Molecular dynamics simulation of the self-retracting motion of a graphene flake

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The self-retracting motion of a graphene flake on a stack of graphene flakes is studied using molecular dynamics simulations. It is shown that in the case when the extended flake is initially rotated to an incommensurate state, there is no barrier to the self-retracting motion of the flake and the flake retracts as fast as possible. If the extended flake is initially commensurate with the other flakes, the self-retracting motion is hindered by potential energy barriers. However, in this case, rotation of the flake to incommensurate states is often observed. Such a rotation is found to be induced by the torque acting on the flake on hills of the potential relief of interaction energy between the flakes. Contrary to carbon nanotubes, telescopic oscillations of the graphene flake are suppressed because of high dynamic friction related to the excitation of flexural vibrations of the flake. This makes graphene promising for the use in fast-responding electromechanical memory cells.

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I. INTRODUCTION

Because of the extraordinary electrical and mechanical properties of graphene,1 this novel two-dimensional nanostructure is considered promising for use in nanoelectromechanical systems (NEMS). For example, a nanoresonator based on flexural vibrations of suspended graphene has been implemented.2 The experimentally observed self-retracting motion of graphite (i.e., retraction of graphite flakes back into graphite stacks on their extension, arising from the van der Waals interaction between graphene layers) led to the idea of an oscillator based on the telescopic oscillation of graphene layers.3 Nanorelays based on the telescopic extension and self-retracting motion of carbon nanotube walls were realized experimentally.4,5 By analogy with these nanotube-based devices, a nanorelay based on the telescopic motion of graphene layers was proposed.6,7

The gigahertz oscillator based on the telescopic oscillation of carbon nanotubes walls8,9 has been widely considered a model system in studies of fundamental aspects of tribological properties and dynamic behavior of nanoscale systems (see, e.g., Refs. 10–26). However, there are significant differences in the potential reliefs of the interlayer interaction energy for graphene layers and carbon nanotube walls. The magnitude of the energy cost,29,30 it was shown to play a significant role in the static friction34–36 and thermally activated diffusion25,30 of graphene flakes on graphene layers. Here, we show that this phenomenon also has implications for the telescopic motion of graphene flakes.

Therefore, investigation of the self-retracting motion of graphene flakes is of interest both for elaboration of graphene-based NEMS and for study of basic tribological properties of matter at the nanometer scale. In the present paper, we examine the self-retracting motion of graphene flakes by molecular dynamics (MD) simulations. The analysis of simulation results shows that the differences in the potential energy reliefs for the graphene layers and nanotube walls listed above lead to essentially different dynamic behavior of these systems. First, telescopic oscillations are suppressed for graphene flakes because of the excitation of flexural vibrations of the flakes. Second, the self-retracting translational motion of the extended flake is often accompanied by the rotation of the flake. The influence of temperature, the direction of telescopic extension, and the initial orientation and position of the extended flake on the possibility and characteristics of the self-retracting motion of the flake are investigated.

The paper is organized in the following way. In Sec. II, we analyze the potential energy relief corresponding to the telescopic motion of one graphene flake on another. In Sec. III, we describe the model considered for the MD simulations and discuss the results of the MD simulations. Our conclusions are summarized in Sec. IV.

II. ANALYSIS OF POTENTIAL ENERGY RELIEF

Because the relative motion of graphene flakes is determined by the potential relief of their interaction energy, we first analyze the potential energy relief corresponding to the telescopic extension of one graphene flake on another. We have calculated the potential energy relief for graphene flakes of 34 Å × 34 Å size at the equilibrium distance between the flakes of 3.4 Å. The van der Waals interaction between...
atoms of the flakes is described using the potential developed recently on the basis of calculations in the framework of the dispersion-corrected density functional theory.\footnote{6,7} This potential was shown to describe adequately the properties of graphite and the small relative vibrations of graphene layers.\footnote{6,7} The cutoff distance of the van der Waals potential is taken equal to 25 Å. The covalent carbon-carbon interactions in the flakes are described by the Brenner potential.\footnote{40} To calculate the binding energy of the graphene flake on the periodic graphene layer,\footnote{29,30,34–36} the interaction energy between the graphene flake and the graphene layer can be considered a sum of two components: a constant negative binding energy $-\varepsilon_0 = -46.9$ meV/atom (for the potential\footnote{6,7} used in the present paper) and a positive corrugation describing the dependence of the interaction energy on the stacking of the flake and the layer and equal to zero at minima of the potential energy relief. Maxima and minima of the potential energy relief of the flake commensurate with the underlying graphene layer correspond to the AA and AB stackings [see Fig. 1(c)], respectively. The energy difference between these states is found to be $\varepsilon_{\text{max}} = 19.4$ meV/atom. The barriers for transitions of the graphene flake between adjacent energy minima correspond to the saddle point (SP) stacking [see Fig. 1(c)]. The magnitude of these barriers is $\varepsilon_{\text{com}} = 2.1$ meV/atom. With the relative rotation of the flake, the magnitude of corrugation of the potential energy relief decreases and becomes negligibly small at rotation angles exceeding $\delta \varphi \approx a_0/L$, where $a_0 = 2.46$ Å is the lattice constant of graphene and $L$ is the size of the flake. The energy required for the relative rotation of the graphene flake to the incommensurate states is $\varepsilon_{\text{in}} = 6.4$ meV/atom. The total binding energy of the graphene flake on the periodic graphene layer and the magnitude of corrugation of the potential energy relief are proportional to the overlap area between the flake and the layer and are constant at any displacement of the flake relative to the layer.

We now discuss potential energy relief calculated for the telescopically extended graphene flakes (see Fig. 2). Analogous to the graphene flake on the periodic graphene layer,\footnote{29,30,34–36} the interaction energy between the graphene flakes can roughly be considered a sum of the binding energy and the corrugation describing the dependence of the interaction energy on the stacking of the flakes. However, different from the case of the graphene flake on the periodic graphene layer, the overlap area between the flakes changes with the relative displacement of the extended flake, providing the dependence of the binding energy and the magnitude of corrugation on the relative position of the flakes [see Fig. 2(a)]. The dependence of the binding energy on the overlap area of the flakes is the cause of the self-retracting motion of the extended flake. To analyze the dependence of the barrier to the relative motion of the flakes on their relative position, we introduce the barrier $E_{\text{bar}}$ to the self-retracting motion of the commensurate flake. The barrier $E_{\text{bar}}$ is defined as the energy

![Image](https://via.placeholder.com/150)

**FIG. 1.** (Color online) (a) Commensurate ($\varphi = 0^\circ$) and (b) incommensurate ($\varphi = 15^\circ$) states of graphene flakes. (c) Stackings of commensurate graphene layers. (d) Schematic representation of the rotation of the extended graphene flake around its center of mass induced by corrugation of the potential energy relief.

![Image](https://via.placeholder.com/150)

**FIG. 2.** (Color online) Calculated interaction energy (eV) of graphene flakes $34 \times 34$ Å (446 atoms) at an equilibrium interlayer spacing of 3.4 Å as a function of the relative position $x$, $y$ (Å; axes $x$ and $y$ are chosen along the armchair and zigzag directions, respectively) of the center of mass of the extended flake and the rotation angle $\varphi$ (in degrees) of the flake around its center of mass: (a) $\varphi = 0^\circ$, (b) $\varphi = 30^\circ$, (c) $y = 0$, and (d) $x = 0$. Equipotential lines are drawn with a step of (a, b) 0.6 eV and (c, d) 0.2 eV. Energy is given relative to the global energy minimum. (c, d) Dashed lines correspond to the critical rotation angle $\delta \varphi = a_0/L$, above which the extended flake is assumed to be incommensurate. Arrows demonstrate energy favorable rotation of the extended flake.
FIG. 3. Schematic representation of scattering on the hills of potential energy relief for a graphene flake extended along the (a) armchair and (b) zigzag directions. Energy minima are denoted AB, AB1, and AB2. Energy hills are denoted AA. Saddle points are denoted SP, SP1, and SP2. The direction of flake motion is indicated by the arrows.

difference between the local energy minimum around which the flake is placed initially and the nearest saddle point opposite the direction of extension. This barrier can be estimated as

\[ E_{\text{bar}} = \frac{1}{\sigma} \left( \varepsilon_{\text{com}} L - \varepsilon_0 \frac{a_0}{2\sqrt{3}} L \cos \alpha \right) \],

(1)

where \( l \) is the overlap length of the flakes in the direction of extension, \( \alpha \) is the angle between the direction from the energy minimum to the saddle point and the direction opposite to the direction of extension, and \( \sigma \) is the area per atom in graphene. The first term in this formula is related to an increase of the magnitude of corrugation of the potential energy relief with an increase of the overlap area of the flakes and is independent of the direction of extension. The second term in Eq. (1) is related to an increase of the binding energy of the flakes in magnitude with the retraction of the extended flake. This term does not depend on the overlap length of the flakes but depends on the direction of extension. For the case of extension along the zigzag direction, the angle \( \alpha = 30^\circ \) for any energy minima around which the flake is placed initially. For the flake extended along the armchair direction, the energy minima are not equivalent. The angle \( \alpha \) takes the values \( 60^\circ \) and \( 0^\circ \) for displacements from the energy minima denoted by AB1 and AB2 in Fig. 3(a) to the saddle points denoted by SP1 and SP2, respectively. As follows from Eq. (1), the dependences of the barrier \( E_{\text{bar}} \) to the self-retracting motion of the flake on the overlap length \( l \) are shifted relative to each other for different directions of extension. With increasing the overlap length of the flakes \( l \gg a_0 \), the barrier to the self-retracting motion of the flake tends to \( E_{\text{bar}} = \varepsilon_{\text{com}} l / \sigma = 0.8 \text{ meV}/\AA^2 \cdot L \), which is the barrier to the relative motion of the graphene flake of size \( l \times L \) on the periodic graphene layer.

By calculations of the energy difference between the SP and AB stackings, we have confirmed that the barrier \( E_{\text{bar}}/L \) to the self-retracting motion of the flake per unit width of the flake perpendicular to the direction of extension depends linearly on the overlap length \( l \) of the flakes with the same coefficient \( 0.8 \text{ meV}/\AA^2 \) for the armchair and zigzag directions (see Fig. 4). However, as the dependences are shifted, the barriers are different for the cases of extension along the armchair and zigzag directions. There is no barrier to the self-retracting motion of the flake extended along the zigzag direction at overlap lengths less than 10 Å. For the flake extended along the armchair direction there is also no barrier to the self-retracting motion of the flake at overlap lengths less than 15 Å for the energy minima denoted by AB2 in Fig. 3(a), whereas for the energy minima denoted by AB1, this barrier is nonzero for any overlap length. For example, the barrier for an AB1 energy minimum is about 0.08 eV at the extension of the considered flake by 30 Å along the armchair direction. Such a barrier can hinder the start of the self-retracting motion of the flake even at room temperature.

In the present paper, we perform MD simulations of the self-retracting motion of the extended flake for initial overlap lengths less than 10 Å. For these overlap lengths, the start of the self-retracting motion of the flake is energetically favorable for any initial position of the flake extended along the zigzag direction, whereas for the flake extended along the armchair direction, there are states around the AB1 energy minima for which the start of the self-retracting motion is possible only in the result of thermodynamic fluctuations. Therefore, the dynamic behavior of the extended flake at these initial overlap lengths is expected to be different for the armchair and zigzag directions of extension.

Upon the relative rotation of the graphene flakes [see Fig. 1(b)], the potential energy relief of the flakes becomes smooth [see Fig. 2(b)]. This should facilitate the retraction of the extended flake initially rotated to an incommensurate state, which is confirmed for flakes of micrometer size by the experiment\(^3\) and for flakes of nanometer size by our MD simulations (see Sec. III). Moreover, our simulations (see Sec. III) reveal that the rotation of the extended flake from the commensurate to incommensurate states often takes place during the self-retracting motion of the flake. To analyze the reasons of this rotation, we consider the interaction energy of the flakes as a function of the rotation angle of the extended flake [see Figs. 2(c) and 2(d)]. It is seen from Figs. 2(c)
and (2d) that on the hills of the potential energy relief, the extended flake experiences a torque which induces rotation of the flake (as indicated by the arrows). The extended flake can be placed initially on a potential energy hill, or the flake can start the self-retracting motion and acquire the kinetic energy sufficient for climbing the potential energy hills on the way of retraction of the flake.

As opposed to the case of a graphene flake on a periodic graphene layer, 29,30 the telescopically extended flake experiences a nonzero torque, even at the zero rotation angle. The origin of this additional torque, which leads to the start of the rotation of the extended flake with the initial commensurate orientation, can be explained as follows. The force of the interaction between the flakes is applied only to the atoms of the extended flake located in the overlap area of the flakes [see Fig. 1(d)]. Therefore, the force acting on the flake on slopes of the potential energy hills perpendicular to the direction of extension exerts the torque inducing the rotation of the flake around its center of mass.

Note that the described mechanism of rotation of the extended flake to the incommensurate states can take place only for the flake that is able to start the self-retracting motion. The rotation of the commensurate flake locked near a local energy minimum is possible only because of thermodynamic fluctuations, similar to the thermally activated diffusion of the graphene flake on the periodic graphene layer.29,30 The thermally activated rotation takes a long time and is of minor importance for the operation of graphene-based NEMS in which the fast retraction of the extended flake is desirable.

The patterns of equipotential lines in Figs. 2(c) and 2(d) demonstrate that the rotation of the flake to the incommensurate states by the angle $\delta \phi$ is energetically favorable for the flake extended along the armchair direction, whereas for the flake extended along the zigzag direction, the rotation by angles smaller than $\delta \phi$ is expected. Thus, the probability for the extended flake to rotate to the incommensurate states should depend on the direction of extension. This can be explained as follows. For the flake extended along the armchair direction, the potential energy hills lie directly on the direction of retraction of the flake [see Fig. 3(a)]. In this case, the chances for the flake to be on potential energy hill slopes where torque is sufficient for rotation to the incommensurate states are high. For the flake extended along the zigzag direction, the potential energy hills lie beside the direction of retraction [see Fig. 3(a)], and the probability for the flake to experience torque sufficient for rotation to the incommensurate state should be lower than in the case of extension along the armchair direction.

On the basis of the above analysis of the potential energy relief, the following features of the self-retracting motion of the flake can be predicted. First, because of significant variation in the interaction energy of the commensurate flakes at the scale of the lattice constant of graphene, the behavior of the extended flake with the initial commensurate orientation should be highly sensitive to the initial position of the flake on the subatomic scale. Second, the rotation of the flake to incommensurate states should facilitate retraction of the flake. Third, different flake behavior is expected for cases in which the flake is extended along the armchair and zigzag directions because of differences in barriers to the self-retraction motion and probabilities of rotation to the incommensurate states. To check these predictions, we have performed MD simulations of the self-retracting motion of a graphene flake.

III. MOLECULAR DYNAMICS SIMULATIONS

The MD simulations of the self-retracting motion of a graphene flake are performed for a system of three graphene flakes of $34 \, \text{Å} \times 34 \, \text{Å}$ at the equilibrium distance of $3.4 \, \text{Å}$ from each other (see Figs. 1 and 5). The Molecular Dynamics–kinetic Monte Carlo (MD-kMC) 41 Kintech Lab Ltd. version 2.0, Moscow, Russia) code is used. The integration time step is 0.6 fs. The temperature of the middle flake is maintained by rescaling atomic velocities every 0.1 ps (the Berendsen thermostat42). All atoms of the bottom flake are fixed. At the beginning of simulations, the upper flake is extended telescopically by about $30 \, \text{Å}$. The extended flakes at different initial positions within the unit cell of graphene are considered, with initial orientations corresponding to the commensurate ($\varphi = 0^\circ$) and incommensurate states ($\varphi = 30^\circ$), displaced along the armchair and zigzag directions and at temperatures 4 and 300 K.

The simulations show that the self-retracting motion of the extended flake with the initial commensurate orientation proceeds in diverse ways, even for nearly the same initial conditions (different only in the initial distribution of thermal velocities of the atoms, in the initial position of the extended flake within the unit cell of graphene, or both; see Fig. 6 and supplemental movies43). In most cases, retraction of the extended flake occurs. The self-retracting motion of the flake

![Figure 5](image_url)

FIG. 5. (Color online) Schematic representation of the telescopic motion of a graphene flake (the system under consideration).

![Figure 6](image_url)

FIG. 6. (Color online) Different calculated dependences of displacement $x (\text{Å})$ of the flake with initial commensurate orientation extended in the armchair direction on time $t$ (ps) at temperature 300 K. The coordinate $x = 0$ corresponds to the ground state position of the flake before extension.
can be fast (at times $\sim 10$ ps) or slow (at times $\sim 50$ ps). Sometimes, the flake performs one or two damped oscillations; rarely, flake retraction is time lagged. In some cases, no retraction at all is observed at simulation times of hundreds of picoseconds. This diversity of the dynamic behavior of the graphene flake is provided by thermodynamic fluctuations, similar to NEMS based on carbon nanotubes, as well as by the properties of the potential energy relief of the flake discussed in the previous section.

As expected from the potential energy relief (see Sec. II), the behavior of the flake initially in the commensurate state is found to be strongly sensitive to the initial position of the flake at the scale of the lattice constant of graphene. For example, the initial positions of the commensurate flake extended by $30$, $31$, and $32$ Å in the armchair direction correspond to the positions near an AB2 energy minimum [see Fig. 3(a)] and slopes of a potential energy hill with attractive and repulsive forces, respectively. For each of these initial positions, we have performed $10$ simulations of $50$ ps duration at temperature $4$ K. The complete retraction of the flake is observed in zero, nine, and two simulations, respectively. However, experimentally, it can be difficult to control the initial position of the flake with such high accuracy. Therefore, the results of calculations for a particular initial extension of the flake in the commensurate state are averaged over the unit cell of graphene.

To characterize the diversity of the dynamic behavior of the flake, we determine the fractions $\chi$ and $\zeta$ of simulations in which the rotation of the flake to incommensurate states and several oscillations of the flake are observed, respectively, for different temperatures $T$ (K), initial rotation angles $\varphi$ (degrees) of the extended flake, and directions of the initial extension of the flake. The results are obtained on the basis of $25$–$35$ simulations of $50$ ps duration, with the initial position of the flake within a unit cell of graphene at a distance of about $30$ Å from the global energy minimum. The axes $x$ and $y$ are chosen along the armchair and zigzag directions, respectively.

In several simulations at $300$ K with the initial extension of the flake along the armchair direction, a time lag of $5$–$30$ ps for the start of the self-retracting motion of a flake is also seen. To give an account of these observations two average times are calculated: the average time $\tau_r$ of retraction of the flake (the time in which the relative displacement of the flake along the direction of extension changes from the initial value to zero, or the final value if the flake stops before it crosses the position corresponding to the zero displacement) and the average time $\tau_s$ of complete stop of the flake. The average $x$, $y$ coordinates of the final position of the extended graphene flake and root mean square deviations $\sigma_x$ and $\sigma_y$ of the final coordinates of the flake are also found. These data, obtained on the basis of the MD simulations, are given in Table I.

The simulations for the extended flake with the initial commensurate orientation show almost no telescopic oscillations of the extended graphene flake ($\zeta \ll 1$ in Table I). Furthermore, the self-retracting motion of the flake is often found to be accompanied by rotation to the incommensurate states ($\chi \sim 1$ in Table I), see also supplemental movies.

<table>
<thead>
<tr>
<th>$T$</th>
<th>Extension $\varphi$</th>
<th>$\tau_r$</th>
<th>$\tau_s$</th>
<th>$\zeta$</th>
<th>$\chi$</th>
<th>$x$</th>
<th>$y$</th>
<th>$\sigma_x$</th>
<th>$\sigma_y$</th>
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<td>$x$</td>
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<td>300</td>
<td>$x$</td>
<td>15.2</td>
<td>23.5</td>
<td>0.04</td>
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<td>0.8</td>
<td>-0.3</td>
<td>4.7</td>
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<tr>
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<td>$y$</td>
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<td>13.4</td>
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<td>26.3</td>
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FIG. 7. (Color online) Calculated displacement $y$ (Å) of the extended graphene flake with initial commensurate orientation in the zigzag direction (perpendicular to the direction of extension) and rotation angle $\varphi$ (in degrees) of the flake around the center of mass as functions of displacement $x$ (Å) of the flake in the armchair direction (the direction of extension) at temperature $4$ K. Coordinate $x = 0$ corresponds to the commensurate state. The critical angles $\pm 6\varphi$ at which the flake becomes incommensurate are shown with dashed lines.
and Fig. 7). As seen from Fig. 7, the rotation of the flake proceeds simultaneously with the displacement of the flake perpendicular to the direction of extension. This supports the hypothesis that the rotation is induced by the torque of the force acting on the flake on steep slopes of potential energy hills perpendicular to the direction of extension. Rotation of the flake to incommensurate states on the potential energy hills is also indicated in Fig. 8 for trajectories of the flake. It follows from Fig. 8 that the rotation of the flake occurs as a result of getting off the potential energy hill on which the flake is placed initially or because of scattering on the potential energy hills during retraction of the flake.

The commensurate flake extended along the armchair direction is found either to retract poorly or to rotate to the incommensurate states and to retract completely (see Table I). In 80% and 85% of simulations at temperatures 4 and 300 K, respectively, the flake starts the self-retracting motion and rotates to incommensurate states. In 17% and 12% of simulations, the flake is observed to be trapped in the initial local energy minimum. In 3% and 4%, the flake starts the self-retracting motion but gets trapped in another energy minimum due to the energy dissipation. The fractions listed above weakly depend on temperature, indicating that the probabilities for the flake to start the self-retracting motion and to rotate to incommensurate states are determined by the initial position and energy of the flake rather than by thermodynamic fluctuations. Figure 8(a) shows that most trajectories of the flake initially extended along the armchair direction go directly through the potential energy hills on which the flake experiences scattering, accompanied by rotation to incommensurate states.

As shown in the previous section, for the flake initially extended along the zigzag direction, there is no barrier to the self-retracting motion for overlap lengths less than 10 Å (see Fig. 4). In this case, complete retraction of the flake is observed in all simulations independent of rotation to incommensurate states (see Table I). The fraction \( \chi \) of simulations in which the flake rotates to incommensurate states is relatively small at 4 K and increases with temperature (see Table I). The analysis performed in the previous section showed that the potential energy relief of the flake extended along the zigzag direction favors rotation of the flake only to the angles below\( \delta \varphi \approx \varphi_0 / L \), which are insufficient to eliminate completely the corrugation of potential energy relief [see Fig. 2(d)]. In agreement with this conclusion, most trajectories of the flake extended along the zigzag direction at temperature 4 K lie around the potential energy hills, and the rotation angle of the flake does not reach the critical angle \( \delta \varphi \) at which the flake becomes incommensurate with the other flakes [see Fig. 8(b)]. However, with increasing temperature, rotation of the flake to angles greater than \( \delta \varphi \) becomes possible.

The extended flake initially rotated by 30° to the incommensurate state is found to retract in all simulations (see the data in Table I for \( \varphi = 30° \)). The fraction of simulations in which several telescopic oscillations of the flake are observed increases compared with the case of the initial commensurate orientation of the flake (see Table I). However, this fraction is still much less than unity, which means the telescopic motion of graphene flakes cannot be used in oscillators proposed in Ref. 3.

The initial orientation of the flake also determines the time of retraction. If the extended flake is initially in the commensurate state, the corrugation of the potential energy relief slows the self-retracting motion of the flake. On the contrary, for the flake initially rotated to the incommensurate state, there are no barriers to the motion of the flake, and its...
retraction occurs as fast as possible with the smallest average time $\tau_0$ of retraction (see Table I).

The final position of the retracted flake does not always correspond to the global energy minimum. The flake can stop in numerous metastable states on the potential energy relief. The dispersion of the final coordinate of the flake in the direction of extension has a significant value of 4−10 Å for all the considered cases (see Table I). This dispersion is somewhat higher for the flake extended along the armchair direction than for the flake extended along the zigzag direction. The dispersion further increases when the flake is initially rotated to the incommensurate state.

To clarify the role of rotation of the extended flake to the incommensurate states, we have performed the MD simulations for the flakes with the fixed commensurate and incommensurate orientations extended along the armchair direction. For the flake with the fixed commensurate orientation, no telescopic oscillations are observed. The average final position of such a flake in the armchair direction is found to be 15.5 Å at 300 K and 21.2 Å at 4 K on the basis of 10 simulations at each temperature. The flake with the fixed incommensurate orientation (rotated by 30° with respect to the commensurate orientation) performs telescopic oscillations with the Q-factor $Q = 2.00 \pm 0.08$ at 300 K and $Q = 2.25 \pm 0.07$ at 4 K. The time of retraction of this flake corresponding to one quarter of the oscillation is 9.5 ps. These results confirm that the rotation of the flake to incommensurate states facilitates retraction of the flake.

Because the visual analysis of the simulation results shows a high excitation of flexural vibrations of graphene flakes, such a way of dissipation seems to be dominant for the telescopic motion of the extended flake. To check this assumption, we have performed simulations of telescopic oscillations of the graphene flake with the fixed incommensurate orientation, which is also constrained in the plane. In this case, the Q-factor of the oscillations along the armchair direction at temperature 300 K is found to increase up to $Q \sim 10$. Therefore, out-of-plane vibrations of atoms of the graphene flake considerably increase the dissipation of the kinetic energy of the flake. The Q-factors calculated for the graphene flake are orders of magnitude smaller than the Q-factors $Q \sim 100−1000$ for the telescopic oscillations of carbon nanotube walls.23,25 This can be explained by the fact that carbon nanotubes are stiffer than graphene, and no significant flexural vibrations are detected in typical simulations of the telescopic oscillations of nanotube walls.12−20

The results obtained in the present paper can be extended to the case of experimentally studied graphene flakes of micrometer size.3 For flakes of size $L \sim 1 \mu$m, the critical rotation angle $\delta \psi$ at which the flakes become incommensurate is very small $\delta \psi \sim a_0/L \sim 10^{-4}$ (see Refs. 29, 30, 35, and 36).

Therefore, it could be difficult to detect such a small angle in experiments. We believe that most of the extended flakes in the experiment3 were initially rotated to incommensurate states, explaining why retraction was observed with 100% probability for the flakes of 1−2 μm size. For larger flakes, the probability of retraction decreased, which could be attributed to nonelastic deformations of these flakes during pull-out.3 Assuming that time of retraction of the flake scales with size of the flake as $\tau_0 \sim \sqrt{m}$ (see Ref. 25), where $s$ is the length of the initial extension and $m$ is the mass of the extended flake, and using the data from Table I, we estimate the time of retraction for flakes of micrometer size to be on the order of microseconds, in agreement with observations.3

IV. CONCLUSION

We have performed MD simulations of the self-retracting motion of a graphene flake telescopically extended from its equilibrium position on a stack of graphene flakes. It is shown that almost no telescopic oscillations of the graphene flake occur because of the high corrugation of the potential energy relief in the commensurate states and the high dynamic friction force related to the excitation of flexural vibrations of the flake in both the commensurate and incommensurate states. It is demonstrated that the potential energy relief becomes smooth upon rotation of the extended flake to incommensurate states, which facilitates the self-retracting motion of such a flake. Rotation of the extended flake from the commensurate to incommensurate states is often observed in MD simulations and is shown to be induced by torque acting on the flake on potential energy hills. The flake is found to stop in numerous metastable states on the potential energy relief, with dispersion of the final position of up to 10 Å for the considered system.

Mechanical oscillations (followed by the oscillation of the tunneling current) arising after switching on were shown to be the main problem, which restricts the response speed of memory cells based on bending14 and telescopic motion45 of carbon nanotubes. The observed ultrafast damping of telescopic oscillations of the graphene flake makes us expect the absence of mechanical oscillations after switching on for memory cells based on the telescopic motion of an extended graphene flake. Thus, graphene is a promising material for use in fast-responding memory cells.

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