Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

Nano-architected Functionalized Origami Metamaterials

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Abstract

Graphene, a two-dimensional (2D) single layer of graphite, is one of the leading nanomaterials for designing high-performance multifunctional materials in several fields of materials science, owning to its outstanding features such as ultra-high stiffness, extremely high thermal conductivity, chirality-dependent electrical conductivity, and large specific surface area. In this study, we propose a novel approach, inspired by the art of paper folding (so-called *origami*), to construct graphene-based three-dimensional (3D) nano-architected mechanical metamaterials. The foldable graphene origami is constructed out of a flexible graphene sheet with creases introduced by surface functionalization that forms a new sp^3 bond between the carbon and hydrogen atoms. The 3D graphene origami metamaterials are built by assembling the graphene origami strips. The thermo-mechanical properties of (strip and 3D) graphene origami metamaterials are systematically studied using molecular dynamics simulation. The atomistic simulation results demonstrate that a vast range of thermal conductivity can be obtained by tailoring the topological parameters of the graphene origami, altering hydrogen density, and applying mechanical strains. The thermal conductivity can be increased by applying tension and decreased by applying compression, presenting a feasible strategy for tuning the thermal conductivity of engineered nanomaterials. In addition, the constitutive graphene sheets are nonporous and therefore retain high strength when used to form 3D nano-architected metamaterials. Owning to the intrinsic foldability of origami structures, the stretchability of graphene origami is also increased compared to the pristine graphene. Further results of phonon density of states and phonon group velocity show that the softening of phonon modes and decreased phonon group velocity result in the decreased thermal conductivity of graphene origami metamaterials. The origami approach imparts a new platform for designing shape-changing 3D graphene metamaterials with tunable thermo-mechanical properties and controllable functionalities.