SIZE EFFECT IN THE ELASTIC RESPONSE OF ZNO NANOWIRES, El. E. Gdoutos[1], R. Agrawal[1], B. Peng[1], H. D. Espinosa*[1], Northwestern University[1], Department of Mechanical Engineering, Evanston, IL 60201

Understanding the mechanical properties of ZnO nanowires is central to their application in sensors, transducers and actuators used in micro- and nano- electromechanical systems (MEMS and NEMS). In this work the results of Molecular Dynamics simulations of ZnO nanowires of crystallographic orientation [0001] are presented. The Buckingham interatomic potential in conjunction with the summation proposed by Wolf was used to model nanowires with more than a million atoms at room temperature. It was found that the Young's modulus of hexagonal [0001] oriented ZnO nanowires increases from 169 GPa to 194 GPa as the wire diameter decreases from 20 nm to 5 nm. This size effect originates from surface reconstruction, which becomes more important with increasing surface to volume ratio. These results are in agreement with experimental data [1] showing an increase in the Young's modulus of ZnO nanowires with a decrease in diameter in a range smaller than 80 nm.

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1. R. Agrawal, B. Peng, E. Gdoutos, and H. Espinosa, *Elasticity Size Effects in ZnO Nanowires - A Combined Experimental-Computational Approach*. Nano Letters (Accepted for Publication)