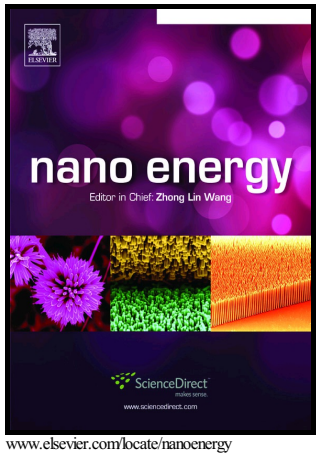
Mechanisms underlying the shape effect on nano-piezoelectricity

R.J. Wang, C.Y. Wang, Y.T. Feng, Chun Tang



www.elsevier.com/locate/nanoenergy

PII: S2211-2855(18)30675-X
DOI: https://doi.org/10.1016/j.nanoen.2018.09.031
Reference: NANOEN3036

To appear in: *Nano Energy*

Received date: 19 July 2018
Revised date: 6 September 2018
Accepted date: 14 September 2018

Cite this article as: R.J. Wang, C.Y. Wang, Y.T. Feng and Chun Tang, Mechanisms underlying the shape effect on nano-piezoelectricity, *Nano Energy,* https://doi.org/10.1016/j.nanoen.2018.09.031

Mechanisms underlying the shape effect on nano-piezoelectricity

R.J. Wang[1], C.Y. Wang[1*], Y.T. Feng[1], Chun Tang[2]

[1]Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, Bay Campus, Swansea, SA1 8EN, UK

[2]Faulty of Civil Engineering and Mechanics, Jiangsu University, No. 301 Xuefu Road, Zhenjiang, Jiangsu, P.R. China 210013

*Corresponding author: chengyuan.wang@swansea.ac.uk

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 20.6*nm* 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