

Coupled atomistic-continuum simulation of the mechanical properties of single-layered graphene sheets

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The purpose of this work is the multiscale modeling of a single-layered graphene sheet. The model is divided into three parts. One is an atomistic domain which is simulated with the atomic-scale finite element method (AFEM). Another is a continuum domain. In this domain, the mechanical properties are investigated by using a finite element based on a nonlocal continuum shell model with a high order strain gradient. To be exact, it is a 4-node 60-generalized degree of freedom (DOF) Mindlin–Reissner finite shell element with a second order strain gradient. In the third part, a new transitional finite element is developed for smoothing the transition between the atomistic domain and continuum domain.

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1 Introduction

Due to the exceptional features of graphene sheets, a lot of research projects are focused on them. Besides experiments, numerical simulations are also necessary for studying their mechanical properties. Coupled atomistic-continuum simulation of graphene sheets is essential for studying their mechanical properties. While effects on the atomic scale can be described explicitly with molecular mechanical models on some selected positions, continuum mechanical models enable the efficient calculation of large and technical relevant structures. In this work, a coupled atomistic-continuum model is used to simulate the mechanical behavior of a single-layered graphene sheet. The atomistic domain is described by the atomic-scale finite element method (AFEM) [3,6]. The mechanical properties of the continuum domain are investigated by using a finite element based on a nonlocal continuum shell model with a high order strain gradient. Between the atomistic and continuum domain, transitional finite elements are applied for smoothing the transition.

2 Multiscale modeling

The model of atomistic domain is based on the finite element formulation of molecular mechanics in [3,6]. The total energy of the atomic structure in this domain is formulated as the sum of the internal energy of every atom and the external work on it. In the equilibrium state of the system, the first variation of the total energy should be zero. In this work, it is the static analysis of graphene sheets. The internal energy of the system is equal to the sum of the interatomic potential of each atom which is determined with DREIDING approach [4] here. In the atomistic domain, 3 DOFs are considered per atom: $\mathbf{u}_J^e = \{u_J \ v_J \ w_J\}^T$.

For formulating the model of the continuum domain, the higher order strain gradient theory [1]

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} + g^2 \nabla^2 \tilde{\varepsilon}_{kl}) \quad \text{with} \quad \varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad \tilde{\varepsilon}_{kl} = \varepsilon_{kl}, \quad g = \frac{d}{\sqrt{12}} \quad (1)$$

is applied in this work. According to this theory, the stress components σ_{ij} are not only dependent on the strain ε_{kl} but also on its second-gradient. And with the parameter g and the internal length d , the size effects can be considered. The internal length d depends on the underlying deformation mechanisms and the microstructure. In this work, it's the interatomic distance in x-direction (see Fig. 1).

In the FE approximation, a 4-node finite shell element is formulated. The equation for conservation of momentum, kinematic and constitutive equation of this shell element are the same as those for classical shell element. There are totally 15 generalized DOFs per node. Each node I of the finite shell element e has the following set of DOFs:

$$\mathbf{v}_I^e = \{u_I \ v_I \ w_I \ \phi_{xI} \ \phi_{yI} \ u_{I,x} \ v_{I,x} \ w_{I,x} \ \phi_{xI,x} \ \phi_{yI,x} \ u_{I,y} \ v_{I,y} \ w_{I,y} \ \phi_{xI,y} \ \phi_{yI,y}\}^T. \quad (2)$$

The shape functions having a degree of maximum three in each coordinate direction, are applied to keeping the C^1 continuity. In transitional domain, the finite elements from atomistic and continuum domain overlap with each other (see Fig. 1). The 3-DOF displacements of atoms \mathbf{u}_J^a from atomistic domain a are coupled with the 15-DOF displacements of spatial points \mathbf{u}_I^c from continuum domain c in transitional domain by using the (3×15) -matrix \mathbf{L} :

$$\mathbf{u}_J^a = \mathbf{L} \mathbf{u}_I^c = \begin{bmatrix} \mathbf{1}_{3 \times 3} & \mathbf{0}_{3 \times 2} & d_x \cdot \mathbf{1}_{3 \times 3} & \mathbf{0}_{3 \times 2} & d_y \cdot \mathbf{1}_{3 \times 3} & \mathbf{0}_{3 \times 2} \end{bmatrix}_{3 \times 15} \mathbf{u}_I^c. \quad (3)$$

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It means, the displacements of atoms \mathbf{u}_J^a are approximated by the Taylor polynomial of the displacements of spatial points \mathbf{u}_I^c . d_x and d_y are the distances in x - and y -direction between the atom J and the spatial point I .

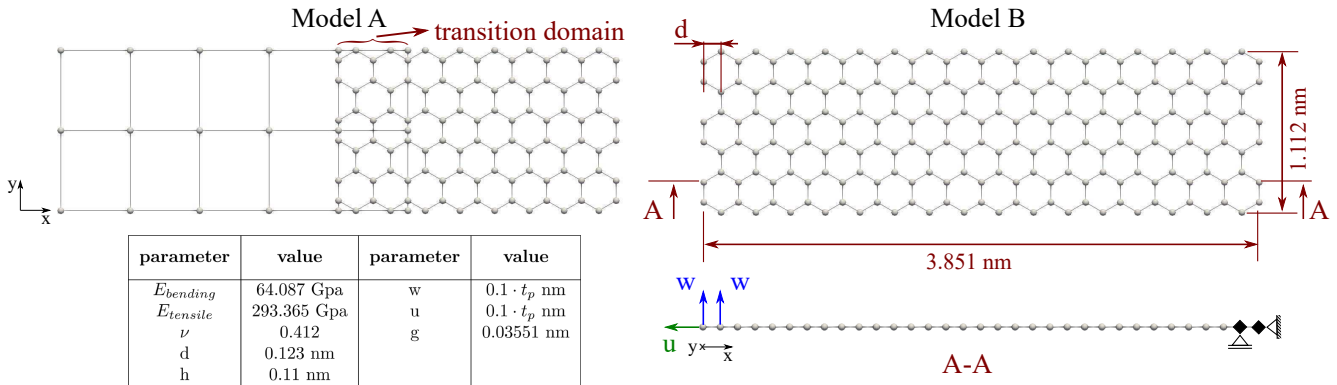


Fig. 1: (up left) The multiscale modeling of a graphene sheet. (up right) The full atomistic modeling of a graphene sheet and its geometry. (down left) Parameters of the simulation. (down right) Boundary conditions of the simulation.

3 Numerical example

This multiscale modeling was evaluated by tensile tests and bending tests. The geometric definition and boundary conditions of the cases are shown in Fig. 1. The Young's modulus $E_{bending}$, $E_{tensile}$ and the Poisson's ratio ν are determined with the numerical tensile and bending tests. According to [5], the equilibrium thickness h of the finite shell element is 0.11 nm. The loads u and w are functions of pseudo-time t_p . The in-house code dockSIM was used to perform these calculations.

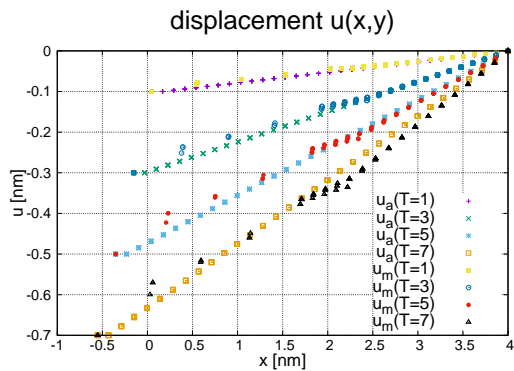


Fig. 2: The results of tensile tests.

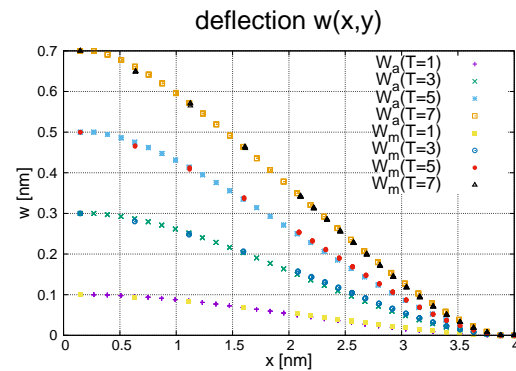


Fig. 3: The results of bending tests.

4 Conclusion

The results of tensile and bending tests are shown in Fig. 2 and 3. The multiscale modeling and the full atomistic modeling are denoted with indices m and a . And $T = t_p$ is the pseudo-time. The results show that the error increase with the strain. This results from the ghost forces, which are not eliminated yet. In the future work, a coupling method, likes QC-GFC-Model [2], should be implemented to eliminate the ghost forces. This multiscale modeling is economical, only for the situation that more than 5 atoms, which has 3 DOFs, are replaced by a spatial point, which has 15 DOFs in continuum modeling. Then the total system DOFs in the multiscale modeling will be fewer than these in the full atomistic modeling.

References

- [1] H. Askes et al., Arch Appl Mech **72**, 171-188 (2002).
- [2] W. A. Curtin and R. E. Miller, MSMSE **11**, R33-R68 (2003).
- [3] B. Liu et al., Phys Rev B **72**, 035435 (2005).
- [4] S. L. Mayo et al., J Phys Chem **94**, 8897-8909 (1990).
- [5] F. Scarpa et al., Nanotechnology **21**, 125702 (2010).
- [6] J. Wackerfuß, Int J Numer Methods Eng **77**(7), 969-997 (2009).
- [7] B. Zhang et al., Eur J Mech A Solids **42**, 63-80 (2013).