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Atomistic Mechanical Testing of Nanostructures – Seeing the Invisible and Bridging Theory and Experiments

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Recently there has been a major thrust to develop novel nanomaterials exhibiting unique electro-mechanical properties. These nanostructures are envisioned as building blocks for the next generation of electronic and energy harvesting systems. In this context, identification of size dependent properties is essential. Here, a MEMS-based device for in-situ electron microscopy testing of one dimensional nanostructures will be introduced and used to identify mechanical property size effects in ZnO and GaN nanowires. The validity of force fields commonly used to model these semiconducting materials will be discussed by comparison to experimental findings and quantum mechanical simulations. It will be shown that force fields are accurate enough to capture elasticity but that higher order theories are needed to interpret nanowire failure. Furthermore, while both ZnO and GaN possess the same crystal structure, they exhibit quite different elastic and piezoelectric size dependences. Opportunities arising from such size effects in energy harvesting applications will be given as conclusion.

Keywords: Nanowires;Nanotubes;In-situ TEM;Atomistic Simulations;Size-Effects;

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