Multiscale modeling of piezoelectric nanowires with surface effects based on ab initio calculations

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A multiscale procedure for modeling piezoelectric crystalline nanostructures such as nanowires is proposed. The size effects exhibited by nano objects are captured by taking into account a surface energy, following the classical Gurtin-Murdoch surface elasticity theory and related extensions in the case of piezoelectricity. An appropriate variational form and a finite element approach are provided to model and solve the relevant problems numerically. We describe a simplified technique based on projection operators for constructing the surface elements. The methodology is completed with a computational procedure based on *ab initio* calculations to extract elastic and piezoelectric coefficients of general anisotropic surfaces. The FEM continuum model is validated by comparisons with full *ab initio* models of nanowires with different diameters where size- dependent electro-mechanical properties are observed. The piezoelectric FEM continuum model can then be used to model similar nanostructures in ranges of sizes or geometries where analytical or atomistic model are limited. The validated model is applied to energy harvesting systems made of AlN, Zno, and GaN nanowires.

Keywords: Surface effects, nanowires, piezoelectricity, size-effects, multiscale methods.