A structural mechanics approach based on peridynamics for fracture of carbon nanomaterials

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ABSTRACT
The structural mechanics approach to analysis of carbon nanomaterials models carbon nanomaterials as planar or spatial framed structures [1]. Carbon atoms and covalent bonds between the atoms are treated as nodes of the structures and beams between the nodes. This method, as one of the three mainstream approaches to analyse carbon nanomaterials, has a high computational efficiency compared with molecular dynamics simulations, and it can consider scale effect compared with the method of an equivalent continuum structure. However, this method encounters a difficulty in analysing the fracture of nanomaterials. When the deformation of the bond exceeds the equilibrium state, the interaction force between the atoms decreases with the increase of the deformation. This instability phenomenon cannot be simulated by a linear elastic beam. A nonlinear elastic beam model may result in iterative solutions, and thus high computational cost. In this work, we propose the beam model to simulate the covalent bonds between the atoms within the framework of peridynamics. The beam can undergo stretching, bending and twisting deformation modes. The damage model of peridynamics can accurately describe instability phenomena. We simulate the unidirectional tensile failure of graphene, the unidirectional compressive failure of fullerene, and the failure of carbon nanotubes under tension, bending and torsion. Through comparison with the experimental results, we demonstrate that the structural mechanics approach using the peridynamic beam model is more accurate than the one using the classical linear elastic beam model for the analysis of the ultimate load and the failure profile, and that the peridynamic approach is more efficient than the one using the nonlinear beam model in terms of computational time.

REFERENCES