Extreme Mechanics Letters 1 (2014) 83–89

Contents lists available at ScienceDirect

Extreme Mechanics Letters

journal homepage: www.elsevier.com/locate/eml

Directional transport of molecular mass on graphene by straining

Yinjun Huang [1], Shuze Zhu [1], Teng Li *

Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, USA

HIGHLIGHTS

- We reveal a fundamental law of directional transport of molecular mass by straining.
- Directional transport of molecular mass is programmable by devising straining scheme.
- Generally applicable to a wide range of molecular mass and platform materials.

ARTICLE INFO

Article history:
Received 22 October 2014
Received in revised form 5 December 2014
Accepted 5 December 2014
Available online 26 December 2014

Keywords:
Graphene
Molecular mass transport
Strain gradient
Strain engineering

ABSTRACT

Directional transport of molecular mass is essential in enabling desirable functions in nanodevices, but is often challenging to achieve. In this letter, we combine theoretical analysis and molecular simulations to demonstrate a facile mechanism of directional transport of molecular mass on graphene by a simple stretch. We reveal that stretch-induced strain gradient in graphene leads to a net transport force that is sufficient to drive molecular cargo on the graphene in a directional fashion. The large elastic deformability of graphene and the van Der Waals nature of the transport force allow for programmable directional transport of various types of molecular cargo (e.g., graphene flake, carbon nanotube, fullerene, and gold nanoparticle) under the same mechanism. The present findings suggest a fundamental law of directional transport of molecular mass by straining.

1. Introduction

Directional transport of molecular mass is of great importance in designing novel molecular devices and machines, and has a wide range of potential applications in fields such as micro/nanofluids and nanorobotics and nanoelectromechanical systems [1–6]. External mechanical, electrical or magnetic excitations have been shown to induce directional motion of molecular mass [2,7–10]. For example, an excited vibrating carbon nanotube cantilever can act as an efficient and simple nanopump [7]. The presence of a gradient in a potential field can also cause directional motion of molecular mass, mimicking the fact that in macroscopic regime objects tend to fall toward lower gravity potential direction. For example, thermal gradient has been experimentally and theoretically studied on its role of enabling fullerene, graphene flakes, and other molecular cargos to migrate toward lower temperature region on a graphene surface [3,11–13]. Surface chemical gradient, surface tension gradient, surface structural-scale gradient have been demonstrated to be effective to transport water droplet [14–17]. It has been theoretically shown that controlled variations of the intensity or phase of a DC/AC electric field can pump water molecules through carbon nanotubes [18,19]. The above transport mechanisms of molecular mass, however, suffer from either complicated multi-physics actuation scheme, or lack of active control of the transport direction. A facile mechanism of directional transport of molecular mass is still highly desirable.

Introducing strain in graphene by wrinkling [20–22], folding [23–25] and functionalization [26–31] in a programmable fashion have received enormous attention

* Corresponding author.
E-mail address: LiT@umd.edu (T. Li).
[1] These authors contribute equally to this work.

http://dx.doi.org/10.1016/j.eml.2014.12.006
2352-4316/

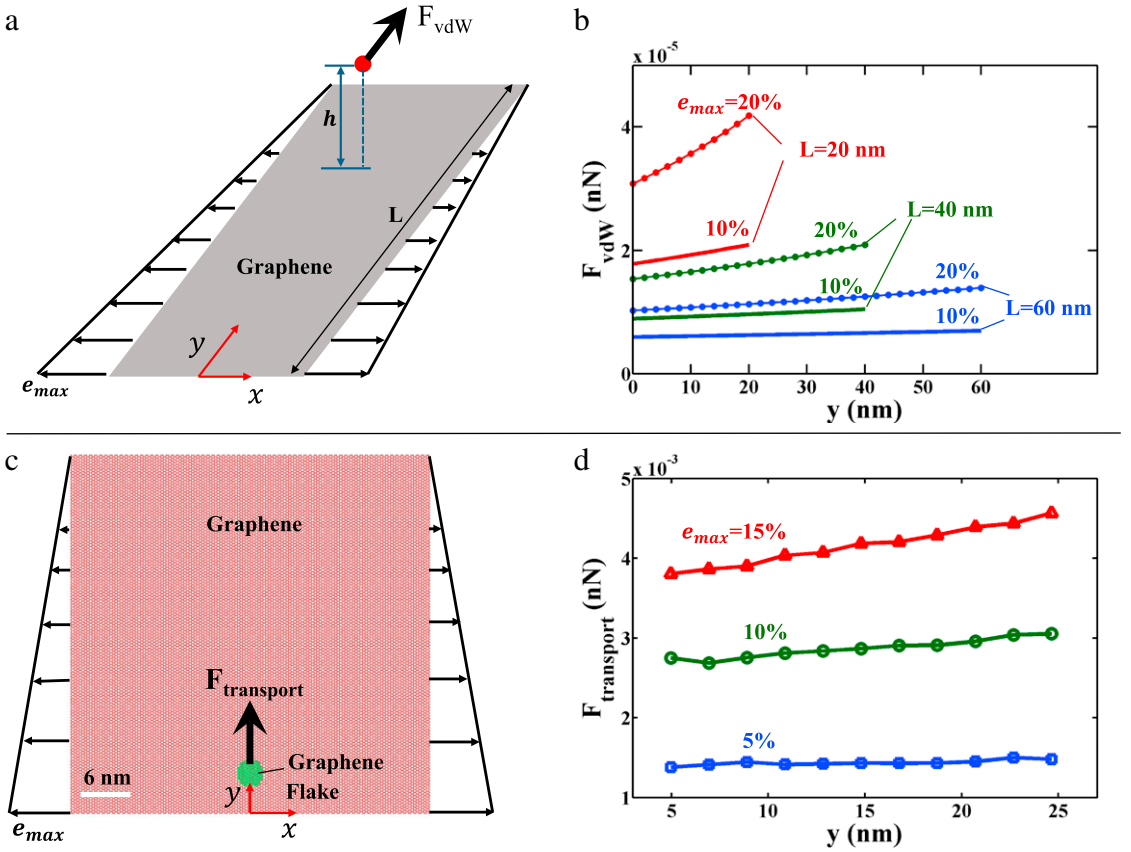

Fig. 1. (a) Schematic showing a net force F_{vdW} acting on an atom (red dot) positioned above on a basal graphene subject to a strain gradient. (b) F_{vdW} as a function of position along y direction for various lengths of basal graphene and strain gradients. (c) Molecular mechanics model of a round graphene flake on a basal graphene subject to a strain gradient to compute the overall net force $F_{transport}$ acting on the graphene flake, which is plotted as a function of position along y direction for various strain gradients (d).

largely due to the need to actively control the electronic and structural properties of graphene [32–38]. Nevertheless few efforts have been made to explore the effect of straining graphene on directional transport of molecular mass. In this Letter, through theoretical modeling and molecular dynamics simulations, we show that a strain gradient in graphene can generate a net transport force on a molecular cargo on the graphene that is sufficient to drive the motion of the molecular cargo in a controlled direction. Given the high elastic deformability of graphene and the facile reversibility of applied straining, programmable transport of molecular mass on graphene can be achieved. The net transport force is essentially van der Waals (vdW) type, therefore such a transport mechanism can be applicable to transport a wide range of molecular cargos. Results from the present study can potentially offer a fundamental law of directional transport of molecular mass by straining.

2. Net transport force on molecular mass induced by a strain gradient in graphene

For an atom positioned above a pristine graphene, the total interaction force between the atom and the graphene can be determined by summing up all atomic-pair potentials between the atom and all carbon atoms in the graphene. Such a potential for an atomic pair of distance r due to vdW force is usually represented by a Lennard-Jones 6–12 potential, $V(r) = 4\epsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6}\right)$, where $\sqrt[6]{2}\sigma$ is the equilibrium distance between atoms and ϵ is the bond energy at the equilibrium distance. Due to the symmetry of graphene lattice, such a total interaction force zeros out when the atom is positioned with a separation distance from graphene of $h = \sqrt[6]{2}\sigma$. As a result, the atom reaches equilibrium and does not move in a preferred direction. By contrast, when the basal graphene is subject to a strain gradient, the graphene lattice symmetry is broken; there exists a net force acting on the atom, essentially due to the uneven distribution of the carbon atoms in the graphene, as to be detailed below.

Consider a rectangular basal graphene of length L, subject to uniaxial in-plane tension perpendicular to its length direction (Fig. 1(a)). The applied tension linearly decreases from $e_{\max}$ at one end to zero at the other end of the graphene. In other words, the graphene is subject to a strain gradient of $e_{\max}/L$. An atom is positioned above the graphene with a separation distance of h. In order to establish a semi-continuum cohesive law between the atom and the graphene, we homogenize carbon atoms in the graphene and represent them by an area density ρ_s. The cohesive energy Φ between the atom and the graphene is