International Journal of Engineering Science 133 (2018) 109–131

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

On the molecular mechanics of single layer graphene sheets

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ARTICLE INFO

Article history:
Received 26 June 2018
Revised 31 August 2018
Accepted 3 September 2018

MSC:
74K20
74E15

Keywords:
Graphene
Molecular mechanics
Molecular structural mechanics
Mechanical moduli

ABSTRACT

The molecular structural mechanics (MSM) method is developed by applying beam elements to model bonded interactions between carbon atoms in the atomic lattices of single-layer graphene sheets (SLGSs). The novelty of the approach developed in this paper lies in the accurate adjustment of the geometric and material parameters of Bernoulli–Euler beam elements to simulate reference mechanical moduli (2D Young's modulus, Poisson's ratio, and bending rigidity modulus) of graphene. The MSM method with an advanced geometric and material parameter set of Bernoulli–Euler beam elements is implemented by means of the commercial MSC.Marc finite element (FE) code. We also employ the standard molecular mechanics (MM) method using the DREIDING force field (see Mayo et al. The Journal of Physical Chemistry, 1990, 94: 8897–8909). We implemented this force field in the homemade PIONER FE code using a modified parameter set which reproduces the mechanical moduli of graphene reasonably well. Computer simulations show that the free vibration frequencies and modes of SLGSs obtained using the standard MM and MSM methods converge. However, the buckling forces of compressed SLGSs obtained by the two methods provide acceptable convergence only for the lowest values of the critical forces.

1. Introduction

Graphene is a structural material for sp2 carbon nanoforms Suarez-Martinez, Grobert, and Ewels (2012) (low-dimensional carbon nanostructures) such as single-layer graphene sheets (SLGSs), single-walled carbon nanotubes (SWCNTs), fullerenes, etc. The molecular dynamics/mechanics (MD/MM) methods are widely used to simulate the deformation, vibration, and buckling of sp2 carbon nanoforms. These methods are based on solving the classical Newton equations of motion for material points (in the present paper, by material points are meant carbon atoms) in force fields (see, e.g., Lee (2017)).

The MD method (see, e.g., Lee (2017)) uses schemes of explicit integration of the motion equations of nanostructures. The MM method (see, e.g., Burkert & Allinger (1982)) was initially developed to determine the static equilibrium of nanostructures. In the present study, the method of step-by-step integration of the equations of quasi-static and dynamic motion of nanostructures based on implicit integration schemes is also referred to as the MM method because the numerical implementation of these schemes is close to that in the method of determining the static equilibrium of nanostructures (solution of systems of nonlinear algebraic equations with the refinement of the solution by the Newton–Raphson method). Each integration step in the MM method is more labor-consuming than that in the MD method. However, in the MM method, the

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https://doi.org/10.1016/j.ijengsci.2018.09.001
0020-7225/

restriction on the time integration step is less stringent than that in the MD method[1] In addition, the MM method allows an easier solution of problems of free vibrations and linear buckling of nanostructures than the MD method, and in solutions of nonlinear buckling problems, the MM method allows the use of buckling criteria of nanostructures and a reliable determination of both the critical states (external forces, prescribed displacements, time, etc.) and buckling modes of nanostructures Korobeynikov, Alyokhin, Annin, and Babichev (2012).

In turn, the MM method can be divided into the standard MM method, based on the direct use of the force fields of atomic interactions (cf., Alyokhin, Annin, Babichev, and Korobeynikov (2013); Annin, Alekhin, Babichev, and Korobeynikov (2012); Feng, Liew, He, and Wu (2014); Ghaderi and Hajiesmaili (2013); Giannopoulos and Georgantzinos (2017b); Guo, Leung, Jiang, He, and Huang (2007); Gupta, Agrawal, and Batra (2016); Gupta and Batra (2010); Haghbin and Khalili (2014); Hollerer (2012, 2014); Hollerer and Celigoj (2013); Korobeynikov, Alyokhin, Annin, and Babichev (2014, 2015); Korobeynikov, Alyokhin, and Babichev (2014, 2018b); Liu, Zhang, and Chen (2008); Majzoobi, Payandehpeyman, and Nojini (2011); Merli, Lazaro, Monleon, and Domingo (2015); Nasdala and Ernst (2005); Nasdala, Kempe, and Rolfes (2010, 2012, 2015); Safaei, Naseradinmousavi, and Rahmani (2016); Theodosiou and Saravanos (2013, 2014); Tserpes and Papanikos (2014); Wackerfuß (2009); Wilmes and Pinho (2014); Xiao, Gama, and Gillespie Jr. (2005)) and the molecular structural mechanics (MSM) method, which was first used by Odegard, Gates et al. Gates, Odegard, Frankland, and Clancy (2005); Odegard, Gates, Nicholson, and Wise (2002); Odegard, Gates, Wise, Park, and Siochi (2003) and then by other authors (see, e.g., Awang, Mohammadpour, and Muhammad (2016); Yengejeh, Kazemi, and Öchsner (2015a) and the references therein) to solve problems of deformation, vibration, and buckling of sp2 carbon nanoforms. In the MSM method, the potential energies of bonded and non-bonded atom interactions are approximated by the potential energies of beam and truss elements. In contrast to the standard MM method, the MSM method can only be applied to the simulation of small deformations (but possibly, large rotations and displacements) of sp2 carbon nanoforms since the strain energies of beam and truss elements are determined by harmonic approximation of force field potentials[2] The MM and MSM methods allow the simulation of the mechanical moduli of sp2 carbon nanoforms, in particular, graphene (cf., Cao (2014)). In the latter case, it is important to use force field and beam element parameters that provide the most accurate simulation of the mechanical moduli of graphene.

In Gates et al. (2005); Goldstein and Chentsov (2005); Goldstein, Chentsov, Kadushnikov, and Shturkin (2008); Odegard et al. (2002, 2003), the potential energies of bonded and non-bonded atom interactions are approximated by the potential strain energies of truss elements. However, this implementation of the MSM method using truss elements for carbon atom interactions, first, leads to cumbersome finite element (FE) models of nanostructures and, second, does not provide a sufficiently accurate simulation of the mechanical moduli of nanostructures[3] The alternative, more advanced approach proposed in Alzebdeh (2012); Ansari and Mahmoudinezhad (2015); Georgantzinos and Giannopoulos (2017); Georgantzinos, Giannopoulos, and Anifantis (2010, 2016); Georgantzinos et al. (2011a); Georgantzinos, Giannopoulos, Pierou, and Anifantis (2015); Georgantzinos, Katsareas, and Anifantis (2011b); Georgantzinos, Markolefas, Giannopoulos, Katsareas, and Anifantis (2017); Giannopoulos (2012, 2014, 2017); Giannopoulos and Georgantzinos (2017a); Giannopoulos, Kakavas, and Anifantis (2008); Giannopoulos, Liosatos, and Moukanidis (2011); Giannopoulos, Tsiros, and Georgantzinos (2013); Mahmoudinezhad and Ansari (2013); Mahmoudinezhad, Ansari, Basti, and Hemmatnezhad (2014); Meo and Rossi (2006); Rafiee and Heidarhaei (2012); Zhao et al. (2013) is based on the joint use of truss and spring elements. This approach provides an adequate simulation of the graphene mechanical moduli.

One more implementation of the MSM method is based on simulating the potential energies of bonded atom interactions by beam element potential strain energies. This approach was pioneered by Li and Chou Li and Chou (2003c) (see also Li & Chou (2003a,b, 2004a,b,c)), who proposed a simple and elegant way to approximate the potential energies of bonded atom interactions using Bernoulli–Euler beam elements, which was subsequently used to simulate the deformation, buckling, and vibrations of sp2 carbon nanoforms Alzebdeh (2012, 2014); Ansari, Rouhi, and Aryayi (2013); Arghavan and Singh (2011a,b); Avila, Eduardo, and Neto (2011); Awang et al. (2016); Dominguez-Rodriguez, Tapia, and Aviles (2014); Ghadyani and Öchsner (2015); Ghadyani, Soufeiani, and Öchsner (2016); Haghbin and Khalili (2014); Harik, V. (ed.) (2014); Majzoobi et al. (2011); Miao, Li, and Guo (2012); Rahmandoust and Öchsner (2012); Rouhi and Ansari (2012); Sakhaee-Pour (2009a,b); Sakhaee-Pour, Ahmadian, and Naghdabadi (2008a); Sakhaee-Pour, Ahmadian, and Vafai (2008b); Sakharova, Pereira, Antunes, Brett, and Fernandes (2015); Shokrieh and Rafiee (2010); To (2006); Tserpes and Papanikos (2005); Yengejeh, Kazemi, and Öchsner (2014a, 2015a); Yengejeh, Zadeh, and Öchsner (2014b, 2015b); Ziaee (2014)). Similar versions of the MSM method, based on Timoshenko beam elements were developed in Haghbin and Khalili (2014); Hu et al. (2005); Hu, Nunoya, Pan, Okabe, and

[1] The MD and MM methods belong to the classes of explicit and implicit schemes of integration of Cauchy problems, respectively. Therefore, from the standpoint of the effectiveness of integration of Newton's motion equations, the MD and MM methods have different applications: the MD method is more suitable for simulating high-rate deformation of nanostructures, and the MM method is more suitable for simulating low-rate (including quasi-static) deformation of nanostructures. A detailed discussion of the ranges of application of the explicit and implicit methods of integration of Newton's motion equations is given in, for example, Bathe (1996).

[2] Some studies use mixed standard MM/MSM methods (cf., Annin, Alekhin, Babichev, and Korobeynikov (2010, 2012); Annin, Korobeynikov, and Babichev (2009); Georgantzinos, Giannopoulos, Katsareas, Kakavas, and Anifantis (2011a); Korobeynikov et al. (2012)), which can also be applied to the study of large strains of sp2 carbon nanoforms.

[3] Using truss elements to model the bonded interactions of graphene yields a value of 1/3 for the Poisson's ratio of this material Hu, Fukunaga, Lu, Kameyama, and Yan (2005); Scarpa, Adhikari, and Phani (2009), whereas based on the results of experimental studies and quantum mechanical simulations of the deformation of graphite, SWCNTs, SLGSs, and graphene Korobeynikov, Alyokhin, and Babichev (2018b), we assume that the Poisson's ratio of graphene is 0.17.