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Editorial

Graphene Mechanics

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Graphene might be one of the most important materials in human history [1–4]. As a monatomic layer of carbon atoms in a honeycomb lattice, graphene possesses extraordinary mechanical properties, in addition to other amazing properties. The mechanical properties are of extreme importance for several potential applications, including tailoring other properties with strain engineering [5]. It is worth noting that the first fabrication of graphene is through mechanical exfoliation. As a fact, Mechanical exfoliation is still a popular approach for the scalable production of graphene [6].

In this Special Issue, we focus on the cutting-edge studies of graphene mechanics, from both theoretical and experimental investigations. In particular, this collection covers current areas of research that are concerned with the effect of the production method and/or the presence of defects upon the mechanical integrity of graphene, the work related to the effect of graphene deformation upon its electronic properties and the possibility of employing strained graphene in future electronic applications, and reviews of the experimental and theoretical results to date on mechanical loading of freely suspended or fully supported graphene.

The Special Issue on “Graphene Mechanics" is intended to provide a unique international forum aimed at covering a broad description of results involving mechanical properties, mechanical loading and engineering, and applications. This special issue is very successful and contains 21 articles. Worldwide researchers working in a wide range of disciplines have contributed to this special issue.

There are 21 papers in this special issue, with three review papers [7–9] and 18 original research papers [10–27], from experimental, computational, and theoretical investigations. Among them, there are seven experimental investigations. Here, we have a brief introduction of these 21 works in order of their publication date as follows.

As the first paper on this special issue, Chi et al. reported the influence of epitaxial crystallization on the mechanical properties of polyamide 66/reduced graphene oxide nanocomposite injection bar using differencital scanning calorimeter and other various techniques [10]. Their tensile test results showed that the presence of fewer epitaxial crystals can improve the mechanical properties of a polymer.

Using first-principles calculations, Yan et al. studied the strain effects on gallium nitride adsorption on defective and doped graphene [11]. Their calculations reveal that the vacancy defect core enhanced the adsorption stability of the adatom on graphene, whereas the incorporation of oxygen impurity greatly reduced the stable adsorption of the gallium and nitrogen adatoms. The lattice expansion led to increased stability for all adsorption sites and configuration surfaces, except for the nitrogen adatom adsorbed over the gallium atom in Ga-doped graphene.

By local-probe techniques including three-dimensional force field spectroscopy, Ashino and Wiesendanger investigated the out-of-plane elasticities of convexly curved graphene [12]. The substantially small intrinsic modulus that complies with continuum mechanics has been found to increase significantly at atomically specific locations, where sp^2 to sp^3 re-hybridization would certainly take place.

The research group led by Prof. Pengwan Chen reported a method to fabricate the Fe–FeO–graphene nanocomposite material by pulsed wire discharge in graphene oxide (GO) suspension [13]. The as-prepared samples were characterized by various techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and transmission electron microscopy (TEM). The formation mechanism during the pulsed wire discharge process was revealed.

A three-dimensional (3D) hierarchical graphene–hydroxyapatite hybrid bioscaffolds (GHBs) has been prepared by Xie et al. [14]. The GHBs is a calcium phosphate salt electrochemically deposited onto the framework of graphene foam (GF). The as-prepared GHBs show a high elasticity with recoverable compressive strain up to 0.8, and significantly enhanced strength with Young's modulus. The GHBs can more effectively promote the proliferation of MC3T3-E1 osteoblasts with better biocompatibility than pure GF and the control group.

Adak et al. [15]reported a study about thermally reduced graphene oxide (TRGO) as a reinforcing filler in the epoxy resin. They have investigated the effect on the mechanical properties of carbon fiber (CF)/epoxy composites. The epoxy matrix was modified by adding different weight percentages of TRGO. The prepared TRGO was characterized by using Fourier transform infrared spectroscopy, Raman spectroscopy and field emission scanning electron microscopy (FE-SEM) techniques. Their study suggested that TRGO could be used as an effective nanofiller to resist matrix and fiber fracture.

Using molecular dynamics simulations, the influence of vertical vibration on nanoscale friction was investigated by Cheng et al. [16]. They found that the average friction increases in a high-frequency range due to the vibration of the tip following vibration excitation, which results in peaks of repulsive interaction between tip and substrate and leads to higher friction.

Using MATLAB code, Crisafulli et al. analytically investigated the sliding dynamics between two parallel rigid graphene sheets, to understand how the interlayer force due to van der Waals interactions along the sliding direction changes with the geometrical characteristics of the configuration, namely size and interlayer spacing [17]. They found that metastable equilibrium positions with completely faced sheets, namely a null force along the sliding direction, whereas net negative/positive forces arise when the sheets are approaching/leaving each other. This behavior resembles a molecular spring, being able to convert kinetic into potential energy (van der Waals potential), and vice versa. The amplitude of both storable energy and entrance/exit forces is found to be proportional to the sheet size, and inversely proportional to their interlayer spacing.

Using molecular dynamics simulations, Wang et al. [18] have investigated the interaction between an edge dislocation and a pair of graphene nanosheets (GNSs) in GNS reinforced iron matrix composite (GNS/Fe). The GNS reinforcement can effectively hinder dislocation motion, which improves the yield strength. The interaction between the edge dislocation and the GNS pairs are nonisotropic. The remarkable enhancement (14 times) of the yield stress was revealed and attributed to the Orowan "by-passing" strengthening mechanism.

Using DFTB in addition to molecular dynamics simulations employed in KVAZAR, Slepchkov et al. [19] proposed a new structure of a graphene nanoblister. They found that such a 2D matrix of nanoscale cells in the form of a few-layer graphene substrate and nanoblister of a graphene monolayer is mechanically stable, and they are promising for environmentally friendly technologies. Particularly, they proposed that this graphene nanoblister can effectivly store molecular hydrogen under normal pressure.

Using molecular dynamics simulations, Li and Song studied the influence of hydroxyl groups on friction of graphene [20]. They found that the friction does not always go up with the rising of the hydroxyl groups ratio, and reaches the maximum when the hydroxyl groups ratio between interfaces is about 10%. The reason is that hydrogen bonds tend to form in interlayers when the hydroxyl groups ratio is high. The van der Waals forces are dominant in friction, which can be attributed to the influence of interface distance on friction.

Using home-made optically induced electrodeposition (OIED) experimental system, Zhang et al. [21] fabricated large-scale and mask-free graphene transistors. This is a convenient,

rapid, and large-scale assembly method for deposition of Ag electrodes. Transfer curves of different samples reveal similar trends of slightly p-type characteristics, which shows that this method is reliable and repeatable.

Using molecular dynamics simulations, Lei et al. [22] investigated the mechanical properties of defective graphyne. They found that the Young's modulus and the tensile strength of the four kinds of graphyne were remarkably high, though still lower than graphene. Their Young's moduli were insensitive to various types of point defects, in contrast to the tensile strength. When a crack slit was present, both the Young's modulus and tensile strength dropped significantly.

Using pulsed discharge in graphite micro-flake suspension at room temperature, Gao et al. [23] fabricated few-layer graphene nanosheets. The as-prepared samples were recovered and characterized by various techniques, such as TEM, SEM, Raman, XRD, XPS, FT-IR, etc. The presence of few-layer graphene (3–9 L) in micrometer scale was confirmed. The size of recovered graphene nanosheets are influenced by the initial size of utilized graphite micro-flake powder. The formation mechanism of few-layer graphene was discussed.

Using molecular dynamics simulations, Xie et al. [24] investigated the effects of stretching direction, temperature, and vacancy defects on the mechanical properties of PSI-graphene, a novel carbon allotrope with two-dimensional structure. The non-isotropic mechanical properties are discovered, with a peak value of the Young's modulus of 2082 GPa along 155.2°. The number of points removed from PSI-graphene sheet also seriously affected the tensile properties of the material. In addition, PSI-graphene does not have the negative Poisson's ratio during stretching along various angles.

Using theoretical derivation and soft simulation, the excellent transmission characteristics of graphene surface plasmon polaritons (SPPs) in mid-infrared band were analyzed and verified effectively by Wang et al. [25]. The graphene SPPs show unique properties in the mid-infrared region including ultra-compact mode confinement and dynamic tunability, which allow these SPPs to overcome the defects of metal SPPs and traditional silicon-based optoelectronic devices.

Using molecular dynamics simulations, He et al. [26] investigated the effect of the grain boundary on the nanofriction of graphene on a Au substrate. They found that grain boundaries could reduce the friction between graphene and the gold substrate with a small deformation of the latter. Large lateral forces were observed under severe deformation around the grain boundary. The fluctuation of lateral forces was bigger on surfaces with grain boundaries than that on single-crystal surfaces. Friction forces induced by the armchair grain boundaries was smaller than those by the zigzag grain boundaries.

Using molecular dynamics simulations, Wang et al. [27] studied the graphene adhesion mechanics on iron substrates. Two Fe–C potentials are examined as Lennard–Jones (LJ) pair potential and embedded-atom method (EAM) potential. The results suggest that the LJ potential describes a weak bond of Fe–C, opposed to a hybrid chemical and strong bond from the EAM potential. The average vertical distances between monolayer graphene nanosheets and four iron surfaces are 2.0–2.2 Å from the LJ potential and 1.3–1.4 Å from the EAM potential. These separations are nearly unchanged with an increasing number of layers. The ABA -stacked GN is likely to form on lower-index 110 and 100 surfaces, while the ABC-stacked GN is preferred on the higher-index 111 surface.

Besides these 18 original research contributions, there are three review papers. Mondal et al. [9] have reviewed the relevant optical properties and the applications areas with available results in various fields in a wavelength related regime that depends on strain modulus and position with field arrangements. Graphene shows a saturation and reverse saturation process due to the increase of light intensity. In addition, strong absorption is observed from the visible to mid-infrared (MIR) wavelength range. Moreover, the application areas of graphene including optics, photonics, plasmonics, mode-locked laser, optical modulator, etc., and the comparison of various results obtained from different sources are presented.

Cao et al. [8] presented a brief review of current development of graphene mechanics. The focus includes tension and compression, fracture, shearing, bending, friction, and dynamics properties

of graphene from both experiments and numerical simulations. The graphene derivatives are also reviewed, including graphane, graphone, graphyne, fluorographene, and graphene oxide, which carve some interesting mechanical properties out from graphene. This short review summarizes the current achievements of graphene mechanics, and then shows the future prospects.

Lan et al. [7] reviewed the method of characterization of graphene by Raman spectroscopy. This review summarizes basic aspects of Raman spectroscopy in crystallographic orientation of graphene nanosheets, determination principles, the determination methods, and the latest achievements in the related studies.

With the success of this Special Issue, we continue on the collection of the special topics in graphene mechanics. As a result, the Special Issue of "Graphene Mechanics (Volume II)" is on its way. It is currently open for submission through "https://www.mdpi.com/journal/crystals/special_issues/Graphene_II".

In addition to traditional nanomechanics of graphene, the mechanical properties of various graphene-like materials and structures are within the scope. The extended scope includes *g*-BN, *g*-BNC, graphane, graphone, grapphyne, *g*-GaN, *g*-TlN, *g*-ZnO, *g*-ZnS, *g*-GeC, *g*-MoS2, *g*-C_6O, *g*-Boron, *g*-InN, and their derivatives, as well as hybrid or heterostructures [28–60]. The research includes other properties related to mechanical properties, especially strain engineering. Both original research and reviews are welcome.

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