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Anisotropic Toughness and Strength in Graphene and its Atomistic Origin

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Abstract

This paper presents the implication of crystallographic orientation on toughness and ideal strength in graphene under lattice symmetry-preserving and symmetry-breaking deformations. In symmetry-preserving deformation, both toughness and strength are isotropic, regardless of the chirality of the lattice; whereas, in symmetry-breaking deformation they are strongly anisotropic even in the presence of vacancy defects. The maximum and minimum of toughness or strength occur along the zigzag direction and the armchair direction, respectively. The anisotropic behavior is governed by a complex interplay among bond-stretching deformation, bond-bending deformation, and the chirality of the lattice. Nevertheless, the condition for crack-nucleation is dictated by the maximum force required for bond rupture, and it is independent of the chiral angle of the lattice or loading direction. At the onset of crack-nucleation a localized *nucleation zone* is formed, wherein the bonds rupture locally satisfying the maximum bond-force criterion. The nucleation zone acts as the physical origin in triggering the fracture nucleation process, but its presence is undetectable in the macroscopic stress-strain data.

Keywords. Toughness, Strength, Anisotropy, Graphene, Chirality

1 Introduction

Two-dimensional materials such as graphene, MoS₂, phosphorene, silicene, and their derivatives (such as the van der Waals heterostructures [1]) have drawn a wide attention in an array of application areas including nanotechnology, nanoelectronics, and nanocomposites [2–5]. Scalable production and fabrication of these materials, which are mostly brittle in character, constitute a major obstacle to foreseeing their practical applications [6–9]. To establish pathways for novel fabrication and synthesis methodologies as well as for discovering new functional attributes, a deeper understanding of the correlation among toughness, strength, and crystal structure is needed. Taking graphene as an example material, we investigate the role of crystallographic direction on toughness and strength using a combination of density functional theory (DFT) [10] and molecular dynamics (MD) simulations [11].

Among the diverse family of 2D materials, graphene is the most popular material and it is known to exhibit strong anisotropic electronic and thermal properties within the linear regime of elastic deformation [2, 12–15]. Its crystallographic structure is described by a geometric parameter called chirality [16], or the chiral vector $\mathbf{c} = m\mathbf{a}_1 + n\mathbf{a}_2$, where \mathbf{a}_1 and \mathbf{a}_2 are the basis vectors; and, the integer choices of the indices (m, n) gives various atomistic configurations [17], and form the basis for attaining a wide variety of disparate directional properties and macroscopic features.

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