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DFT Study of ZnO Nanowire with Wurtzite (0001) Structure
XIAO SHEN, PHILIP B. ALLEN, Stony Brook University, MARK R. PEDERSON, Naval Research Laboratory, JIN-CHENG ZHENG, JAMES W. DAVENPORT, JAMES T. MUCKERMAN, Brookhaven National Laboratory — The most commonly reported ZnO nanowires have the (0001) wurtzite growth axis. We report two first-principles calculations using density-functional theory (DFT) for a small model nanowire with diameter 0.9 nm, containing 26 atoms in one periodic repeat unit cell, arranged as a fragment of a wurtzite (0001) crystal. One calculation is done on an infinite wire and the other on a truncated piece. The two calculations show excellent agreement. In both calculations, the atomic coordinates were relaxed to the nearest stable minimum. The exposed $(1\bar{1}00)$ surfaces resemble closely the relaxed surface found in bulk[1]. Our calculation shows that the c axis has a $\sim$2% elongational strain. We also compute the change of the Young's modulus relative to the bulk, and compare our prediction with experiment[2]. The electrical polarization of this non-centrosymmetric nanowire will be discussed, and also the assignment of a rotational quantum number m to the Bloch band states.

[1]U. Diebold et al., Appl. Surf. Sci. 237, 336 (2004)
[2]C. Q. Chen et al., Phys. Rev. Lett. 96, 075505 (2006)

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