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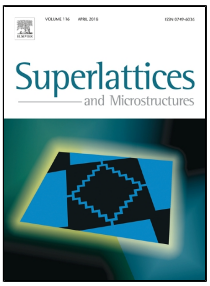

First-Principles Investigation of Size-Dependent Piezoelectric Properties of Bare ZnO and ZnO/MgO Core-Shell Nanowires

Ye Wu, Zi-Chang Zhang, Shaikh Ahmed

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First-Principles Investigation of Size-Dependent Piezoelectric Properties of Bare ZnO and ZnO/MgO Core-Shell Nanowires

Ye Wu, Zi-Chang Zhang, and Shaikh Ahmed

Department of Electrical and Computer Engineering, Southern Illinois University at Carbondale
1230 Lincoln Drive, Carbondale, IL 62901, USA. (E-mail: yewu@siu.edu, zichang@siu.edu, ahmed@siu.edu)

Abstract:

Using first-principles density functional theory (DFT) calculations, we evaluate and compare the piezoelectric properties in *bare* ZnO and ZnO/MgO *core-shell* nanowires. The study confirms that effective piezoelectric coefficient in bare ZnO nanowires is a highly diameter sensitive parameter. In the thinnest ZnO nanowire, with only one layer of atoms, the effective piezoelectric coefficient attains a maximum value of 12.21 C/m^2. On the other hand, for the first time, we report that piezoelectricity in MgO-passivated ZnO nanowires exhibits a *lesser* size dependence than in the bare ones, a finding that may prove useful in the design of emerging ultraviolet optoelectronic devices.

Keywords:

ZnO; ZnO/MgO nanowire; DFT calculation; piezoelectric properties; surface passivation