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Molecular Dynamics Study on Mechanical Responses of Circular Graphene Nanoflake under Nanoindentation

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Abstract : Graphene, a single-atom sheet, has been considered as the most promising material for making future nanoelectromechanical systems as well as purely electrical switching with graphene transistors. Graphene-based devices have advantages in scaled-up device fabrication due to the recent progress in large area graphene growth and lithographic patterning of graphene nanostructures. Here we investigated its mechanical responses of circular graphene nanoflake under the nanoindentation using classical molecular dynamics simulations. A correlation between the load and the indentation depth was constructed. The nanoindented force in this work was applied to the center point of the circular graphene nanoflake and then, the resonance frequency could be tuned by a nanoindented depth. We found the hardening or the softening of the graphene nanoflake during its nanoindented-deflections, and such properties were recognized by the shift of the resonance frequency. The calculated mechanical parameters in the force vs deflection plot were in good agreement with previous experimental and theoretical works. This proposed schematics can detect the pressure via the deflection change or/and the resonance frequency shift, and also have great potential for versatile applications in nanoelectromechanical systems.

Keywords : graphene, pressure sensor, circular graphene nanoflake, molecular dynamics
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