

Orientation effects in morphology and electronic properties of anatase TiO₂ one-dimensional nanostructures. II. Nanotubes

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Abstract

In the first part [D. B. Migas *et al.*, *Phys. Chem. Chem. Phys.*, 2014, DOI: 10.1039/C3CP54988G] by means of *ab initio* calculations we have analyzed and discussed anisotropy effects on electronic properties of <001>-, <100>- and <110>-oriented anatase TiO₂ nanowires. In this part we present results indicating crucial changes in morphology of anatase TiO₂ nanotubes originating from TiO₂ nanowires by making a hole along the wire axis. The critical wall thickness has been found to exist for the nanotubes with <001> and <110> axes: at smaller thickness their shape can be rounded, squeezed, viewed as conglomerates of nanocrystals and even represented as cylindrical and 'single-walled'-like structures formed without rolling up a thin titania layer into a nanotube. In general, band dispersion near the gap region of TiO₂ nanotubes is close to the one of TiO₂ nanowires with the same orientation. We have also revealed that optimization of the unit cell parameter along the wire axis and consideration of quantum confinement and surface state effects are important to provide an interpretation of band-gap variation with respect to wall thickness in TiO₂ nanotubes.