Elastic and piezoelectric properties of nanowires: from atoms to continuum,from chemistry to mechanics

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Abstract

Experimentally, mechanical and piezoelectrical properties of individual nanowires have been extensively explored. However, predicting properties of structures or composites based on electromechanic nanowires is highly challenging and remains an open problem for the following reasons: (a) the multiscale nature of the problem: the response of the composite is macroscopic, while the structure is defined at the nanoscale level, and the properties of the constituents, as well as the interactions (interfaces mechanics) between the constituents must be predicted at the atomic scale. Furthermore, determining the different coefficients associated with the properties at the nano/atomic level requires ab initio quantum mechanics calculations; (b) electromechanical models for continuum mechanics describing surface effects due to the nanoscale have not been proposed so far; (c) the computational costs can be out of scope if we do not introduce appropriate couplings between scales and models to take maximum advantage of each model in its range of validity. Thus, multiscale modelling strategies as well as novel numerical methods seem the only way to fully describe electromechanical nanowire-based composites.

Starting from fully atomistic calculations, we have developed a classical, continuous mechanics, model of wurtzite nanowires, using FEM discretization. Ab initio calculations of AlN and ZnO wurtzite [0001] nanowires have been performed with diameters up to 4 nm. It is shown that the nanowires can be well represented by an internal part with AlN bulk elastic properties, and one-atomic surface layer with its own elastic behaviour. To deal with more nanostructures/nanoparticles complex geometries, a finite element method using surface elements with their own elastic properties is developed. The surface elastic coefficients are provided by ab initio calculations through a slab procedure. The finite element model is compared with the full ab initio nanowires calculations and a good agreement is demonstrated.