Nonlocal Parameter Estimation for Tensile Single-Walled Carbon Nanotubes by Molecular Structural Mechanics

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Introduction

This work is concerned with the estimation of nonlocal parameters for tensile Single-Walled Carbon Nanotubes (SWCNTs) by means of Molecular Structural Mechanics (MSM) simulations.

Molecular Structural Mechanics

In MSM, atomic systems are modeled as discrete systems of balls and springs. Knowing the position of the atoms and the stiffness of the chemical bonds that hold them together allows to predict Young’s modulus and mechanical response of a tensile SWCNT (see Figs. 1 and 2, respectively).

Nonlocal Elastic Tensile Rod

As shown in Fig. 3, tensile SWCNTs have been modeled as nonlocal elastic rods.

According to the integro differential formulation of nonlocal elasticity [1], the stress \( \sigma_{xx} \) at a point \( x \) is calculated as a weighted integral of the strain field \( \varepsilon_{xx} \) at surrounding points according to

\[
\sigma_{xx}(x) = E_{xx} \left( \xi_1 \varepsilon_{xx}(x) + \xi_2 \int_0^L g(|x - \bar{x}|, m, n) \varepsilon_{xx}((\bar{x}) \, d\bar{x} \right)
\]

where \( E_{xx} \) is the Young’s modulus of the SWCNT, \( g(x, \bar{x}, m, n) \) the atomistically based nonlocal kernel shown in Fig. 4, and the dimensionless quantities \( \xi_1, \xi_2, m \) and \( n \) are nonlocal parameters. The solution of this problem is derived numerically by means of B-spline finite elements [2].

Results

Nonlocal parameters have been estimated for several tensile armchair and zigzag SWCNTs with different length and diameter through a parameter estimation procedure. Moreover, an analytical relation between the nonlocal parameters and the nanotubes geometric characteristics has been derived [3]. As depicted in Fig. 5, the nonlocal model yields a good approximation of the axial strain field in tensile SWCNTs.

References