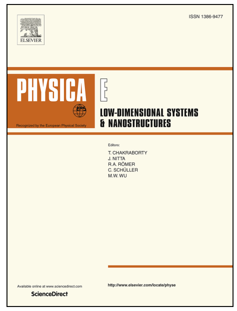
Accepted Manuscript



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PII: S1386-9477(17)30828-7

DOI: 10.1016/j.physe.2017.10.005

Reference: PHYSE 12932

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 7 June 2017

Revised Date: 16 September 2017

Accepted Date: 10 October 2017

Please cite this article as: X. Yang, H. Li, M. Hu, Z. Liu, J. Wärnå, Y. Cao, R. Ahuja, W. Luo, Mechanical properties investigation on single-wall ZrO_2 nanotubes: A finite element method with equivalent Poisson's ratio for chemical bonds, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2017.10.005.

Mechanical properties investigation on single-wall ZrO_2 nanotubes: A finite element method with equivalent Poisson's ratio for chemical bonds

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Abstract

A method to obtain the equivalent Poisson's ratio in chemical bonds as classical beams with finite element method was proposed from experimental data. The UFF (Universal Force Field) method was employed to calculate the elastic force constants of Zr-O bonds. By applying the equivalent Poisson's ratio, the mechanical properties of single-wall ZrNTs (ZrO_2 nanotubes) were investigated by finite element analysis. The nanotubes' Young's modulus (Y), Poisson's ratio (ν) of ZrNTs as function of diameters, length and chirality have been discussed, respectively. We found that the Young's modulus of single-wall ZrNTs is calculated to be between 350 to 420GPa.

Keywords: Signal-wall ZrO_2 nanotubes; Mechanical properties; Finite element method; Poisson's ratio

1. Introduction

Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima[1], the interests on one-dimensional nanotube materials has been growing for decades. This seminal work has made tremendous impact to the field of nanoscience and nanomaterials. Following this report, there has been subsequent attempts for the synthesis and characterisation of different types of nanotubes other than CNT, such as boron nitride, boron carbide, metal halides, transition metal dichalcogenide, and metal oxides. Among the nanotubes, metal oxides constitute an important class owing this to their significance in potential technology applications and basic scientific research[2]. Zirconia is considered to be

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