Molecular dynamics simulation of self-retracting motion of graphene flakes

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Graphene exhibiting extraordinary electrical and mechanical properties holds great promise for the use in nanoelectromechanical systems (NEMS). Recently a self-retracting motion of graphite microflakes, i.e. retraction of graphite flakes back into graphite stacks on their extension arising from the van der Waals attraction between the flakes, was observed [1]. An idea of the oscillator based on the telescopic oscillation of graphene flakes was suggested [1]. We perform atomistic simulations to analyze perspectives of using telescopic motion of graphene flakes in NEMS.

Our calculations show that the potential relief of interlayer interaction energy for the extended flake with the commensurate orientation (Fig. 1) has high potential energy barriers (Fig. 2). Therefore, if such a flake is placed near a local energy minimum, it is not able to start the self-retracting motion. If the flake initially has enough energy to start the self-retracting motion, this motion is slowed down by the corrugation of the potential energy relief. However, upon rotation of the flake to incommensurate states (Fig. 2), the potential energy relief becomes smooth. Thus, rotation of the flake to incommensurate states should facilitate its retraction.

Molecular dynamics simulations demonstrate that the self-retracting motion of the extended flake with the initial commensurate orientation proceeds in diverse ways even at almost the same initial position (see Fig. 3, movies are also available). The extended flake can retain its commensurate orientation and be locked near a local energy minimum or retract slowly. However, in majority of the simulations, fast retraction of the flake accompanied by its rotation to incommensurate states is observed. Analysis of the flake trajectories reveals that rotation of the extended flake with the initial commensurate orientation to incommensurate states occurs when the flake passes potential energy hills. In fact, the force of interlayer interaction is applied to atoms of the flake only in the overlap area between the neighbour flakes. Therefore, the force acting on the extended flake in the direction perpendicular to the direction of extension exerts a torque inducing rotation of the flake to incommensurate states.

One-two damped telescopic oscillations of the extended flake are very scarce. Therefore, as opposed to carbon nanotube walls which can perform telescopic oscillations with the Q-factor ~ 100-1000 [2], graphene flakes are not suitable for the use in oscillators. On the other hand, this result means that graphene flakes are perfect for the use in fast-responding electromechanical memory cells.

It should also be noted that even if the extended flake is fixed in the incommensurate state, the Q-factor of the telescopic oscillations of the flake does not exceed 3. Therefore, the absence of telescopic oscillations for graphenes flake is related to two factors: (1) high barriers to motion of the extended flake with the commensurate orientation, and (2) high dynamic friction force.

References

[1] Q. Zheng, B. Jiang, S. Liu, Yu. Weng, L. Lu, Q. Xue, J. Zhu, Q. Jiang, S. Wang, L. Peng, Phys. Rev. Lett., **100** (2008) 067205.
[2] I. V. Lebedeva, A. A. Knizhnik, A. M. Popov, Yu. E. Lozovik, B. V. Potapkin, Nanotechnology, **20** (2009) 105202.

Figures

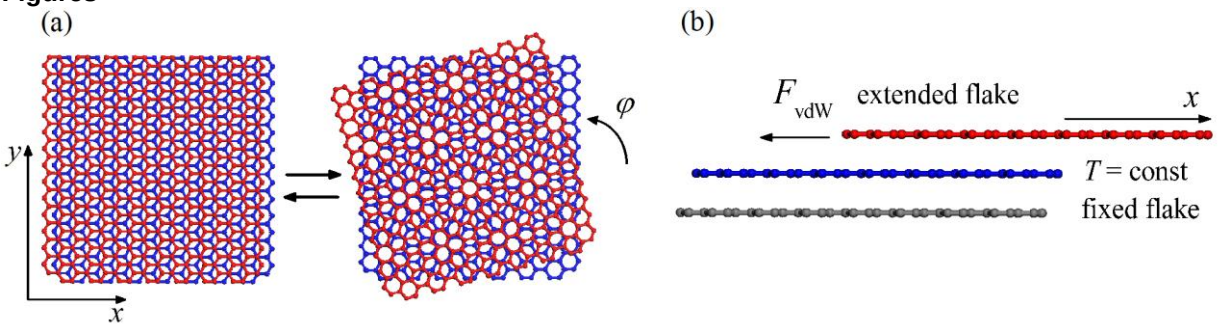

Fig. 1. (a) Commensurate ($\varphi = 0^\circ$, left) and incommensurate ($\varphi = 15^\circ$, right) states of graphene flakes. (b) Schematic representation of the telescopic motion of a graphene flake (system under consideration).

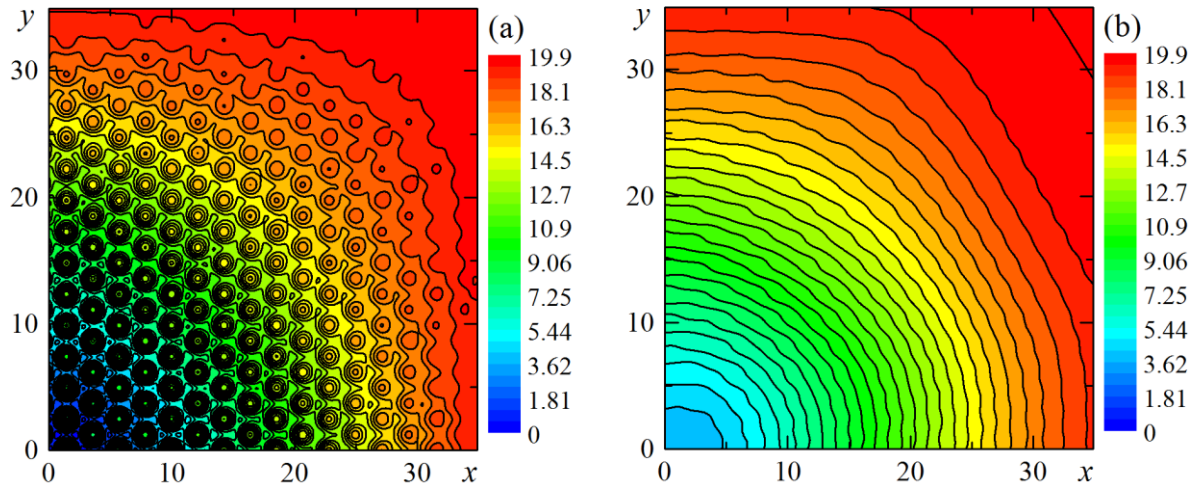

Fig. 2. Calculated interaction energy (in eV) of the graphene flakes of 34 Å x 34 Å size (446 atoms) at the equilibrium interlayer spacing 3.4 Å as a function of the relative position x, y (in Å; axes x and y are chosen along the armchair and zigzag directions, respectively) of the center of mass of the extended flake at the rotation angles of the flake (a) $\varphi = 0^\circ$ and (b) $\varphi = 30^\circ$. The equipotential lines are drawn with a step of 0.6 eV. The energy is given relative to the global energy minimum.

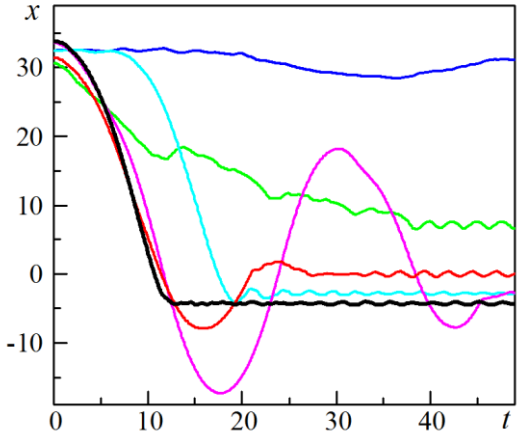

Fig. 3. Different types of calculated dependences of displacement x (in Å) of the flake with the initial commensurate orientation extended in the armchair direction on time t (in ps) at temperature 300 K.