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Modeling Nanomechanical Behavior of ZnO Nanowires as a Function of Nano-Diameter

Authors : L. Achou, A. Doghmane

Abstract : Elastic performances, as an essential property of nanowires (NWs), play a significant role in the design and fabrication of modern nanodevices. In this paper, our interest is focused on ZnO NWs to investigate wire diameter (D_{wire}≤ 400 nm) effects on elastic properties. The plotted data reveal that a strong size dependence of the elastic constants exists when the wire diameter is smaller than ~ 100 nm. For larger diameters (D_{wire} > 100 nm), these ones approach their corresponding bulk values. To enrich this study, we make use of the scanning acoustic microscopy simulation technique. The calculation methodology consists of several steps: determination of longitudinal and transverse wave velocities, calculation of refection coefficients, calculation of acoustic signatures and Rayleigh velocity determination. Quantitatively, it was found that changes in ZnO diameters over the ranges 1 nm ≤ D_{wire} ≤ 100 nm lead to similar exponential variations, for all elastic parameters, of the from: A = a + b exp(-D_{wire}/c) where a, b, and c are characteristic constants of a given parameter. The developed relation can be used to predict elastic properties of such NW by just knowing its diameter and vice versa.

Keywords : elastic properties, nanowires, semiconductors, theoretical model, ZnO
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