Analysis of Sb dopant influence on SnO_2 nanoparticles morphology and growth mechanism

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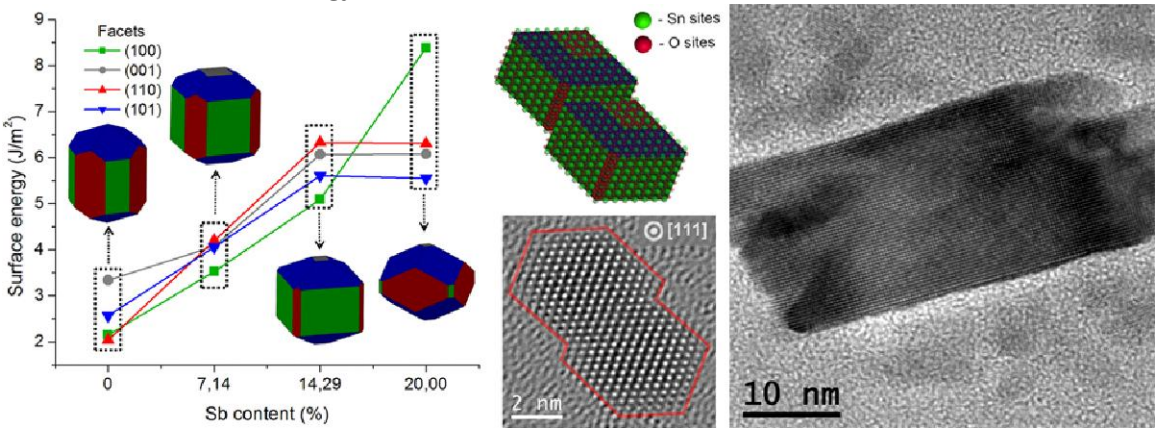
The development of novel and reliable nanostructured devices requires the ability to synthesize and characterize materials on the atomic scale. Among the most significant challenges in nanostructural characterization is the evaluation of crystal growth mechanisms and their dependence on the distribution of doping elements.

This work provides an evaluation of Sb dopant influence on SnO_2 nanoparticles morphology and growth mechanism by the combined use of HRTEM characterization and *ab initio* calculations for surface energy. SnO_2 and Sb:SnO_2 ($18\%_{atom}$) nanocrystals were obtained by a nonaqueous synthesis route. HRTEM characterization was performed using a JEM-3010 URP at 300 kV with a LaB_6 electron gun. Wulff construction using the *ab initio* calculated surface energies was applied to model the nanocrystals.

Oriented attachment was identified as the growth mechanism for both systems and the preferential growth directions, [110] for the SnO_2 nanocrystals and [100] and [101] for Sb:SnO_2 nanocrystals, could be successfully described by the *ab initio* calculated surface energy distribution.



a) Wulff constructions using *ab initio* calculated surface energies for different Sb dopant concentration, b) Nanocrystals modeling and HRTEM image simulation for Sb:SnO_2 oriented attachment and c) highly crystalline SnO_2 nanoparticle.

Keywords: HRTEM, Dopant Distribution, Oriented Attachement, Surface Energy *ab initio* Calculation.

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