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Elastic properties of lattice-like 2D materials using continuum mechanics

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ABSTRACT

Elastic properties of lattice-like two-dimensional (2D) materials can be formulated based on the molecular mechanic parameters of atomic bonds (i.e. stretching and bending stiffness) that can be estimated using molecular mechanics/dynamics simulation, ab-initio calculations, or experimental investigations. Initially, the inter-atomic potential energy of the materials experienced bonding interactions (e.g. bond bending, stretching, and torsion) and nonbonding interactions (e.g. core repulsion and van der Waals forces) is evaluated. In the perspective of structural mechanics, atomic bonds work as an elastic uniform circular beam whose strain energy under axial forces and bending moments can be explicitly formulated. By comparing corresponding terms in the inter-atomic potential energy and elastic strain energy, effective elastic properties of atomic bonds can be expressed in terms of their molecular mechanic parameters. This study focuses on hexagonal 2D materials that can be categorized based on their homogeneity (i.e. uniform (e.g. graphene, stanene) and non-uniform atomic constituents (e.g. (hBN, MoS2)) and their structural configurations (i.e. mono-planar (e.g. graphene, hBN) and multi-planar configurations (e.g. stanene, MoS2)). Due to the symmetry of hexagonal configurations, one general unit cell with multi-planar configuration subjected to mechanical loads is analyzed. Under different uniaxial loading conditions, displacements of the unit cell can be determined as the results of classical structural mechanics for beams, from which, corresponding strain terms, and thus, elastic moduli, shear moduli, and Poisson's ratio can be explicitly formulated based on their definitions. The reciprocal theorem for the general multi-planar hexagonal 2D materials is satisfied. From a broader viewpoint, the presented approach can be used to estimate elastic properties of any mono-layer and multi-layer lattice-like 2D materials with known structural configurations and molecular mechanic parameters of interatomic bonds, which is important for characterizing these 2D materials in various electromechanical devices.

Keywords: Elastic property; 2D materials; Continuum mechanics.