Tearing Graphene

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ABSTRACT

Experiments on free standing graphene can expose the graphene sheets to out-of-plane forces. Here we show that out-of-plane forces can cause free standing graphene to fracture. This fracture mode is known as the tearing mode and is common in materials such as paper. We present a numerical study of the propagation of cracks in clamped, free standing graphene as a function of the out-of-plane force. We observe that the cracks' path and the edge structure produced are dependent on the initial crack length. We also obtain an analytical expression for the the minimum force required to tear a two dimensional sheet, such as graphene, in terms of the initial crack length. This work may help avoid the tearing of graphene sheets and aid the production of samples with specific edge structures.

Keywords: graphene, fracture, tearing, molecular dynamics

1 INTRODUCTION

Graphene presents many attractive properties to basic science and to industry. It is light, flexible, and thermally stable (in a non-oxidizing environment). It has a high electrical conductivity (the Fermi velocity of electrons in graphene is 10^6 m/s [1]) and a high Young's modulus of about 1 TPa [2], making it one of the stiffest material known. Nevertheless in some experimental setups free standing graphene samples show cracks and holes, and sometimes the samples even break [3], [4]. The back-gate voltage experimental setup is an example of a setup where samples have been observed to break. In this setup the free standing graphene sheet is clamped and exposed to a downward force from an external electric field.

In this work we study the fracture mechanics of a free standing graphene sheet under a downward force. In Sec. 2 we present an analytical study of the tearing of a two dimensional sheet, such as graphene. Sec. 3 shows a numerical simulation of the propagation of cracks in clamped, free standing graphene, as a function of the out-of-plane force.

Previous studies of fracture dynamics in graphene have focused on in-plane fracture, also called fracture mode 1 [5], and tearing of graphene nanoribbons [6], [7]. We observe similarities between the tearing of clamped graphene and the tearing of nanoribbons.

2 ANALYTICAL APPROACH TO TEARING A TWO DIMENSIONAL SHEET

We are interested in a two dimensional sheet, such as graphene, with an initial crack of length l under a downward force f. Here we present an analytical method to obtain the minimum force needed for the crack to run.

Cracks on graphene sheets have been observed to come in multiple sizes and shapes [3]. It is intuitive that the force required for a crack to run will depend on the initial crack length. For sheets of paper, for example, it is easier to tear a sheet with a long crack, than to tear one with a short crack. Most experimenters focus on electronic properties, and do not look at initial cracks on the samples. Consequently, the shapes of the cracks are in general unknown.

We follow a procedure similar to the one developed by M. Marder [8] for the propagation of a crack in a strip (a three dimensional problem).

Consider a system with an initial crack of length l and total energy $U_{tot}(l)$. The crack can run a length dl if that reduces the total energy of the system, that is:

$$U_{tot}(l) > U_{tot}(l + dl) \tag{1}$$

The total energy of the system can be written as the energy contained within the crack tip region plus the energy outside of it, U_{out}. The energy to move the crack tip (region) is proportional to the energy of the new surface opened up by the crack. Therefore the total energy of a 2D sheet, such as graphene, with a crack of length l is given by:

$$U_{tot}(l) = \gamma l + U_{out}(l) \tag{2}$$

where γ is the surface energy density. The surface energy density is material-dependent, and it can be measured experimentally.

From Eqs. 1 and 2 we get the Griffith's criterion for a crack to propagate on a 2D sheet:

$$\frac{dU_{out}}{dl} + \gamma < 0 \quad (3)$$

The energy outside the crack tip, U_{out}, depends on the geometry of the system. As the exact shape of the cracks is unknown, for simplicity we will consider a crack at the very edge of the sheet. The downward force will then tear the sheet at the edge making it bend diagonally, as seen on Fig. 1. The energy outside the crack tip is then equivalent to the energy required to bend a 2D sheet.

Consider a two dimensional sheet of diagonal length L. The energy for bending the sheet diagonally is given by:

$$U_{out} = \int_0^L dx \left[k \left(\frac{d\theta}{dx} \right)^2 + f_{area} \cdot y(x) \right] (L - x) \quad (4)$$

where k is the bending modulus. The θ term refers to the bending energy and the f_{area} term refers to energy due to the external downward force (per area) applied to the sheet. Also for simplicity we assume small bending, therefore:

$$\frac{d\theta}{dx} \approx y''(x) \quad (5)$$

Minimizing Eq. 4 gives us the energy outside the crack tip in terms of the minimum force required for the crack to run:

$$U_{out} = -\frac{f_{area}^2 L^6}{864k} \quad (6)$$

Note that $L = l\sqrt{2}$.

Using this result with the Griffith's criterion, Eq. 3, we obtain the expression that relates the minimum force (per area) required for a crack to run on a 2D sheet to the initial crack length, l:

$$f_{area} = \sqrt{\frac{18k\gamma}{l^5}} \quad (7)$$

The bending modulus, k, and the surface energy density, γ, of graphene have been measured experimentally (and also obtained numerically) [9]–[11].

This simple analytical study offers insight into the tearing of graphene, it suggests the order of magnitude for the forces to be used in the numerical study.

3 NUMERICAL STUDY OF TEARING GRAPHENE

We present a numerical study of the propagation of cracks in clamped, free standing graphene as a function of the out-of-plane force. Here we use the MEAM semi-empirical potential, shown to reproduce well the properties of graphene and to support crack propagation [11], [12]. The energy minimization is done through damped molecular dynamics. To better model the experimental conditions, all the simulations in this work are of finite-sized graphene sheets, and no periodic boundary conditions are used. These simulations were done at zero temperature, to show only the fracture mechanics of the graphene sheet. In the near future we will include temperature effects.

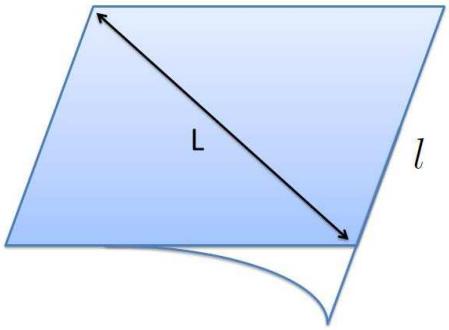

Figure 1: Two dimensional sheet with an initial crack of length l at the right hand side. Because of an external downward force the crack runs, and the sheet bends diagonally.

As an example of an initial condition, Fig. 2 shows a crack of $10\mathring{A}$ at the edge of a suspended graphene sheet, as discussed in Sec. 2. Once sufficient downward force is applied on the sheet, the crack starts running, as seen in Fig. 3. We have also made videos of crack propagations.

The simulations show that, depending on the initial condition, a crack will not run straight through the sheet, as initially expected (see Fig. 4.) Short initial cracks run straight, while longer cracks do not. We are currently looking for the threshold value of the initial crack length that determines the dynamics of the crack propagation.

Another interesting result is that, depending on the initial crack length and orientation (zigzag or armchair), the propagation pattern will be different (see Fig. 4.). The edge orientation of a graphene sheet determines its electronic properties, therefore it will be most useful to be able to predict the edge orientation of produced samples.

4 CONCLUSION

We presented an analytical study of the tearing of a two dimensional sheet, such as graphene, and obtained the minimum force required for a crack to run in terms of the initial crack length.

We performed computer simulations of a clamped, free standing graphene sheet exposed to of an out-of-

Figure 2: Initial crack of $10\mathring{A}$ in a $100\mathring{A}$ by $100\mathring{A}$ clamped, free standing graphene sheet.

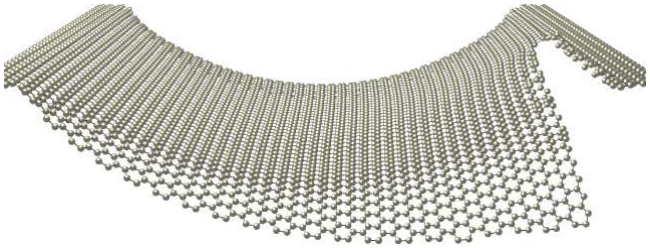

Figure 3: Downward constant force is applied on the sheet of Fig. 1. First the sheet wrinkles and bends and then the crack propagates.

plane force, as expected for back-gate voltage experiments. Preliminary results of the numerical fracture forces show good agreement with the analytical fracture force for small initial cracks. But for initially large cracks the analytical result appears to be lower than the numerical result. Numerically we observed that as the initial crack length gets bigger the crack does not run straight, which could explain the disagreement between numerical and analytical calculations, as the analytical calculation does not account for this type of crack dynamics. Another behavior that is different in the analytical and numerical studies is that numerically the sheet first wrinkles and bends and then the crack runs. This is also not accounted for in the analytical study.

Numerically we also observe that, depending on the initial crack length and orientation (zigzag or armchair), the propagation pattern will be different. Similar dynamics have been seen in simulations of tearing graphene nanoribbons [6].

We are currently working on obtaining the threshold for the graphene fracture energy and the threshold value of the initial crack length that determines the dynamics of the crack propagation. This information can be useful not only to avoid graphene fracture, but also to produce specific types of edges in the process of fracture, as the edge orientation of a graphene sheet determines its electronic properties. In the near future we intend to simulate different initial crack shapes and introduce impurities.

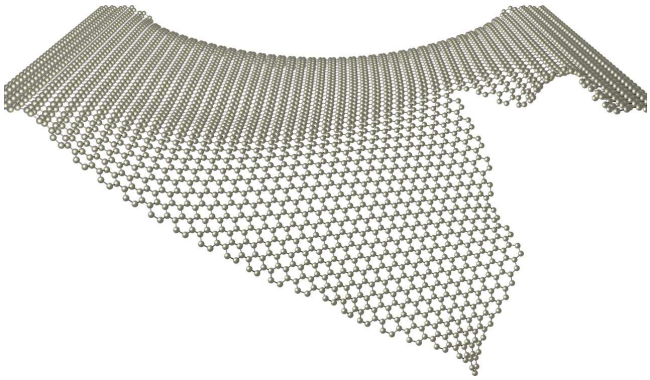

Figure 4: Non-straight crack propagation in a $100\mathring{A}$ by $100\mathring{A}$ graphene sheet with an initial crack of $25\mathring{A}$. Note that the initial zigzag crack propagates as armchair.

We thank Allan MacDonald for pointing out this problem to us, Fulbright and CAPES for scholarship funding, and the National Science Foundation for funding through DMR 0701373.

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