

Accepted Manuscript

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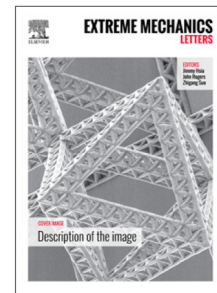
PII: S2352-4316(18)30074-9
DOI: <https://doi.org/10.1016/j.eml.2018.07.006>
Reference: EML 392

To appear in: *Extreme Mechanics Letters*

Received date: 9 April 2018
Revised date: 20 July 2018
Accepted date: 26 July 2018

Please cite this article as: Y. Pinto, D. Mordehai, Size-dependent coupled longitudinal-transverse vibration of five-fold twinned nanowires, *Extreme Mechanics Letters* (2018), <https://doi.org/10.1016/j.eml.2018.07.006>

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Size-Dependent Coupled Longitudinal-Transverse Vibration of Five-Fold Twinned Nanowires

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Abstract

The use of nanowires in nano-electro-mechanical resonators is envisioned owing to their high transverse fundamental frequency spectrum. While the natural frequencies are customarily calculated using linear beam theory, nonlinear continuum theories suggest that different vibration modes may be coupled. In this study, we employed molecular dynamics (MD) simulations to examine the coupling between longitudinal and transverse oscillations in nanowires. Five-fold twinned nanowires in a cantilever configuration with an initial tensile strain were constructed in the MD simulations. After relaxation, the nanowire started oscillating longitudinally and the dynamics of the systems was studied. Several atoms on the main axis were tracked, from which the natural longitudinal and transverse frequencies of the nanowire were calculated. In some cases, the longitudinal vibration of nanowires transformed into a transverse motion, a case that we term a coupled motion. We show that the coupling is a geometrical phenomenon that depends on the slenderness ratios of the nanowires. We found that for ratios in the range of $\sim 68-95$ the main transverse mode of deflection is the third one, whereas for ratios above ~ 117 , the first transverse mode prevails. We propose that geometrical nonlinear higher order contributions, which are considered in the continuum theory, rationalize the coupling and its size dependency.

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