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ScienceDirect
Comput. Methods Appl. Mech. Engrg. 294 (2015) 278–298
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Mechanical modeling of graphene using the three-layer-mesh bridging domain method

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Received 9 December 2014; received in revised form 30 May 2015; accepted 3 June 2015
Available online 25 June 2015

Highlights

- A framework for concurrent atomistic/continuum simulation of graphene is developed.
- The TBDM is re-formulated based on the Nosé–Hoover thermostat.
- The AIREBO potential is used, which is carefully weighted in the bridging zone.
- The Q1STs solid-shell element is modified to include the energy scaling function.
- A thermodynamically rigorous high-order continuum constitutive model is parameterized.

Abstract

Recently developed three-layer-mesh bridging domain method (TBDM) enhanced the conventional bridging domain method (BDM) by (1) mitigating the temperature cooling effect on the atoms in the bridging domain, and (2) employing a mesh-independent physics-based discrimination between thermal and mechanical atomic motions. In this paper, we present the new enhancements for the TBDM to achieve an appropriate framework for concurrently coupled atomistic–continuum simulation of graphene. To capture the mechanical behavior of graphene accurately, we employed the adaptive intermolecular reactive bond order (AIREBO) potential in the atomistic model, which is carefully weighted by the atomic energy scaling function in the bridging zone. In the continuum model, a thermodynamically rigorous high-order continuum description, considering the symmetries of graphene, is used which is parameterized using full molecular dynamics (MD) simulations. To accurately capture the bending behavior of graphene, a recently developed explicit finite-deformation solid-shell element is used to discretize the continuum domain, and its formulation is modified to include the continuum energy scaling function. To achieve realistic constant-temperature condition (canonical ensemble), the Nosé–Hoover thermostat is used in the full MD domain and also as local thermostats in the bridging domain. 5-value Gear predictor–corrector time integrator is implemented, which is well-suited to be used with the Nosé–Hoover thermostat. Accordingly, the TBDM formulation is modified to work with this time integrator. Some modifications are also made in the TBDM formulation to increase the robustness of the multiscale simulations. Finally, the effectiveness of the proposed

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http://dx.doi.org/10.1016/j.cma.2015.06.001

multiscale method for graphene is demonstrated by running in-plane shear, out-of-plane bending, and nanoindentation simulations and comparing the results with those obtained from full MD and full finite-element simulations.

Keywords: Graphene; Multiscale methods; Coupled atomistic–continuum simulations; Bridging domain method; Temperature

1. Introduction

Two-dimensional graphene, the one-atom-thick honeycomb lattice of carbon, is the conceptual building block for a number of carbon allotropes, e.g. graphite (three-dimensional), carbon nanotubes (one-dimensional), and buckyballs or spherical fullerenes (zero-dimensional) [1,2]. Until recently, graphene existed only within three-dimensional graphite or tightly bound to another solid surface [1]. In a seminal paper in 2004 [3], it was reported that graphene could be obtained by mechanical exfoliation, a process including directly rubbing bulk graphite onto a smooth substrate [3–5]. It has been shown that graphene has many supreme properties such as extreme mechanical strength, exceptionally high electronic and thermal conductivities, and impermeability to gases, which make it highly attractive for numerous applications in electronics, photonics, composite materials, coating, energy generation and storage, sensors, drug delivery, etc. [6]. In graphene, carbon atoms are densely packed in a regular sp^2-bonded atomic hexagonal pattern. Its robust network of sp^2 bonds makes graphene the strongest material ever studied [7,8]. On the other hand, graphene is also incredibly supple, which in combination with its electrical properties can be exploited for strain-based graphene electronics [9,10]. Graphene thermal properties are also extraordinary: extremely high thermal conductivity [11], ∼20 times higher than that of copper, and large and negative thermal expansion coefficient [12], 5–10 times larger than that in ordinary graphite.

Graphene production is now scaled up to centimeter [13,14] or even meter scale [15] and polycrystallinity is unavoidable [16] in large-scale graphene films. It is well-known that the properties of polycrystalline materials are often dominated by the size of their grains and properties of grain boundaries. For graphene, a 2D lattice, these effects have more practical significance because even a line defect can divide and disrupt the whole crystal. Although, atomistic numerical simulations have played an important role in fast advancing graphene research by predicting and elucidating various properties of graphene, e.g., [17–27], modeling "full-scale" grains and their interactions are not feasible using all-atom simulations. Our goal is to provide essential multiscale tools to investigate the mechanical behavior of full-size graphene grains, which has significant implications in the application of large-area polycrystalline graphene, such as for biological membranes and electronic devices. In this paper, we report on the new enhancements for the recently developed three-layer-mesh bridging domain method (TBDM) [28] to achieve an appropriate framework for concurrently coupled atomistic–continuum simulation of graphene. Application of the TBDM in simulation of polycrystalline graphene will be presented in due course.

Generally, multiscale methods aim to seamlessly couple multiple models at different scales. Despite sequential multiscale methods, which have enjoyed long-time success, e.g., [29], concurrent multiscale methods have encountered more challenges associated with energy transmission and changes in the constitutive description of a material across the interface between different models, such as spurious wave reflection. A number of concurrent multiscale methods have been developed so far, including the quasicontinuum method (QM) [30,31], the coarse-grained MD method (CGMD) [32], the macroscopic-atomistic-ab initio dynamics (MAAD) method [33,34], the bridging scale method (BSM) [35], and the bridging domain method (BDM) [36,37]. The BDM is one of the most efficient and widely-used multiscale methods, which couples the molecular dynamics (MD) simulations with finite element (FE) methods. In the BDM, the system is partitioned into three sub-domains: atomistic, continuum, and bridging domains. Lagrange multipliers technique is employed to impose the displacement/velocity compatibility between atomistic and continuum scales in the bridging domain (BD). In the BDM, the Lagrange-multipliers constraint matrix is usually diagonalized using the row-sum technique, which is shown to be essential in eliminating spurious wave reflections at the interface of the atomistic and continuum domains [38]. Accordingly, total Hamiltonian in the BD is divided into three parts: the atomistic Hamiltonian, the continuum Hamiltonian, and the Hamiltonian associated with the Lagrange multipliers. The Hamiltonian of continuum and atomistic domains are weighted by scaling factors to avoid double counting of the Hamiltonian in the BD so the atomistic (continuum) energy is dominant near the purely atomistic