Maria A Caravaca et al., J Nanomater Mol Nanotechnol 2018, Volume 7
DOI: 10.4172/2324-8777-C1-021

Strain effects on the elastic and electronic properties of Core/Shell nanowires of ZnO/X (X=ZnS, BeO)

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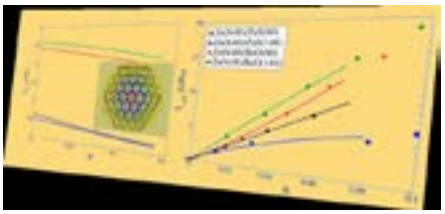
ZnO is an important semiconductor due to its wide range of technological applications, which are based on their properties like as direct band gap, high conductivity and piezoelectricity. Some of them are improved at the nanoscale. In the last years, ZnO/X (X=ZnS, BeO) nanowires have demonstrated an upgrade in piezoelectronic sensons, photovoltaic cells and optoelectronic devices than nanowires based on a singular ZnO. However, the elastic properties have been scarcely explored. For that reason, we present an ab initio study about properties such as Young Modulus, Poisson ratio, band gap and formation energy relative to nanowires sizes diameters. In order to contribute in the design criteria, we have studied the effects on the elastic and electronic properties of uniaxial strain along the [0001] direction on hexagonal cross-sectional nanowires whose diameters range from 1.0 to 2.88 nm. We found an improved in elastic properties with respect to ZnO single crystal. For the case of ZnO/shell nanowires, if the ZnS layers are added the Young modulus, Poisson ratio and gap energy decrease, but if the BeO layers are added, the Young and Poisson ratio decrease while the band gap increase. Respect to the maximum strain, we found is very sensitive to the shell type. Therefore, we could modulate the elastic properties and modify the toughness according to the shell chemical elements and their wide. Apart from this, the calculated effective mass was found larger in nanowires than ZnO single crystal. The addition of ZnS layers increase the surface energy compared with BeO layers of the same sizes. By means of the density of states, we can show the contribution of the surface atoms to states near to the Fermi level and distinguished by the shell type.



Recent Publications

1. Ab-initio study of structural, elastic and electronic properties of core/shell nanowires. Lucy A.Valdez, Ricardo A. Casali. Revista Matéria, v 23, nro 2 (Accepted manuscript, June 2018).
2. H.T. Girão, T. Cornier, S. Daniele, R. Debord, M.A. Caravaca, R.A. Casali, P. Mélinon, D. Machon, Pressure-Induced Disordering in SnO2 Nanoparticles, J. Phys. Chem. C 121, 15463 (2017).

Biography

In memory of Ricardo A. Casali, who was our respected and enthusiastic collaborator. He was completed his PHD at IFLISYB Universidad Nacional de La Plata, Argentina and postdoctoral studies at AARHUS University of Denmark and at IHP at Frankfurt Oder Germany. He was Director of different projects of PHD students and referee of scientist journals. He was Professor at Universidad Nacional del Nordeste, Argentina and published more than 25 papers in reputed journals. He began his theoretical studies describing the static and dynamic properties of semiconductors with point and complex defects, thermoelastic properties of high hardness oxides and was currently applied to describe the electronic thermodynamic, vibrational properties of SnO2 and TiO2 nanoparticles. His last topic was to characterize the elastic and electronic properties of Core/Shell nanowires.

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