PHÂN TÍCH DẠNG PHÁ HỦY HỖN HỢP (MIXED MODE) CỦA VẬT LIỆU GRAPHENE ĐƠN LỚP BẰNG PHƯƠNG PHÁP PHẦN TỬ HỮU HẠN

ANALYSIS MIXED-MODE FRACTURE TOUGHNESS (MODE I/II) OF A SINGLE LAYER GRAPHENE SHEET BY FINITE ELEMENT METHODS SIMULATION

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ABSTRACT

The mode I and mode II fracture behavior of a single-layer graphene sheet (SLGS) containing a center crack was characterized with the results of an finite element method (FEM) and an analytical model. Finite element method based micromechanical analysis is used to understand the fracture behavior of functionally SLGS. The in-plane shear fracture of a cellular material was analyzed theoretically for deriving the K_{IC}, K_{IIC} of SLGS, and FEM results were obtained. Crack is created by removing certain number of cells pertaining to a crack length. The inputs to the model are the geometric parameters required to model the repeating unit cell and tensile strength of the strut. Mixed-mode fracture of armchair direction graphene sheet was studied for various angle mode I/II ratios. The effect of mixed-mode loading on the Arcan specimen was investigated, all the systems considered in this study mimic real service conditions. Applying rotation boundary conditions does not influence the calculated fracture toughness significantly. The mixed-mode fracture criterion was determined, and the obtained fracture envelope was in good agreement with that of another study.

Keywords: *fracture of graphene; mixed mode of fracture toughness; stress intensity factor graphene; fracture toughness of graphene; micromechanic of graphene;*

TÓM TẮT

Dạng phá hủy thứ nhất và thứ hai của tấm graphene đơn lớp với vết nứt ở giữa tấm là mô hình điển hình với những kết quả đã được nghiên cứu bởi mô hình phân tích cơ học và phần tử hữu hạn. Phương pháp phần tử hữu hạn dựa trên phân tích vi mô được sử dụng để hiểu rõ ràng hành vi phá hủy của graphene đơn lớp. Bằng phương pháp phân tích lý thuyết cũng như phương pháp phần tử hữu hạn, người ta đã tìm ra hệ số cường độ tới hạn của dạng phá hủy thứ nhất K_{IC} và dạng hai K_{IIC}. Vết nứt được tạo ra bằng cách loại bỏ số lượng các bond theo chiều dài vết nứt. Các thông số đầu vào của mô hình là những thông số hình học, thuộc tính của vật liệu graphene cần thiết để tính toán mô phỏng và xác định cường độ kéo của bond ngay đầu vết nứt. Dạng phá hủy hỗn hợp của dạng I và II theo hướng armchair đã được nghiên cứu với các góc pha khác nhau. Mô hình thực hiện dạng phá hủy hỗn hợp này được thiết lập với hướng tải và điều kiện biên dựa vào mô hình của Arcan. Áp dụng điều kiện biên quay không ảnh hưởng đến kết quả tính toán. Giá trị hệ số cường độ ứng suất ở từng góc pha đã được xác định và được so sánh đánh giá với các kết quả nghiên cứu trước.

Từ khóa: *Sự phá hủy vật liệu graphene; phá hủy hỗn hợp vật liệu graphene đơn lớp; hệ số cường độ ứng suất graphene; cường độ phá hủy tới hạn graphene; mô hình cơ học vi mô graphene*

1. INTRODUCTION

A fundamental understanding of the fracture mechanisms in graphene is not only scientifically interesting, but also practically important for preventing or controlling fracture in graphene [1]. Honeycombs are widely used in lightweight structures [2] and proposed a bending model of cell walls to analyze mechanical properties of cellular materials. They found that mechanical properties of cellular materials are related to cell geometry and material properties of solid cell-wall materials. They have made an

analytical estimate for the fracture toughness of elastic–brittle hexagonal honeycombs.

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.

Recently, Zhang *et al* [3] and models on the fracture toughness of shear 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. Datta *et al* [4] performed classical molecular dynamics (MD) simulations on a graphene sheet with crack like flaw and investigated the complex mixed-mode fracture behavior of grapnene.

However, the effect of the mixed-mode fracture of graphene has not been performed by FEM simulation. In this study, the effect of crystal orientation armchair directions on the mixed mode fracture behavior of graphene sheet needs to be studied. We investigate the effect of applying rotations as boundary conditions in addition to prescribed translational displacement boundary conditions on the predicted fracture toughness. This method has been used by Prasanna Thiyagasundaram [5] and S. Choi [6]. We directly apply displacements based on the *K-field* on the boundary of the micromechanical model. A modified version of the Arcan specimen is made for the mixed-mode fracture. Mixed-mode fracture analysis using FEM simulations was conducted to determine the fracture toughness of SLGS for various angles. A commercial software ANSYS is used for FEM calculations and comparison with previous results.

2. MODELS AND METHODOLOGIES

For the finite element analysis, a grid of 100x60cells was employed (Fig 1) where W(width) and H(high). Here, ANSYS 14.5 [7] was utilized to model the struts with the armchair model. The stress distribution along the outermost layer of cells is uniform and the stress field far away from the crack tip is undisturbed. The analysis gives the forces and moments at both ends of each strut from which the critical skin stress of the first unbroken cell edge ahead of the crack tip can be calculated. Failure occurs when the critical skin stress reaches the modulus of rupture of the cell wall, which is assumed to be constant at this point in the study [8]. The thickness (d) and length (l) of a graphene sheet vary depending on the study, and different values have been reported by Duplock [9], Zhou [10], Tu and Ou-Yang [11] and Pantano [12], Kudin [13], Goupalov [14], Reddy [15]. We used AMBER force constants [16], where the thickness of the C–C bond is 0.84Å and Poisson's ratio is 0.186 and Young's modulus is 1.05TPa for an equilibrium length *l* of 1.38 Å.

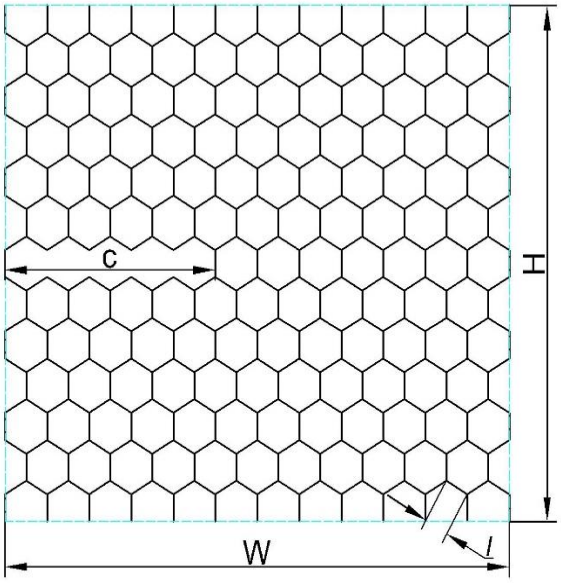


Fig.1. *The geometry for the finite element analysis of SLGS having a central crack with a length of 2c.*

The results of the analysis [17] indicate that if the crack length is higher than 10 cells the fracture toughness is constant. Only one crack length is used in present work with c= 25 cells. Modulus of rupture, σ_{fs} of SLGS is used to [18], so that the SLGS is linear elastic to fracture and that it has constant modulus of rupture, σ_{fs} of 27.89 MPa is calculated as follows. The micro model uses beam elements to model the struts and to determine the maximum stresses at crack tip and contained approximately 273,000 elements. From the failure criterion for the strut material the fracture toughness of the graphene sheet is estimated. A known uniform tensile stress, σ, is applied to the SLGS. This generates an internal stress in the cell wall ahead of the crack tip of:

$$\sigma = M\frac{y}{I} + \frac{P}{A} =$$

$$= \sigma_{Bending\ stress} + \sigma_{Axial\ tress} \quad (1)$$

where $\sigma_{Bending\ stress}$ and $\sigma_{Axial\ tress}$ are found directly from the FEM analysis. Fracture occurs when the internal stress in the cell wall ahead of the crack tip reaches the modulus of rupture of the cell wall, σ_{fs}, at an applied stress of, $\sigma = \sigma_{fs}$. Mode-I and Mode-II stress intensity factors [17,18] were evaluated as

$$K_{IC} = \sigma_{fs}\frac{\pi\sqrt{\pi}d^2}{4\sqrt{\sqrt{3}\,l(2\sqrt{3}l+d)}} \quad (2)$$

$$K_{IIC} = \tau_{fs}\frac{\pi\sqrt{\pi}\,d^3}{12\sqrt{2}\,l^2\sqrt{l}} \quad (3)$$

where, σ_{fs} and τ_{fs} are the tensile and shear stress values at the instant of first bond rupture.

The fracture toughness of SLGS was determined from FEM with the modified version of the Arcan specimen [19, 20] under different mixed-mode loading conditions. In this section, a modified version of the Arcan specimen is made for the mixed-mode fracture of SLGS, which allows mode-I, mode-II, and almost any combination of mode-I and mode-II loading with the same specimen configuration.

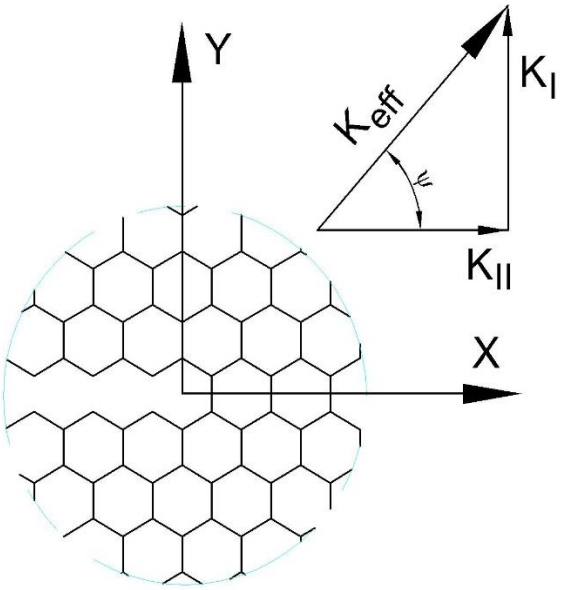


Fig.2. *Model of the mixed-mode loading.*

Phase angle Ψ (mixed mode parameter or equivalent crack angle) is defined as

$$\Psi = tan^{-1}\left(\frac{K_I}{K_{II}}\right) \quad (4)$$

and an effective SIF, K_{eff}, at the initial crack length is evaluated as

$$K_{eff} = \sqrt{(K_I)^2 + (K_{II})^2} \quad (5)$$

Therefore the far-field behavior of pristine graphene is assumed to be well represented by the solution since the stress singularity decreases apart from the crack tip. The geometry and boundary conditions are shown in Fig 3. The average value of mode I fracture toughness (K_{IC}) obtained from the [17,18] with FEM simulations with c= 25cells at Ψ = 90° is 2.63 MPa$\sqrt{m}$ and also mode II fracture toughness (K_{IIC}) obtained from this chapter by FEM simulations at Ψ = 0° is 1.68MPa$\sqrt{m}$.

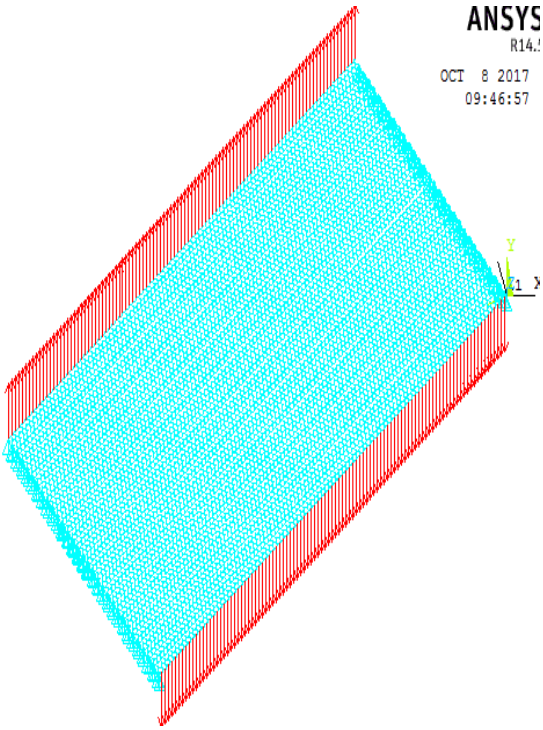
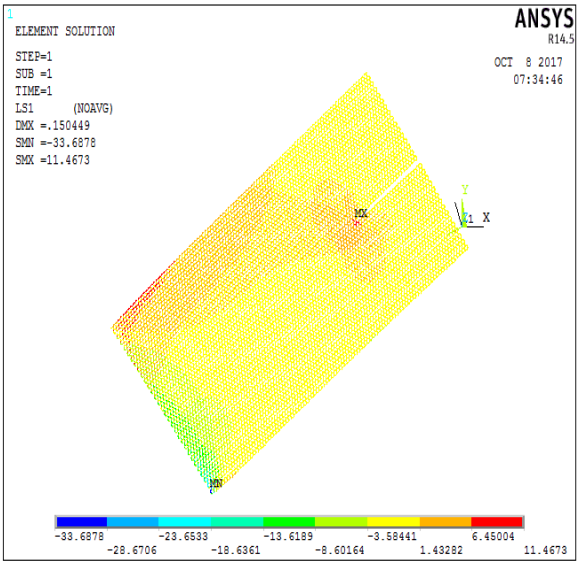
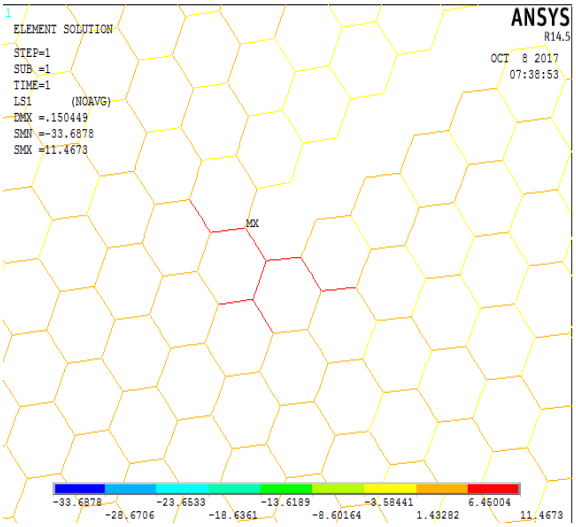


Fig.3. *Finite element model of a typical Arcan specimen with 45°.*

The model must change with change in maximum normal stress direction. It can be noted from Fig.4-5 that the crack length direction is almost insensitive to the change in loading angle (from 15°, 30^0, 45° for armchair and from 45°, 60°, 75^0 for zigzag sheet), or change in maximum normal stress direction.

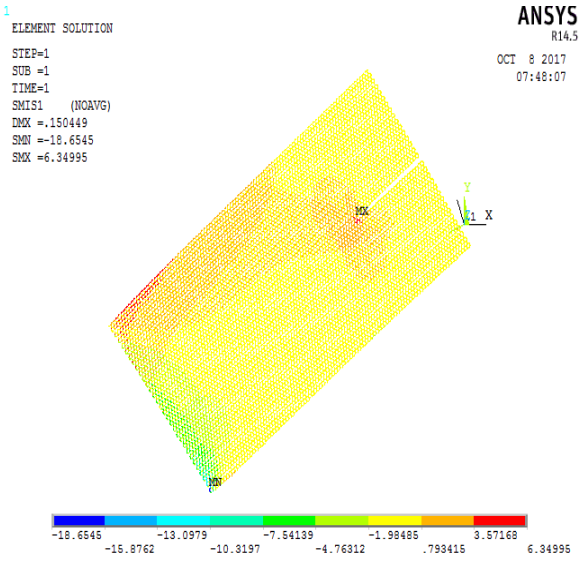


(a)

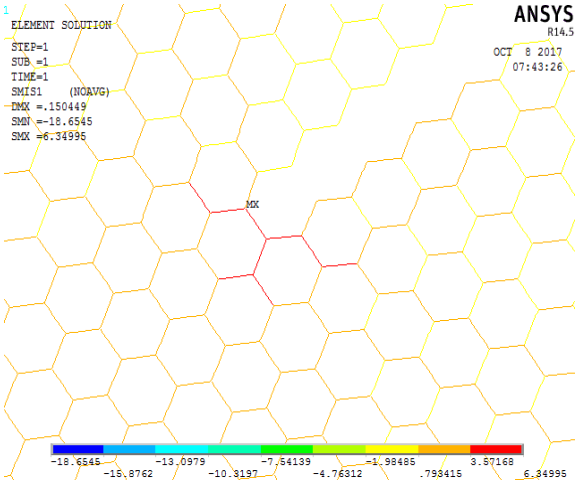


(b)

Fig. 4. *(a) FEM with axial stress results (b) View of detail at crack tip.*



(a)



(b)

Fig.5. *(a) FEM with bending stress results (b) View of detail at crack tip.*

Critical stress intensity factors values were derived from the maximum stress at crack tip. K_I and K_{II} were calculated using FEM simulations. K_I increases and K_{II} decreases as the mode I loading contribution, i.e. as Ψ increases from 0^o to 90^o. It is seen that for loading angles $\Psi \geq 45^o$, the mode-I contribution is greater than that of mode-II and the opening mode fracture becomes dominant. For loading angles $\Psi \leq 45^o$ there is an opposite trend and the shearing mode fracture becomes dominant.

3. RESULTS AND DISCUSSION

We investigate closed form solutions for the fracture properties of SLGS using mechanical cellular solids. The analysis of this field for different loading angle has shown which length must be employed in the fracture toughness evaluation. In order to verify the accuracy of the modeling procedure and the formulation developed in this study a finite element model of a graphene sheet is constructed in ANSYS commercial package [7]. The numerical simulations presented are encouraging (Fig. 4-5). Researches, however, are still seeking a more efficient computational modeling for predicting fracture toughness of SLGS.

It is well known that the fracture energy under mode I loading is different from that under mode II loading in SLGS. For the situation under mixed-mode loading, there is an interaction between the two fracture modes and it is necessary to find a relationship between mode I and mode II stress intensity factors. It is generally

proposed in the form as

$$\left(\frac{K_I}{K_{IC}}\right)^m + \left(\frac{K_{II}}{K_{IIC}}\right)^n = 1 \qquad (6)$$

The fracture toughness of SLGS was determined from FEM with a modified version of the Arcan specimen for various phase angles under different mixed-mode loading conditions. A failure criterion was developed by plotting the average fracture toughness data on a normalized volume diagram (Fig.6). It can be seen that an equal elliptical equation (i.e m=2, n=2 and $K_{IC} \neq K_{IIC}$ is suitable for characterizing the mixed-mode fracture criterion of Bin Zhang [3] and [4].

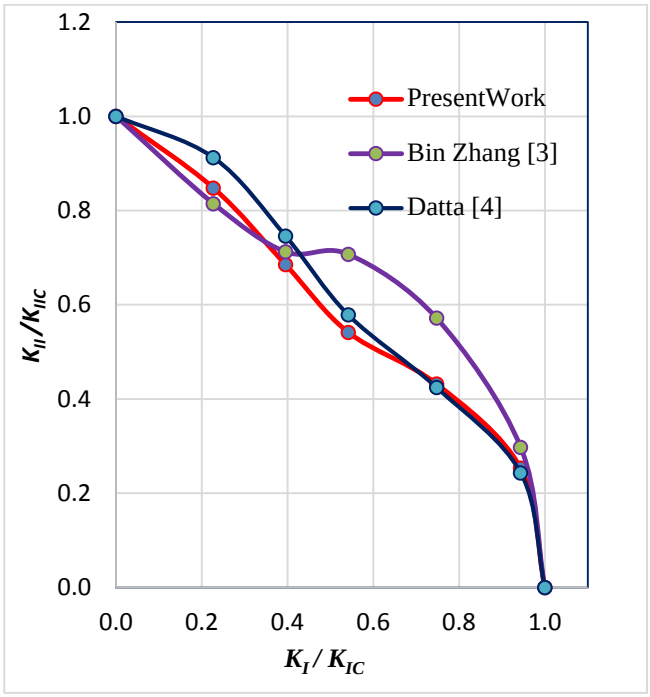


Fig.6. *Normalized mixed-mode fracture envelope and predictions of the mixed-mode fracture criteria with a crack length of 25cells.*

Since the Arcan specimen developed by Arcan [19] has very similar geometry and boundary conditions to the specimen used in the investigation, results were expected to be very close. For the purpose of comparison, in Fig 6, the finite element results together with those calculated MD simulations by Bin Zhang [3], Datta [4] and a homogeneous Arcan specimen are presented. The mixed mode FEM results are shown in Fig. 7 in a K_{II}/K_{IC} versus K_I/K_{IC} diagram and also shown in this figure is the MD simulations prediction of a well-known fracture criterion in [3] and [4].

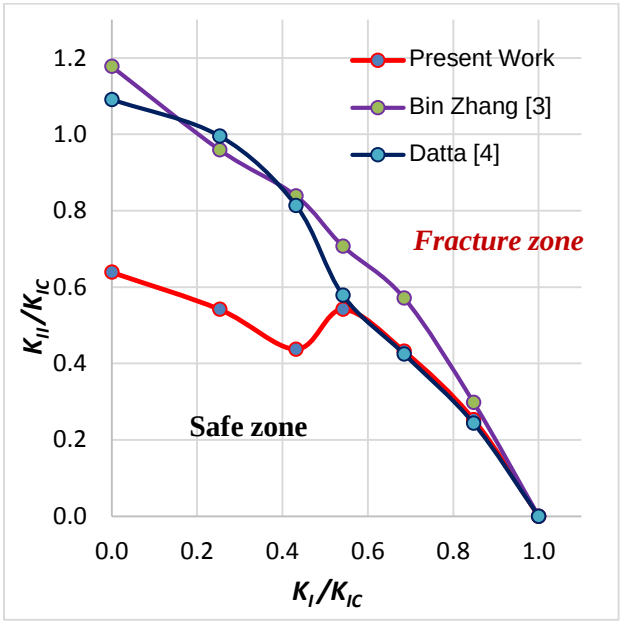


Fig.7. *Normalized prediction of the mixed mode fracture criteria of SLGS.*

The curves in Fig.7 are the mixed-mode (I/II) fracture curves of the Arcan specimen for different phase angle. To use these curves in theory cases, first the phase angle for each stress intensity factors should be calculated for the phase angle for each components under the applied load. These factors are then normalized as K_{II}/K_{IC} and K_I/K_{IC} and the corresponding point is determined in Fig 7. A finite element based method has been used to calculate the fracture toughness of graphene. Increase in K_I can be attributed to the increase in normal stress component at the crack tip with the loading angle from 0^0 to 45^0 and similar previous results. In contrast, the K_{II} values decrease with loading angle from a peak value at $\psi > 45°$ to $\psi = 90°$. Also, the K_{II} values for graphene sheets loaded in amrchair edges are lower compared to previous results for all the loading cases. With this results show that the Mode-II fracture toughness converges to discrete models are not applied and to when the rotations are applied. The mixed mode fracture criteria are determined and fracture surfaces obtained at different loading angles for pristine graphene are discussed.

4. CONCLUSIONS

A FEM model for mixed mode (mode I/ mode II) SLGS has been implemented. One advantage of such approach is that it's easy implementation and considerably lowers computational efforts when compared with

MD techniques. The expression for mixed mode fracture toughness fracture criterion for SLGS and foams are derived. It is found that mixed mode fracture toughnesses of SLGS depend on their cell geometry and the modulus of rupture of materials. When the variation of modulus of rupture is taken into account, the finite element method study indicates that the existing model, based on a continuum approach, is satisfactory for graphene sheet with semi-crack length greater than 10 times the cell size.

For the sake of comparison, the analytical finite element model with the same geometric parameters and material properties as the atomistic graphene sheet was constructed, and the corresponding stress intensity factors were calculated from the crack closure method. Results indicated that the stress intensity factors obtained from the micromechanical model exhibit good agreement with those derived from discrete atomistic model. Comparing the normalized result for fracture toughness given in FEM with the MD results, one can note that the difference is about 15% with Bin Zhang and 5% with Datta. Considering the idealizations made in the model and variations in the unit-cell shape and dimensions and in situ properties of the graphene cell walls, the finite element results seem to be reasonable. Therefore, it is suggested that the SIF is an appropriate parameter, which can be employed in the atomistic model and the micromechanical model for describing the fracture of covalently bonded graphene sheet. Our results suggest that the mixed mode fracture toughness of SLGS is independent from the crack length and predicted toughness of graphene shown in Fig 6 and Fig 7. The simulation of fracture strength is in good agreement with that predicted by the energy-based quantized fracture mechanics.

Generally, the crack propagation in mixed mode I/II can be predicted by the Arcan specimen and the propagation of a mixed-mode crack in a brittle fracture graphene is investigated. The brittle fracture of graphene prefers along armchair edges concerning with its lower toughness and applied complex mechanical stresses in static rupture. The comparison between Bin Zhang [3], Datta [4] and our numerical results shows that the numerical results are in good agreement with the MD simulations results.

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