FRACTURE ANALYSIS OF SINGLE LAYER GRAPHENE SHEETS

PHÂN TÍCH SỰ PHÁ HỦY LAN TRUYỀN VẾT NỨT CỦA VẬT LIỆU GRAPHENE ĐƠN LỚP

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ABSTRACT

The formula is derived analytically from the deformation and bending mechanism of solid-state carbon-carbon bonds to describe the mode I fracture of single layer graphene sheet (SLGS). Fracture of a single layer graphene is governed by the competition between bond breaking and bond rotation at a crack tip. It is demonstrated that in tension the cell walls bend and elongate, leading to the development of tensile stresses on some portions of the outer surfaces of the cell walls. As a result it was found that fracture of graphene sheets can create fracture edges at the middle of bond and bond deformation and rupture are induced by the localized high stress near the crack tip.

Key words: *fracture of graphene; fracture mechanics; fracture toughness; stress intensity factor.*

TÓM TẮT

Một công thức đã được phân tích và thiết lập từ sự biến dạng và chịu uốn cơ học của các xương (bond) ở trạng thái liên kết C-C để diễn tả sự phá hủy theo tiêu chuẩn thứ nhất (open mode hoặc mode I) của vật liệu Graphene đơn lớp. Sự phá hủy của tấm Graphene đơn lớp này do hai yếu tố sinh ra là xương chịu kéo và xương chịu uốn xoay đồng thời sinh ra ở đầu vết nứt. Điều đó chứng tỏ rằng, khi chúng ta dùng tiêu chuẩn thứ nhất để phân tích thì các bond ở đầu vết nứt sinh ra chịu uốn và kéo dọc trục bond và sau đó nó sẽ lan truyền đến các vị trí tiếp theo. Sự phá hủy của tấm vật liệu Graphene đơn lớp được hình thành là do sự gia tăng ứng suất ở đầu vết nứt và nó tập trung vào giữa bond liên kết, biến dạng của bond này vượt quá giới hạn và sinh ra đứt bond.

Từ khóa: *Hệ số cường độ ứng suất graphene; phá hủy vật liệu graphene đơn lớp; cường độ tới hạn graphene.*

1. INTRODUCTION

Single layer graphene sheets (SLGS) are one atom thick two-dimensional layers of sp^2-bonded carbon densely packed to form a honeycomb crystal lattice [1]. The graphene's Young's modulus and thermal conductivity rival the analogous properties of graphite (1.06 TPa and 3000 $Wm^{-1}K^{-1}$, respectively) [2, 3]. Graphene is the strongest material ever measured in the world. It is noticed that the graphene density is even harder than diamond and about 100 times stronger than that of the best steels in the world, while the density is only 2.2 g/cm^3.

Fracture toughness describes the ability of a material containing a crack to resist fracture and it is a critically important material property for design applications. Previous attempts to model the fracture toughness of brittle honeycomb have yielded well-known results by Gibson *et al* [4,5]. Fracture analysis of monolayer graphene sheets with double vacancy defects via molecular dynamics simulation is used to explore the influence of separation distance of double vacancy defects on the mechanical properties of SLGS [6]. The mechanisms of deformation and fracture of

graphene sheets under uniaxial tension were studied on the nanoscale, and their strain characteristics were determined using relations of micromechanics [7]. Research on the nonlinear mechanical properties of graphene nanoribbons [8] is shows that the nominal strain to fracture is considerably lower for armchair graphene nanoribbons than for zigzag ribbons. From the study of the mechanical properties of epoxy nanocomposites with graphene platelets, crack deflection is found to be the process by which an initial crack tilts and twists when it encounters a rigid inclusion [9]. Macroscopic fracture parameters are investigated on 2D graphene systems containing atomic-scale cracks. The atomic stress distributions match very well with those of linear elastic solutions [10]. Rhonda Jack and Markus J. Buehler [11] have carried out systematic studies of the influence of patterns of vacancies in graphene on the dynamics of crack propagation. These studies suggest that engineering vacancy structures ahead of a seed crack can be used to control the fracture behavior of graphene sheets, leading to distinct surface geometries. Recently, new results and models on fracture toughness of open-cell were presented [12–13] and used to calculate the fracture toughness of foams. Sachin S. Terdalkar [14] proposed the fracture of a monolayer graphene is governed by the competition between bond breaking and bond rotation at a crack tip. They have repeated most of the simulations using the Tersoff-Brenner potential but they have not used *K-field* analysis for a crack in graphene.

The main objective of this article is to investigate the fracture toughness of SLGS. In the present study, we first develop a theoretical framework for model fracture tounghness of 2D graphene sheets for both zigzag and armchair cases micromechanics. Using simple mechanics the maximum stress is calculated in each bond at near crack tip on SLGS and hence the whole network can be determined, enabling expressions for the bond breaking and bond rotation at a crack tip. This theoretical model was confirmed by studying several open-cell with short cracks. We use the same approach as L.J. Gibson, M.F. Ashby [5] to determine the fracture toughness for SLGS. We directly apply displacements based on the *K-field* on the boundary of the micromechanical model. A commercial software ANSYS is used for FEM calculations and comparison with theoretical results.

2. EQUIVALENT HONEYCOMB ANALYSIS FOR GRAPHENE SHEETS MODEL

2.1 Fracture toughness behavior of graphene sheets

If graphene sheets are loaded to near it's fracture stress, one cell wall fails, the stress on the neighbouring walls increases and they will fail too. The failed cluster is like a crack, the stress concentration at it's periphery causes further walls to fail, and propagaties across the section. The problem is best approached by the methods of fracture mechanics. Consider the brittle graphene sheets containing a crack cluster of broken cells. When it is loaded in tension the cell walls at first bend elastically. The load is transmitted through the graphene sheets as set of discrete forces and moments acting on each of the cell walls. This condition defines, the fracture toughness of graphene sheets, which we calculate. The method involves a number of assumptions. First, if the graphene sheets is to be treated as a continuum, the crack length must be large relative to the cell size. Second, contribution of the axial forces in the cell walls to the internal stress ahead of the crack tip isn't neglected. Third, we assume that the cell wall material has a constant modulus of rupture, . Crack deflection is the process by which an initial crack tilts and twists when it encounters a rigid inclusion. This generates an increase in the total fracture surface area.

In the present study, we explore the tensile fracture response of a edge-cracked plate (ECP) made from graphene sheets (Fig. 1). The fracture behaviour of the brittle graphene

sheets made use of linear elastic fracture mechanics (LEFM) concepts to estimate the fracture toughness of hexagonal. The stress field of an equivalent linear elastic continuum was used to calculate the stresses on the cell walls of the lattice directly ahead of the crack tip.

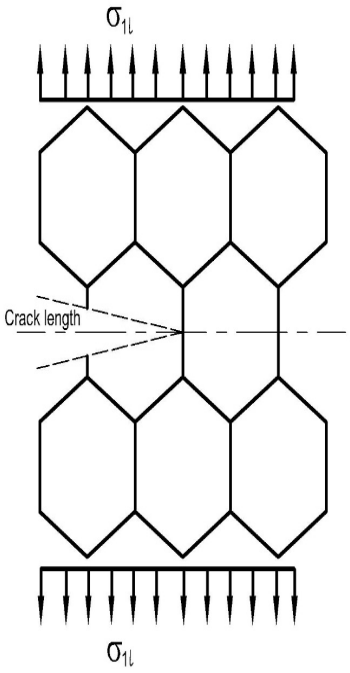


Fig.1*.Edge-cracked plate of graphene sheet*

A crack of length 2c in an elastic solid lying normal to remote tensile stress σ_1 create a singular local stress field, σ_1 [4]:

$$\sigma_l = \frac{\sigma_1\sqrt{\pi c}}{\sqrt{2\pi r}} \quad (1)$$

where r is the distance ahead of the crack tip as half of the width of the cell then and σ_1 is the remote stress perpendicular to the plane of the crack.

2.2 The geometry and deflections for loading in the armchair direction (X_1)

In tension the failure process is different [5]. At some point a cell wall will fail in tension, adjacent walls will also fail as the load transfers to them and create what is effectively a macroscopic crack - an example is shown Fig. 2.

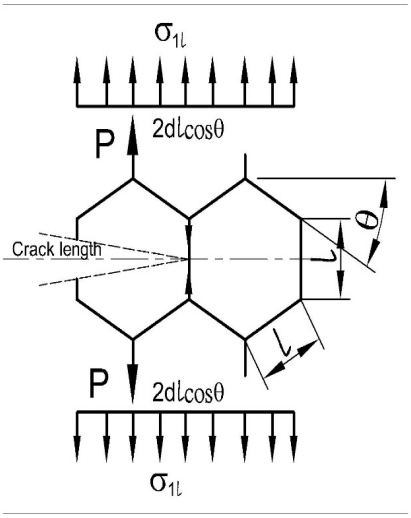


Fig.2. *The local stress field supplemented by the actual tensile stress in the cell wall.*

The bending moment in the vertical beam ahead of the crack exists because of the gradient in stress ahead of the crack tip which results in a larger force pulling on the first column above the end of the crack, than in the second and third columns,.. The moments in the two angled beams are not cancelled out leaving a dual moment rotating the vertical beam ahead of the crack tip. This moment creates a tensile stress on the crack side of the vertical cell wall.

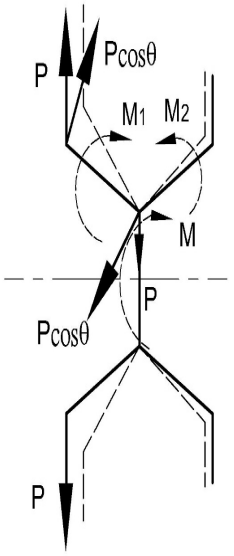


Fig.3. *The forces in the armchair cell wall to the internal stress ahead of the crack tip.*

The bending moment on a cell wall just ahead of the crack tip are as follows:

$$M=M_1- M_2 \quad (2)$$

Where M_1, M_2 are bending moments on the wall exerted by the force.

And we shall assume that $M_1>>M_2$

$$M = M_1 = \frac{Plcos\theta}{2} \quad (3)$$

The force on the cell wall is:

$$P = 2\sigma_{1l}dlcos\theta \quad (4)$$

where d is thickness (diameter) of bond graphene sheet.

The approach can be used for crack propagation when stressed in the armchair (X_1) direction. Stress of the cell wall is:

$$\sigma = M\frac{y}{I}+\frac{P}{A} \quad (5)$$

where M is the moment about the neutral axis, y the perpendicular distance from the neutral axis and I is the second moment of inertia area about the neutral axis.

We obtain:

$$\sigma = \frac{P}{\pi d^3}(16lcos\theta + 4d) \quad (6)$$

With $r = lcosq$, from equation (1)

$$\sigma_{1l} = \sigma_1\sqrt{\frac{c}{2lcos\theta}} \quad (7)$$

From equation (4)

$$P = 2\sigma_1 d\sqrt{\frac{clcos\theta}{2}} \quad (8)$$

From equation (6), we have:

$$\sigma = \frac{4\sigma_1\sqrt{2clcos\theta}}{\pi d^2}(4lcos\theta + d) \quad (9)$$

With graphene sheets of q = 30°

$$\sigma = \frac{4\sigma_1\sqrt{\sqrt{3}\,cl}}{\pi d^2}\left(2\sqrt{3}l + d\right) \quad (10)$$

If fracture occurs when the stress exceeds the fracture strength of the cell wall material:

$$\frac{\left(\sigma_f^*\right)_1}{\sigma_{fs,1}} = \frac{\pi d^2}{4\sqrt{\sqrt{3}\,cl}\left(2\sqrt{3}l+d\right)} \quad (11)$$

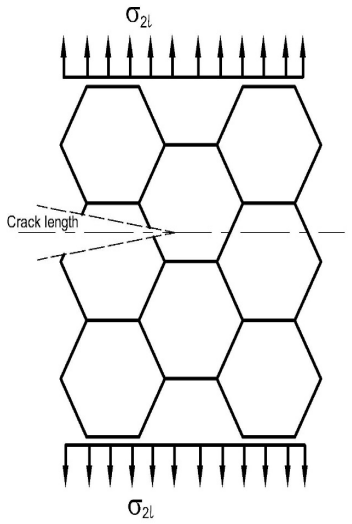
It is helpful to rephrase this result in the terminology of fracture mechanics. Tensile fracture will occur when the fracture toughness is reached:

$$K_{IC}^* = \sigma_f^*\sqrt{\pi c} \quad (12)$$

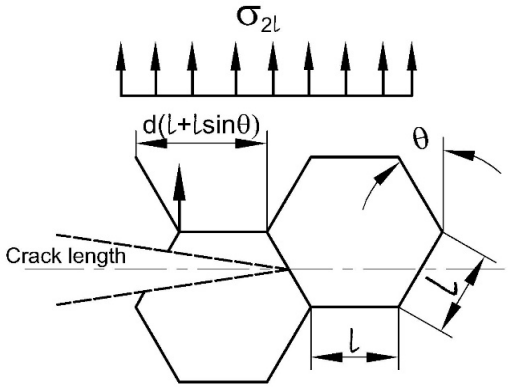
If we re-write the above equation in terms of fracture toughness armchair direction (X_1):

$$K_{IC,1}^* = \sigma_{fs,1}\frac{\pi\sqrt{\pi}d^2}{4\sqrt{\sqrt{3}\,l}\left(2\sqrt{3}l+d\right)} \quad (13)$$

2.3 The geometry and deflections for loading in the zigzag direction (X_2)



(a)



(b)

Fig.4. *Crack propagation leading to brittle tensile failure in graphene sheet. (a) The geometry and deflections for loading in the zigzag direction (X_2); (b) The local stress field supplemented by the actual tensile stress in the cell wall.*

The bending moment in the inclined beam ahead of the crack exists

The bending moment of beam:

$$M = Plsin\theta \quad (14)$$

On average, taking the crack to occupy half the width of the unit cell, then:

$$P = \sigma_{2l} d(L + lsin\theta) \quad (15)$$

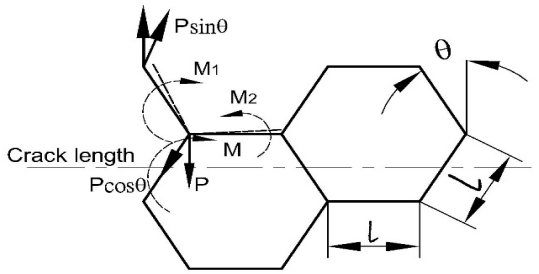


Fig.5. *The forces in the zigzag cell walls to the internal stress ahead of the crack tip and bending moment of beam.*

The stress in the zigzag (X_2) direction:

$$\sigma = M\frac{y}{I} + \frac{Pcos\theta}{A} \quad (16)$$

$$\sigma = \frac{P}{\pi d^3}(32lsin\theta + 4dcos\theta) \quad (17)$$

From equation (1), we have:

$$\sigma_{2l} = \frac{\sigma_2\sqrt{\pi c}}{\sqrt{2\pi r}} \quad (18)$$

Where $r = \frac{l+lsin\theta}{2}$

$$\sigma_{2l} = \sigma_2\sqrt{\frac{c}{l+lsin\theta}} \quad (19)$$

From equation (15)

$$P = \sigma_2 d\sqrt{c(l + lsin\theta)} \quad (20)$$

From equation (17), we have:

$$\sigma = \frac{\sigma_2\sqrt{c(l+lsin\theta)}}{\pi d^2}(32lsin\theta + 4dcos\theta) \quad (21)$$

With graphene sheets of $q = 30^o$

$$\sigma = \frac{\sigma_2\sqrt{2cl}}{\pi d^2}(8\sqrt{3}\,l + 3d) \quad (22)$$

If fracture occurs when the stress exceeds the fracture strength of the cell wall material:

$$\frac{(\sigma_f^*)_2}{\sigma_{fs,2}} = \frac{\pi d^2}{\sqrt{2cl}(8\sqrt{3}\,l+3d)} \quad (23)$$

If we re-write the above equation in terms of fracture toughness zigzag direction(X_2):

$$K_{IC,2}^* = \sigma_{fs,2}\frac{\pi\sqrt{\pi}d^2}{\sqrt{2l}(8\sqrt{3}\,l+3d)} \quad (24)$$

3. FINITE ELEMENT ANALYSIS FOR GRAPHENE SHEETS

The finite element analysis uses a grid of 50x30 cells (Fig.6) and we have used ANSYS 12.1 to model the struts. 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, in this part of the study, we assume to be constant [4]. The thickness (d) and length (*l*) of graphene sheet are known different by different scientists, such as the ones of Duplock [2], Zhou [15], Tu and Ou-Yang [16] and Pantano [17], Kudin [18], Goupalov [19], Reddy [20]. We used AMBER force constants [21], the thickness of the C–C bond would be 0.84A°, with a Poisson's ratio n of 0.034 for an equilibrium length l of 1.38 A°.

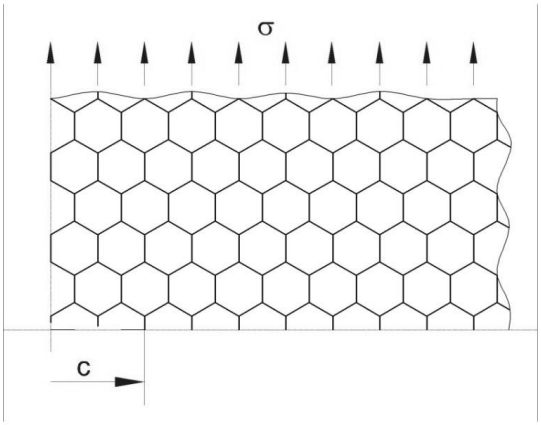


Fig.6. *Loading geometry for finite element analysis of SLGS with central symmetric crack of length 2c.*

Seven different crack lengths are used in present work: c = 2.39, 4.78, 7.17, 9.56, 14.34, 19.21, 23.90A°. However, experimental constant modulus of rupture, σ_{fs} of SLGS is not available, so we assume that the SLGS is linear elastic to fracture and that it has an arbitrary constant modulus of rupture, σ_{fs} of 10MPa is calculated as follows. A known uniform tensile stress, s, is applied to the SLGS. This generates an internal stress in the cell wall ahead of the crack tip of:

$$\sigma = M\frac{y}{I} + \frac{P}{A} = \sigma_{Bending\ stress} + \sigma_{Axial\ tress} \quad (25)$$

Where $s_{Bending\ stress}$ and $s_{Axial\ tress}$ are found 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, s-σ_{fs}. The fracture toughness is then calculated as

$$K_{IC} = \sigma_f\sqrt{\pi c} \quad (26)$$

4. RESULTS AND DISCUSSION

In this work, we develop closed form solutions for the fracture properties of SLGS using mechanical cellular solids. We obtained the equation (13) and (24) which are the fracture toughnesses for the graphene sheet. 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 [22]. Since the fundamental aspect of developed formulation relies on axial stress and bending stress of a carbon–carbon bond, a built-in two-dimensional beam element is employed for finite element analysis on the basis of the same assumption with analytical solution. The geometrical properties of the beam elements are derived using AMBER [21] and fed into the model as input data.

With the hexagonal cells at ratios of c/l >7 the fracture toughness is constant [5] but graphene sheet at ratios of c/l >8 the fracture toughness is constant, independent of crack length. But for *c*/l less than 8, the fracture toughness decreases rapidly. This results shows that from the FEM results the difference in displacement between armchair and zigzag direction is » 5%. The comparison between the fracture toughness obtained from analytical solution and finite element model is shown in Fig.8 and it is found that fracture toughness for case armchair direction is » 18% and zigzag direction is » 20% higher than analytical result.

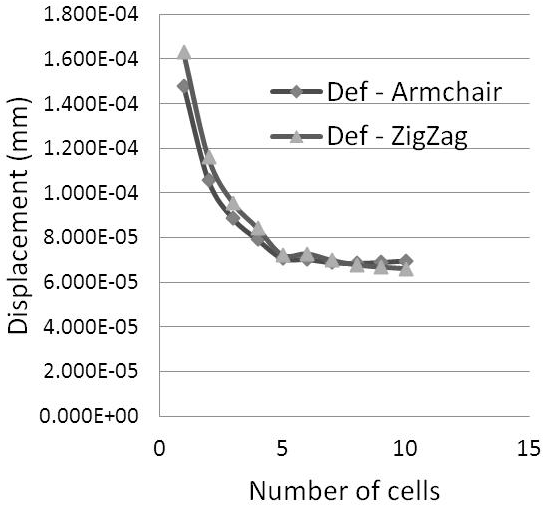


Fig.7. *Displacement of armchair and zigzag models*

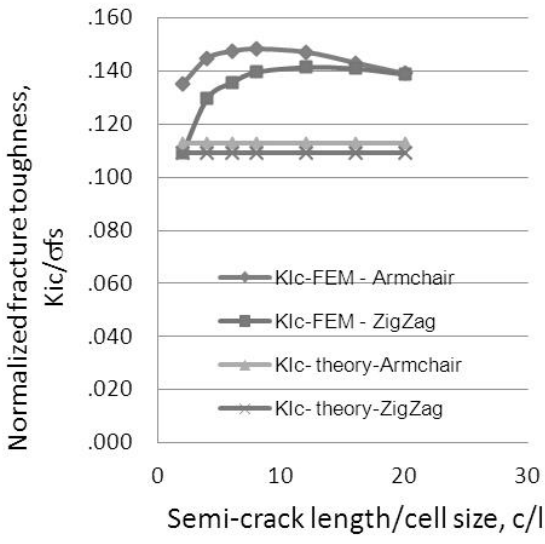


Fig.8. *Comparison of fracture toughness between analytical and FEM analysis*

5. CONCLUSION

The analytical models proposed in this study allow establishing the equivalent homogenized mechanical properties of single

graphene sheet with the different deformation and bending mechanisms of the C–C bonds. We show that the fracture of a single graphene involves the bond rotation and bond breaking. The fracture equation can be accurately evaluated from the local stress field in the immediate vicinity of the crack tip. Moreover, the local stress distributions around the crack tip are studied and calculated by applying remote *K*-field deformations. Our formula can be applied in practice to calculate the fracture toughness of SLGS.

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