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An Atomic Finite Element Model for Mechanical Properties of Graphene Sheets

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Abstract : In this study, we use the atomic-scale finite element method to investigate the mechanical behavior of the armchair- and zigzag-structured nanoporous graphene sheets with the clamped-free-free-free boundary condition under tension and shear loadings. The effect of porosity on Young's modulus and shear modulus of nanoporous graphene sheets is obvious. For the armchair- and zigzag-structured nanoporous graphene sheets, Young's modulus and shear modulus decreases with increasing porosity. Young's modulus and shear modulus of zigzag graphene are larger than that of armchair one for the same porosity. The results are useful for application in the design of nanoporous graphene sheets.

Keywords : graphene, nanoporous, Young's modulus, shear modulus
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