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Effect of crack length and orientation on the mixed-mode fracture behavior of graphene

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ABSTRACT

In almost all practical situations, graphene based nanodevices are subjected to complex loading i.e., combination of shear and tensile stress. Given this situation, mixed-mode fracture is inevitable during tearing of graphene. However, most of the studies on graphene fracture are based on mode-I fracture which is an idealistic situation and rarely occurs in the service conditions. We, therefore, performed classical molecular dynamics (MD) simulations on a graphene sheet with crack like flaw and investigated the complex mixed-mode fracture behavior. Mode-I, mode-II, and mixed-mode stress intensity factors (K_I, K_{II}, and K_{eff} respectively) as a function of Φ and crack length in armchair and zigzag edges were calculated. In addition, we investigated the effect of slit length and angle on the strength of graphene sheet. Effective stress intensity factor increases with flaw size and reaches a plateau (between 3.10 and 3.80 MPa$\sqrt{}$m for armchair, between 2.60 and 3.10 MPa$\sqrt{}$m for zigzag) approximately at a crack length of a/b $\approx$ 0.11 (2a and 2b are crack and model size respectively). For crack with zigzag edge surface, existence of a single bond perpendicular to crack direction facilitates bond-breaking process. While for armchair surface case, two inclined bonds at crack tip offer relatively more resistance. Finally, the effect of mixed-mode loading on the crack propagation path was investigated. All the systems considered in this study mimic real service conditions. Hence, our findings will provide useful guidelines for the design of graphene-based nanodevices.

1. Introduction

Graphene, a two-dimensional (2D) material of one-atom-thick sp^2 hybridized carbon atom, has been the cynosure of Nanotechnology ever since its discovery [1]. Because of its extraordinary properties, graphene has been studied extensively with potential applications in fields such as electrical, thermal, and nano-electronics [2]. Due to its superior mechanical properties, i.e. Young's modulus $\approx$ 1 TPa and breaking strength $\approx$ 130 GPa [3], graphene

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is also being considered as the strengthening agent in nano-composites [4]. The fracture strength of graphene and its allotropes, however, is governed by the impurities and defects that are always present [5] due to the nature of synthesizing process or processing conditions [6]. In addition, effect of functionalization plays a crucial role on fracture of graphene [7,8] and its allotropes [9]. Vacancy type defect significantly reduces its strength [10]. Similarly, defects such as pre-existing cracks will grow under external loads and cause fracture failure [11] and strength reduction. As a result, several studies have been focused on understanding the fracture behavior of graphene.

Omeltchenko et al. [12] studied crack propagation in a graphite sheet with million atom molecular-dynamics simulation based on Brenner's reactive empirical bond-order potential. They have estimated the stress intensity factor (SIF) of graphene sheet to be 4.7 MPa$\sqrt{\text{m}}$. Similar values, 4.21 MPa$\sqrt{\text{m}}$ for zigzag and 3.71 MPa$\sqrt{\text{m}}$ for armchair cracks, were reported by Xu et al. [13] based on coupled quantum/continuum technique. The SIF, generally denoted as K, is a fracture property, which represents the ability of a material to resist crack growth. In a recent experimental study, Zhang et al. [11] measured the SIF of graphene to be 4.0 ± 0.6 MPa$\sqrt{\text{m}}$ which is in agreement with the estimates from earlier theoretical studies [12,13]. In addition, Zhang et al. also observed that the classical Griffith theory could be applied to brittle fracture of graphene with reasonable accuracy. Kim et al. [14] investigated crack formation and propagation mechanism in suspended graphene sheets using transmission electron microscopy (TEM). They found that the tearing direction was predominantly aligned to the armchair and zigzag directions. Meyer et al. [15] performed optical and scanning electron microscopy (SEM) of graphene films on substrate in order to investigate morphologies of fractured graphene. Dewapriya et al. [16] studied the effect of temperature on the fracture of graphene using molecular dynamics (MD) simulations and found that the toughness values decreased with the increase in temperature.

Although the above studies have contributed to the understanding of fracture of graphene, the important issue of mixed-mode fracture, *i.e.* fracture of graphene under combined tensile and shear loading conditions, still needs to be addressed. Graphene fracture under pure tensile loading, also called as mode-I fracture, which was the primary focus of the most of the previous studies, is an idealistic situation and rarely occurs in the service conditions. In almost all practical situations, cracks in graphene are subjected to mixed-mode loading, i.e. a combination of tensile (mode-I denoted with K_{I}) and shear (mode-II denoted with K_{II}) loading conditions and mixed-mode fracture is inevitable during tearing of graphene [17,18]. Recently, Zhang et al. [19] initiated computational study on this important issue. They reported stress intensity factors and direction of crack propagation at room temperature for different orientation of loading conditions. They also observed that the torn edges of fresh cracks were along either zigzag or armchair, where zigzag edges were more preferable. In addition, there have been very few studies on the effect of *slit length* on the fracture strength of graphene [20,21].

However, the effect of crack length on the mixed-mode fracture of graphene has not been addressed. In addition, the effect of crystal orientation (i.e. zigzag and armchair directions) on the mixed-mode fracture behavior of graphene needs to be studied. To this end, the classical molecular dynamics (MD) simulations were performed on two different sets of models. Graphene sheet with cracks of different lengths were subjected to mixed-mode loading conditions. Effect of mode-mixity on stress intensity factors was investigated and crack-kinking behavior under various loading conditions was studied. Crack length effect on fracture strength of graphene sheet under various mixed-mode conditions was also investigated.

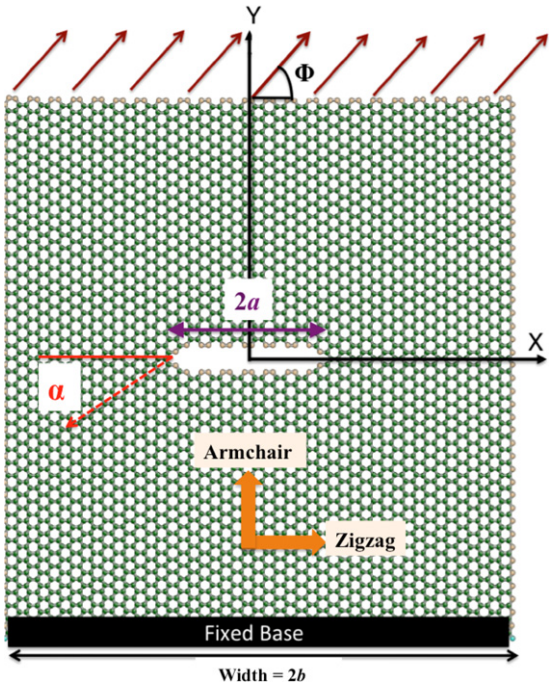

Fig. 1. Graphene nanoribbon (GNR) of size $2b$ ($b \approx 50$ Å) with a slit of length $2a$ ($a = 12$ Å) in the middle of GNR. In this Model-1, the slit (or crack) is oriented in horizontal direction *i.e.* parallel to the fixed base, and the top end of sheet is loaded. Mixed-mode loading condition is obtained by varying '*loading angle*'.

2. Models and methodologies

Two different models of square shaped graphene nanoribbons (GNR) of size $2b$ ($b \approx 50$ Å) with a slit of length $2a$ ($a = 2$ to 12 Å, $2a$ implies the two crack tips) in the middle of GNR, as shown in Figs. 1 and 2(a) were considered for the analysis. The total width of the model and the slit dimensions were chosen to avoid effects from finiteness [22] and unphysical fracture behavior [23]. For example, physical properties such as elastic modulus (E) obtained from a model with free edge length of over 80 Å will converge to that obtained from a model with periodic boundary conditions [3,24,25]. We considered a range of a/b values to understand the effect of flaw size on fracture behavior. In model-1 (shown in Fig. 1), the slit (or crack) is oriented in horizontal direction *i.e.* parallel to the fixed base, and the top end of sheet was loaded. Different loading conditions were obtained by varying the *loading angle*