometer to 1mm), fine sand (20 to 53 micrometers), silt (2 to 20 micrometer) and clay (less than 2 micrometer). Prior to the Rietveld refinement the qualitative constitution of this soil was determined from *in situ* XRD at several temperatures and from X-ray fluorescence, Infra Red and Mossbauer spectroscopy that revealed the presence of the following minerals: HA, HB and HC clay fractions: quartz, hematite, gibbsite, anatase, rutile, hematite, goethite, and the clay minerals of the kaolin group: kaolinite, nacrite and halosite. HA, HB. And HC silt fraction: same as clay except nacrite., HA fine sand fraction: quartz, anatase, hematite, and rutile. HB: same as HA except rutile, HC only quartz and anatase. HA, HB and HC: coarse sand fraction: only quartz. Powder X-ray diffraction data were collected using a Rigaku-Denki rotating anode generator, copper K-alfa radiation, theta-2theta, step mode from 3 to 100 degrees, steps of 0.02 degrees, step counting time 5sec. For the clay fraction the Rietveld refinement attained final Rp values of 0.064, 0.062 and 0.067; for fine sand fraction, final Rp values of 0.130, 0.129 and 0.141, and final Rp values of 0.096, 0.105 and 0.124 for coarse sand. Acknowledgements are due to CAPES, CNPq/PADCT and FAPESP.