Shuze Zhu

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

Teng Li¹

Department of Mechanical Engineering, University of Maryland, College Park, MD 20742 e-mail: LiT@umd.edu

Wrinkling Instability of Graphene on Substrate-Supported Nanoparticles

Wrinkles in graphene with desirable morphology have practical significance for electronic applications. Here we carry out a systematic molecular dynamics study of the wrinkling instability of graphene on substrate-supported nanoparticles (NPs). At a large NP dispersion distance, a monolayer graphene adheres to the substrate and bulges out locally to wrap around individual NPs, forming isolated dome-shaped protrusions. At a small NP dispersion distance, tunneling wrinkles form in graphene to bridge the NPinduced protrusions. A critical NP dispersion distance for the onset of tunneling wrinkle instability of graphene is determined as a function of the NP size. The prediction from the modeling study agrees well with recent experimental observations. Results from the present study offer further insights into the formation of desirable wrinkles in graphene deposited on a substrate with engineered protrusions and, thus, can potentially enable novel design of graphene-based electronics. [DOI: 10.1115/1.4026638]

Keywords: graphene, wrinkling, substrate, nanoparticles, instability

1 Introduction

Graphene is a flexible, atomically thin membrane with remarkable electronic, mechanical, and chemical properties [1-3]. The two-dimensional nature of graphene renders its extra-large surface-to-volume ratio, giving rise to morphological varieties such as intrinsic ripples, extrinsic wrinkles and folds [4-11], and other folded carbon nanostructures [8,12-19]. In particular, the wrinkling formation in graphene has received considerable attention, largely due to its potential in manipulating the electronic properties of graphene [20-23]. For example, when graphene is bent to a certain curvature, a band gap is generated and that locally curved portion is semiconducting while the flat graphene is highly conductive [20-22]. Since the morphology of atomically thin graphene is strongly tied to its electronics properties [24], random wrinkling formation leads to unpredictable graphene properties, which are undesirable for nanoelectronic devices for which precise control is the key. Therefore, controlling the graphene morphology over large areas is crucial in enabling future graphene-based applications.

The extrinsic morphology of graphene on a substrate can be regulated [5,25-30]. When a layer of graphene is placed on patterned substrate surfaces, the graphene conforms to the substrate surface pattern [20,28–30]. In addition, the topological feature of the substrate surface can be regulated by introducing external scaffolds [5,25]. For example, the morphology of graphene intercalated by Si nanowires evenly patterned in parallel on a SiO₂ substrate is governed by the nanowire diameter and internanowire spacing [25]. While the graphene on patterned one-dimensional nanowires is rather regular by forming parallel grooves, the extrinsic graphene morphology regulated by zero-dimensional nanoparticles (NPs) has more complicated features [5,23]. For example, when a small Si NP intercalates in between a graphene bilayer, each layer wraps around the Si NP, forming a conical dome in graphene. As the size of the Si NP increases, both graphene layers wrinkle and form ridgelike morphology. When two neighboring Si NPs intercalate in between two graphene layers, depending on the NP size and spacing, the wrinkling pattern in

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graphene can evolve dynamically [5]. In a recent experiment [23], the wrinkling of graphene deposited on a SiO₂ substrate decorated with SiO₂ NPs is investigated. It is found that the NP dispersion density has a direct influence on the wrinkling pattern in graphene (Fig. 1(b)). For example, when the dispersion density is high enough, the percolation of wrinkles in graphene is observed; when the dispersion density is low, the graphene layer detaches from the substrate only in a small region around the NPs. Such a dependence of graphene wrinkling on NP dispersion is of practical importance as it suggests a feasible approach to programming the electronic signature of graphene through guided formation of wrinkles. Promises aside, the study on graphene morphology regulated by NPs on a substrate is far from mature, with rather empirical understanding from limited experiments. For example, it is expected that such regulated morphology of graphene depends not only on the NP dispersion density but also on the NP size. However, a quantitative understanding is still lacking.

Aiming to address such a knowledge gap, in this paper, we conduct systematic molecular dynamics (MD) simulations to investigate the characteristics of graphene morphology regulated by NPs on a substrate and their quantitative dependence on key underlying parameters. We find that the wrinkling formation in graphene depends strongly on the NP size and the distance between two neighboring NPs, in agreement with the experimental observation [23]. In particular, we identify a critical NP dispersion distance, above which the intercalated local morphology of graphene remains at the proximity of each individual NP, while below which long ridges form to bridge two neighboring NPs. As sharp features in graphene morphology (e.g., long ridges and sharp extrusions) can lead to significant change of the local electronic properties, the research finding from the present study could potentially help guide the design of novel graphene-based electronic devices.

2 Experimental Observation of Graphene Morphology on Substrate-Supported Nanoparticles

Figure 1(a) presents a schematic of graphene covering a substrate with dispersed NPs. This can be experimentally achieved by means of spin coating the NPs onto a substrate [23]. A graphene monolayer is then mechanically exfoliated from graphite onto the substrate decorated with NPs. Figure 1(b) shows a typical atomic

¹Corresponding author.

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Fig. 1 (a) Schematics of graphene covering a substrate with dispersed NPs (not to scale). (b) Atomic force microscopy image of the wrinkled morphology of a monolayer graphene covering a SiO₂ substrate with dispersed SiO₂ NPs. Three representative types of wrinkling morphology (highlighted by red circles) can be observed: (1) wrinkling of graphene on isolated NP; (2) wrinkling of graphene bridging two neighboring NPs; (3) wrinkling of graphene on quasi-isolated NPs. The atomic force microscopy image is reprinted from Ref. 23, under the terms of the Creative Commons Attribution 3.0 License.

force microscopy image of a monolayer graphene covering a SiO₂ NP-dispersed substrate surface. Depending on the NP dispersion distance, three representative types of wrinkling morphology of graphene can be identified. On an isolated NP (sufficiently large distance from other NPs, e.g., labeled area (1) in Fig. 1(b)), the graphene bulges locally to wrap around the NP to form a domeshaped extrusion. On an NP of relatively large size, two wrinkles originate from the bulged graphene dome near the NP protrusion location in opposite directions and gradually terminate after a certain distance, beyond which graphene completely adheres to the substrate surface. For convenience, hereinafter, such a wrinkle that originates from a graphene protrusion and terminates over a distance is termed as a tipped wrinkle. When two NPs are relatively close to each other (e.g., labeled area (2) in Fig. 1(b)), the graphene wrinkles to bridge the two protrusions induced by NP intercalation. Such a wrinkling morphology is hereinafter termed as a tunneling wrinkle. A more delicate third scenario exists when two NPs are separated by a distance that is neither far enough to form two isolated sets of tipped wrinkles near the NPs nor close enough to form a tunneling wrinkle in between the two NPs. Instead, two wrinkles run in parallel between the two NPs and terminate near the middle with a short overlap near their tips. The above experimental observation suggests that a critical distance between two neighboring NPs may exist, below which a tunneling wrinkle forms. Since a regular tunneling wrinkle has the most desirable geometrical features for engineering the electronic properties of graphene [20-22], the dependence of such a critical distance to form tunneling wrinkles on the NP size is intriguing. Motivated by the above observations, we perform systematic MD simulations to shed quantitative insights on these intriguing but less understood phenomena.

3 A Semicontinuum Formulation of Graphene/Substrate Cohesive Law

The origin of the wrinkling is due to the strong adhesion of graphene to its underlying substrate. Such interaction is mainly van der Waals (vdW) type. In order to simulate the graphene/substrate adhesion energy in the experiments with a rationally reduced MD model to ease computational expenses, below we perform theoretical analysis on the relationship between the continuum-scale adhesion energy and the atomic-pair interaction energy. The energy between two atoms of distance r due to vdW force is usually represented by a Lennard–Jones 6–12 potential

$$V(r) = 4\epsilon \left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6}\right) \tag{1}$$

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Fig. 2 A schematic of a flat graphene monolayer on a substrate with a separation distance of h

where $\sqrt[6]{2\sigma}$ is the equilibrium distance between atoms and ϵ is the bond energy at the equilibrium distance. In order to establish a semicontinuum cohesive law between a graphene monolayer and a substrate with a separation distance of h (Fig. 2), we homogenize carbon atoms in the graphene and represent them by an area density ρ_g [31]. We discretize the substrate into multiple atomic layers along its thickness direction but treat each layer as a continuum in its plane so that we can homogenize the substrate atoms in each layer. Taking the substrate surface layer as an example (shaded part in Fig. 2), we represent the atoms in this layer by an area density ρ_s . The distance between a point (0,0) in the graphene and a point (x, y) in the substrate surface layer is $r = \sqrt{x^2 + y^2 + h^2}$. The energy due to the vdW force is given by V(r). For an infinitesimal graphene area dA_g , the energy stored due to the vdW force is

$$\rho_g dA_g \int V(r)\rho_s dA_s = \rho_g \rho_s dA_g \int V(r)dxdy,$$
(2)

The cohesive energy Φ induced by the substrate surface layer is the energy per unit area of graphene and is, therefore, given by

$$\Phi = \rho_g \rho_s \int V(r) dx dy$$

= $\rho_g \rho_s \int 4\epsilon \left(\frac{\sigma^{12}}{(x^2 + y^2 + h^2)^6} - \frac{\sigma^6}{(x^2 + y^2 + h^2)^3} \right) dx dy$
= $4\epsilon \rho_g \rho_s \pi \left(\frac{\sigma^{12}}{5h^{10}} - \frac{\sigma^6}{2h^4} \right)$ (3)

Finally, the total graphene-substrate adhesion energy can be computed by summing up individual cohesive energy induced by all the atomic layers in the substrate. This way, the continuum-scale graphene-substrate adhesion energy is correlated with their atomicpair vdW interaction energy. Furthermore, considering the decaying nature of vdW interaction, a reasonable estimate of adhesion energy can be achieved by adding up the contribution from the first few top atomic layers in the substrate, while the energy contribution from substrate layers underneath is rather negligible. In this sense, the above semicontinuum approach can be readily employed in practice. This approach is used in Sec. 4 to benchmark the parameters in MD simulations to guarantee reasonable agreement with experimental measurement of graphene-substrate adhesion.

4 Wrinkling Morphology of Graphene on Substrate-Supported Nanoparticles

Figure 3(a) depicts the MD simulations model. To reduce computational cost of systematic parametric study using MD, the substrate is represented by two fixed layers of graphene. This strategy

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Fig. 3 (a) MD simulation model. Inset shows the cross-sectional view of the initial configuration. Periodical boundary condition (PBC) is applied in y direction, so that the length of the simulation box along the PBC direction represents the NP dispersion distance S. (b) The typical equilibrium morphology of graphene on a small and isolated NP on the substrate. (c)–(e) Variation of wrinkling morphology of graphene on an isolated NP with increasing size.

is justified considering the decaying nature of the vdW force between graphene and a stiff substrate and further shown below to be reasonable to represent the key underlying interaction between the graphene and the substrate. The monolayer graphene is initially prescribed with a smooth bulged-out geometry to cover the NP that intercalates in between the graphene and the underlying stiff substrate. Periodical boundary condition (PBC) is applied in the y direction. Given the nature of periodical boundary condition, the model in Fig. 3(a) simulates an array of NPs of diameter d_{NP} with a uniform dispersion distance S, intercalating in between the graphene and the substrate.

The simulations are carried out using large-scale atomic/molecular massively parallel simulator (LAMMPS) [32]. All the simulations are carried out in canonical ensemble (NVT) at 300 K. The carbon-carbon interaction in the graphene layer is described by the adaptive intermolecular reactive empirical bond order (AIR-EBO) potential [33]. The NP is modeled as a rigid body and takes the face centered cubic crystal structure. The vdW interaction between each NP atom and each carbon atom in the monolayer graphene or the substrate is modeled by a Lennard–Jones potential $V_{CN}(r) = 4\varepsilon_{CN} (\sigma_{CN}^{12}/r^{12} - \sigma_{CN}^6/r^6)$, where $\varepsilon_{CN} = 0.0127 \text{ eV}$, $\sigma_{CN} = 0.29 \text{ nm}$. The interaction between each carbon atom in the substrate is also modeled by a Lennard–Jones potential $V_{CC}(r) = 4\varepsilon_{CC} (\sigma_{CC}^{12}/r^{12} - \sigma_{CC}^6/r^6)$, where $\varepsilon_{CC} = 0.00852 \text{ eV}$, $\sigma_{CC} = 0.29 \text{ nm}$. Using Eq. (3), the above parameters yield an adhesion energy of the monolayer graphene to the substrate as

$$\Phi_{total} = \Phi_{s1} + \Phi_{s2}$$

$$= 4\varepsilon_{CC}\rho_c^2 \pi \left(\frac{\sigma_{CC}^{12}}{5h_{s1}^{10}} - \frac{\sigma_{CC}^6}{2h_{s1}^4}\right) + 4\varepsilon_{CC}\rho_c^2 \pi \left(\frac{\sigma_{CC}^{12}}{5h_{s2}^{10}} - \frac{\sigma_{CC}^6}{2h_{s2}^4}\right) \quad (4)$$

where the subscripts *s*1 and *s*2 denote the first and second substrate carbon atomic layer in the MD model, respectively, so that $h_{s1} = 0.34$ nm, $h_{s2} = 0.68$ nm, and $\rho_c = 4/3\sqrt{3}l_0^2$, in which l_0 is the equilibrium bond length of graphene and takes the value of 0.142 nm. The corresponding adhesion energy $|\Phi_{total}| \approx 0.5 \text{J/m}^2$ is in good agreement with the recent experimental measurement of monolayer graphene adhesion energy on a SiO₂ substrate (~ 0.45J/m²) [34], which justifies the modeling strategy and the choice of parameters in our MD simulations. To clarify the substrate thickness effect on the adhesion energy, we further calculate the adhesion energy for the situations in which there are two (used in the present paper), three, and four fixed graphene layers in the substrate, with the interlayer spacing of 0.34 nm. The corresponding adhesion energies calculated from the semicontinuum model are 0.5054 J/m^2 , 0.5123 J/m^2 , and 0.5145 J/m^2 for a substrate with two, three, and four fixed graphene layers, respectively. In other words, the adhesion energy calculated from our continuum model by using a substrate of two graphene layers agrees well with those by using a thicker substrate within less than 2%, which further justifies the modeling strategy adopted here.

Figure 3(b) shows a typical equilibrium morphology of graphene when it covers a relatively small NP and the NP dispersion distance S is large (e.g., $d_{NP} = 2 \text{ nm}$, S = 25 nm) so that this NP is isolated. Due to the intercalation by the NP and the strong adhesion of the monolayer graphene to the substrate, a small region of graphene around the NP delaminates from the substrate and locally forms a domelike morphology. Figures 3(c)-3(e) show the variation of graphene morphology as the NP size increases. When $d_{NP} = 3 \text{ nm}$ (Fig. 3(*d*), S = 36 nm), the onset of tipped wrinkles occurs. When $d_{NP} = 4 \text{ nm}$ (Fig. 3(e), S = 60 nm), two long tipped wrinkles extend from the NP-intercalated graphene dome in opposite directions, resembling the experimental observation in Fig. 1(b) (circled area 1). The formation of tipped wrinkles can be understood as follows. As the size of the NP increases, forming a smooth conical dome in the graphene monolayer to wrap around the NP requires deflecting and stretching the graphene in a larger area. The resulting increase in the graphene strain energy and the graphene-substrate interaction energy becomes higher than that due to forming tipped wrinkles. In the wrinkling graphene morphology, even though the curvature of the graphene corrugation along the wrinkles is higher than that of a smooth conical dome, it only requires corrugating a smaller area of the graphene and the graphene portions away from the wrinkles are much less corrugated and have an interlayer distance closer to its equilibrium value. As a result, the formation of tipped wrinkles corresponds to a lower total free energy state and, thus, is more favorable.

We next consider the morphological evolution of the graphene intercalated by NPs on substrate as the NP dispersion distance varies. Similar materials parameters and numerical strategy as those described above are used in the MD simulations. For a given NP size, MD simulations are conducted over a range of NP dispersion distance. Two modes of morphologic evolution emerge from the simulations, as illustrated in Fig. 4. If the NP dispersion distance *S* is sufficiently large (e.g., S = 25 nm for $d_{NP} = 2$ nm), the graphene is intercalated to form two isolated conical domes (Fig. 4(*a*), similar to the results shown in Figs. 3(*b*) and 3(*c*)). If the NP

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Fig. 4 Wrinkling morphology of graphene on NPs with relatively small dispersion distance. For visual guidance, two periodical images are combined along the PBC direction. For $d_{NP} = 2$ nm, (a) the two NP-intercalated graphene domes remain isolated when dispersion distance S = 25 nm. (b) A tunneling wrinkle forms between two NPs when S = 21 nm. For $d_{NP} = 6$ nm, (c) two long tipped wrinkles run in parallel between neighboring NPs and terminate in the middle with a short overlap but their tips remain distinct from each other (inset) when S = 110 nm. (d) When S = 100 nm, a tunneling wrinkle forms between two neighboring NPs.



Fig. 5 A diagram of the wrinkling instability of graphene morphology on substrate-supported NPs in the space of NP dispersion distance and diameter

dispersion distance S is small enough (e.g., S = 21 nm for $d_{NP} = 2 \text{ nm}$), the graphene in between two neighboring NPs is intercalated to form a tunneling wrinkle (Fig. 4(b)). For NPs with larger sizes, similar transition of graphene wrinkling morphology could be observed with more delicate features. As shown in Fig. 4(c), when the dispersion distance S is 110 nm for $d_{NP} = 6 \text{ nm}$, the resulting equilibrium morphology of graphene resembles the typical experimental observation in Fig. 1(b)(circled area 3). From each protrusions, there are two long tipped wrinkles reaching out and orienting toward its nearby protrusions. Although the tip ends have a slight overlap, no signs of further merging into a tunneling wrinkle are observed. This can be interpreted as a critical intermediate transitional state between formations of tunneling wrinkles and tipped wrinkles. Further increase in the NP dispersion distance S results in completely isolated tipped wrinkles, and the morphology of graphene around each protrusion resembles those shown in experiments (e.g., Fig. 1(b), circled area 1). However, further decrease in the NP dispersion distance S leads to the formation of tunneling wrinkles. As shown in Fig. 4(d), when S = 100 nm and $d_{NP} = 6 \text{ nm}$, a long tunneling wrinkle bridges the two graphene protrusions induced by NP

intercalation, resembling the experimental observation in Fig. 1(b) (circled area 2).

5 A Critical Nanoparticle Dispersion Distance for Tunneling Wrinkle Instability of Graphene on Substrate-Supported Nanoparticles

Also emerging from extensive MD simulation study is a critical dispersion distance of NPs Scr for a given NP size, below which tunneling wrinkles form to bridge neighboring NPs and above which isolated tipped wrinkles form, extending from the NPintercalated graphene dome. Figure 5 plots S_{cr} as a function of d_{NP} . Such a curve delineates a boundary that separates the space of NP dispersion distance and NP diameter into two regions of wrinkling morphology of graphene as labeled in Fig. 5. The S_{cr} - d_{NP} curve can be fitted into a second-order polynomial as shown in Fig. 5, with an R-squared value of fitting 0.9997. Results in Fig. 5 can well account for the experimental observation in Ref. 23, in which the mean diameter of NPs is 7.4 ± 2.2 nm. By using the fitted polynomial function, the critical NP dispersion distance is estimated to be around 200 nm, which agrees well with the experimental results (e.g., Fig. 1(b)). In this sense, the diagram depicted in Fig. 5 can, therefore, be used to guide the programmable design of wrinkling formation in graphene on substratesupported NPs.

6 Concluding Remarks

In summary, we conduct extensive MD simulations to investigate the wrinkling morphologic evolution of graphene on substrate-supported NPs from which a critical dispersion distance of the NPs can be determined below which desirable tunneling wrinkles form in graphene. A second-order polynomial dependence of such a critical NP dispersion distance on NP size is revealed, which agrees well with experimental observation. Such a second-order polynomial dependence is of practical importance in the sense that it can be applied to substrates with different adhesion interaction with monolayer graphene. All three coefficients in the second-order polynomial function can be readily parameterized from simple experimental tests. The resulting fitting function can then be used to guide the selection of NP size and dispersion

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density to achieve desirable wrinkling morphology of graphene. Results from the present study offer further insights into the formation of wrinkles in graphene deposited on a substrate surface with engineered protrusions [35–38] and can, thus, potentially enable novel design of graphene-based electronics. For example, by introducing NPs or substrate substructures in an ordered pattern on the substrate surface, even richer features of the wrinkling instability of the covering graphene could be realized. More comprehensive modeling studies are needed to reveal such new features, which will be reported elsewhere. We, therefore, call for further systematic experiments to explore those fertile opportunities.

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