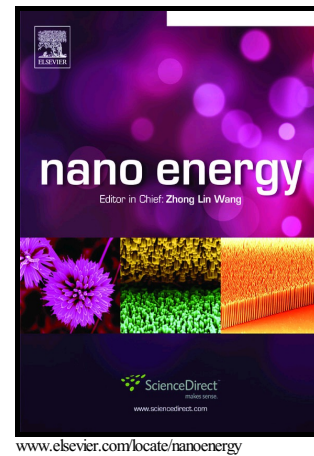


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Mechanisms underlying the shape effect on nano-piezoelectricity

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Abstract

Piezoelectric nanowires (NWs) or nanotubes (NTs) are a vital component in nano-electromechanical and piezo-electronic device development. With various cross-sectional geometries achievable, the piezoelectric property-cross sectional shape relation is of fundamental interest. As existing studies (primarily based on first-principles calculations) are limited to ultrathin NWs or analysis based on continuum theories, the present work employs molecular statics (MS) simulation, which enables the examination of NWs/NTs up to cross-sectional size of $20.6nm$ and elucidation of the underlying mechanisms at the atomic level. Analyses are carried out for NWs/NTs with experimentally observed geometry by comparing their size-dependence of effective piezoelectric constant and the radial distribution of the average dipole moment change with strain. The fraction of strain-sensitive dipoles, initial volume contraction and surface piezoelectricity were shown to control the shape effect on the piezoelectricity of ZnO nanostructures.

Keywords: Zinc oxide Nanowires, shape effect, piezoelectric constants, volume contraction

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