

Chirality-dependent buckling-driven wrinkles in graphene monolayer

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Abstract

It is of great significance to understand the underlying mechanism of buckling-driven wrinkles in graphene monolayer due to its applications in nanoelectromechanical systems (NEMS). In previous macroscopic studies based on continuum theory, the chirality-dependent buckling in graphene monolayer is considered as neglectable. However, we found that the growth of buckling-driven wrinkles in graphene sheet is remarkably chirality- and size-dependent in nanoscale. The preferred growth direction of buckling-driven wrinkles in graphene monolayer behaves as zigzag-preferred, armchair-preferred, and isotropic with increase of buckling geometrical size. It is found that the flexural response of graphene sheet cannot be accurately described by the classical Euler regime in small size, and the non-continuum effect leads to zigzag-preferred buckling. When width/length ratio less than 0.5, the oblique buckling happens in armchair-along compression. Due to the effect of edge warp, the zigzag-along buckling is preferred when width/length ratio is between 0.5 and 1.0. The armchair-along buckling is preferred due to the chiral difference of bending stiffness when width/length ratio is between 1.0 and 3.0. In larger size with width/length ratio over 3.0, the non-continuum effect and chiral bending stiffness can both be neglected, and the buckling in graphene monolayer is isotropic. Knowing the mechanical behavior of buckling in graphene means that the researchers can choose a proper size of graphene according to the application in NEMS, this is especially important for the nanodevices with high frequency response. This should lead to an improved fundamental understanding on the dynamic mechanism of graphene-based nanodevices.

Keywords: graphene, buckling, wrinkles, chirality, size, molecular dynamics simulation