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An Atomistic Approach to Define Continuum Mechanical Quantities in One Dimensional Nanostructures at Finite Temperature

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Abstract : We present a variant of the Irving-Kirkwood procedure to obtain the microscopic expressions of the cross-section averaged continuum fields such as internal force and moment in one-dimensional nanostructures in the non-equilibrium setting. In one-dimensional continuum theories for slender bodies, we deal with quantities such as mass, linear momentum, angular momentum, and strain energy densities, all defined per unit length. These quantities are obtained by integrating the corresponding pointwise (per unit volume) quantities over the cross-section of the slender body. However, no well-defined cross-section exists for these nanostructures at finite temperature. We thus define the cross-section of a nanorod to be an infinite plane which is fixed in space even when time progresses and defines the above continuum quantities by integrating the pointwise microscopic quantities over this infinite plane. The method yields explicit expressions of both the potential and kinetic parts of the above quantities. We further specialize in these expressions for helically repeating one-dimensional nanostructures in order to use them in molecular dynamics study of extension, torsion, and bending of such nanostructures. As, the Irving-Kirkwood procedure does not yield expressions of stiffnesses, we resort to a thermodynamic equilibrium approach to obtain the expressions of axial force, twisting moment, bending moment, and the associated stiffnesses by taking the first and second derivatives of the Helmholtz free energy with respect to conjugate strain measures. The equilibrium approach yields expressions independent of kinetic terms. We then establish the equivalence of the expressions obtained using the two approaches. The derived expressions are used to understand the extension, torsion, and bending of single-walled carbon nanotubes at non-zero temperatures.

Keywords : thermoelasticity, molecular dynamics, one dimensional nanostructures, nanotube buckling
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