The Structure and Morphology of TiO_2-B Nanoparticles

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Nanosized titania, the TiO_2-B phase in particular, show significant promise as an anode material for rechargeable Li batteries, with higher capacity, increased rate capability and decreased capacity fade compared with the bulk material. Superior qualities of nanomaterials are attributed to the size effects, to the arrangement of atoms within the materials and to their morphology. Here we report investigation of the structure and morphology of the TiO_2-B nanoparticles with the dimensions of several nanometers using powder diffraction and computational modeling. Establishing the structure of nanomaterials from diffraction is a challenge because their nm dimensions often precludes the use of crystallographic methods of data analysis. By utilizing the fundamental Debye equation of diffraction and global optimization techniques, the structure and the shape of the particles were refined from X-ray diffraction data without crystallography. The established, non-spherical, shape of the nanoparticulate TiO_2-B has also been obtained from computer simulation, but only by explicit calculation of the total energy of the nanoparticle structure, including bulk and surface atoms, and surface adsorption.