doi：103969/j. issn. 0490-6756. 2017. 01. 017

基于石墨的纳机电系统的外驱动可控振动

李健文[1,2]，刘念华[3]

（1. 南昌大学材料科学工程学院，南昌 330031；2. 南昌工程学院理学院，南昌 330099；
3. 南昌大学高等研究院，南昌 330031）

摘　要：采用数值计算方法研究了基于石墨的纳机电系统在周期性简谐驱动力作用下实现稳定振动的条件. 确定了获得持久稳定的振动的系统和控制力参数. 计算和分析了两块石墨片等长及不等长时纳米振子的操作特性. 结果表明，通过选择合适的驱动振幅和频率，能够实现石墨片的持久稳定振动. 该方法对于进一步研究纳机电系统的设计有重要的参考价值.

关键词：纳机电系统；纳米振子；驱动频率；稳定振动；石墨

中图分类号：TB34　　　**文献标识码**：A　　　**文章编号**：0490-6756(2017)01-0101-07

Controlled driven oscillations of graphite-based NEMS

LI Jian-Wen[1,2], *LIU Nian-Hua*[3]

(1. School of Materials Science and Engineering, Nanchang University Nanchang 330031, China;
2. School of Science, Nanchang Institute of Technology, Nanchang 330099, China;
3. Institute for Advanced Study, Nanchang University, Nanchang 330031, China)

Abstract: The conditions controlling the stable oscillation of graphite-based nanoelectromechanical systems (NEMS) are investigated under periodical harmonic driving force with numerical computational methods. The parameters of the system and control force which allow obtaining the sustained stable oscillation at a constant frequency are determined. The operating characteristics of the nano-oscillator are calculated and analyzed for the equal-length and unequal-length graphite flakes. The calculated results show that the sustained stable oscillation of the graphite flakes can be realized by properly choosing the amplitude and the initial phase of the periodical harmonic driving force. The methods reported here are believed to have important implications in NEMS design.

Keywords: NEMS; Nano-oscillator; Driving frequency; Stable oscillation; Graphite

1　Introduction

Because of the extraordinary mechanical, electrical and thermal properties as well as biocompatibility of graphite, the two-dimensional nanostructures are considered as promising materials for a variety of applications. For example, graphite has widely been used as durable solid lubricants due to the superlubricity between graphite layers and the extreme high elastic moduli and interlayer strengths within the layers[1-4]. New surprising properties of graphite have been discovered at times, such as designable electrical

收稿日期：2015-07-06
基金项目：国家重大基础研究计划(973 计划)(2013CB934200)；国家自然科学基金重点项目(10832005)；国家自然科学基金项目(11264030)
作者简介：李健文(1976－)，男，江西安远人，博士研究生，主要研究领域：纳米表面科学与工程. E-mail：nitljw624@nit. edu. cn
通讯作者：刘念华. E-mail：nhliu@ncu. edu. cn

properties[5-7] and the quantum Hall effect[[8,9]] which provide an ample scope for fundamental research and new technologies[10,11]. There were also a few works devoted to the mechanical properties of graphite which is viewed as an ideal material for the sensing and detection applications based on nanoelectromechanical systems (NEMS)[12]. In particular, self-retracting motion of graphite, i. e. retraction of graphite flakes back into graphite stacks on their extension, was observed experimentally[13,14]. This phenomenon is similar to telescopic oscillation of carbon nanotubes walls arising from their van der Waals (vdW) interaction. The ability of free relative sliding and rotation of carbon nanotube walls and their excellent 'wear proof' characteristics allowed using carbon nanotube walls as movable elements in NEMS[15-17]. By analogy with the gigahertz oscillator based on carbon nanotubes, a gigahertz oscillator based on the telescopic oscillation of graphite layers was suggested[14].

Some researchers studied the frictional properties of graphene flake on small contacts with a friction force microscopy (FFM)[18-20]. Dienwiebel *et al*[1,21] examined the friction between a graphite flake attached to sharp FFM tip and an atomically flat graphite surface, and they also measured the friction as a function of the misfit angle. Friction forces ranging from moderate to vanishingly small depend on the degree of commensurability between the lattices of the flake and the extended surface. Although a relatively smooth and low-frictional sliding can be achieved by choosing an appropriate misfit angle between two graphite flakes, friction induced energy dissipation is still inevitable, resulting in damping motion which limits its practical application because it brings difficulties for the energy supplement and signal detection. Thus how to sustain the graphite oscillatory motion in a precise control down to the molecular level over long periods of time remains a crucial issue. Reducing energy dissipation or applying an external field is two possible approaches.

As we know, for a harmonic oscillator, the natural frequency has nothing to do with the initial displacement. However, the natural frequency of anharmonic oscillator is strongly dependent on the initial displacement. In this work, we introduce a numerical computational method for maintaining and controlling the stable motion of graphite flake with a linear dependence of the friction force on the relative velocity of the graphite flake. Periodical harmonic driving force is applied to the anharmonic nano-oscillator in which the top and bottom graphite flakes are of different lengths. We determine the controllable operating conditions for the stable oscillation by the parameters of the oscillators and the driving force, and investigate the relation of the stable oscillation with the amplitude and the initial phase of the periodical driving force. Our aim is to demonstrate the feasibility of the proposed method for controlling the stable motion of the oscillation system. We wish to explore in detail how we may design systems that persistent oscillation can be exploited for building efficient nanomechanical devices.

The rest of the paper is organized in the following way. The model of bilayer graphite flakes and the numerical computational methods in Section 2 are described briefly. In Section 3, we give the calculated results and demonstrate the possibility of controlling the stable oscillation of graphite flakes. Section 4 is left for conclusions.

2 Model and method

In this work, we perform numerical simulations of the controlled operation of two rectangular graphite flakes to investigate the possibility of realizing the stable oscillation. The distance between two graphite flakes is ~3.4 Å, which is the balance displacement between adjacent flakes of graphite. Since covalent bonds are much stiffer than vdW interaction, the graphite flakes can be modeled as a system of two rigid flakes moving parallelly, as shown in Fig. 1. The interaction energy $U(x)$ of two perfectly rigid graphite flakes can be written as

$$U(x)=\begin{cases}0 & |x|<L_0\\ \frac{1}{2}\beta(|x|-L_0)^2+\frac{1}{6}\eta(|x|-L_0)^3 & L_0<|x|<x_0\\ U_0+\alpha l(|x|-L_0) & |x|>x_0,\end{cases}\tag{1}$$

in the expressions,

$$L_0 = (L_2 - L_1)/2, \tag{2}$$

$$\beta = \frac{2\alpha}{(x_0 - L_0)}, \tag{3}$$

$$\eta = -\frac{2\alpha}{(x_0 - L_0)^2}, \tag{4}$$

$$U_0 = -\alpha l(x_0 - L_0) + \frac{1}{2}\beta(x_0 - L_0)^2 + \frac{1}{6}\eta(x_0 - L_0)^3, \tag{5}$$

where l is the width of the graphite flakes, L_1 is the length of the top flake, L_2 is the length of the bottom flake, α is the binding energy per unit area, and x is the displacement of the top graphite flake. The potential as a function of translational displacement and the concrete relations between the natural frequency and the initial displacement for different sizes of the top graphite flake are shown in Fig. 1(a) and (b), respectively. The natural frequency of the oscillator is defined as the frequency of free oscillation without damping. Fig. 1(b) indicates that the natural frequency of anharmonic oscillator is strongly dependent on the initial displacement, which is quite different from that of a harmonic oscillator. As is known to all, the natural frequency of harmonic oscillator has nothing to do with the initial displacement. Consequently the dynamics of an anharmonic oscillator is quite different from that of a harmonic oscillator.

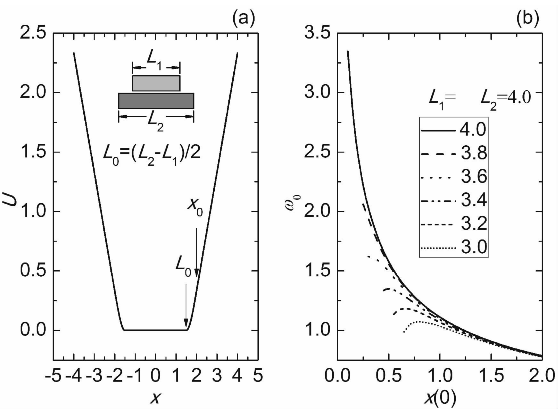

Fig. 1　(a) Potential as a function of translational displacement x, and (b) natural frequency as a function of initial displacement $x(0)$ for different lengths L_1 of top rectangular graphite flake.

In order to study the dynamics of the nanodevice, we consider linearly damped oscillators with numerical computations. The dissipation of the oscillation energy results in the decrease of the oscillation amplitude with time. Consequently, to sustain the stable oscillation of the graphite oscillator, it is necessary to supply the energy to the oscillator. We assume that the dissipated energy is compensated by an external applied periodical harmonic force. If neglecting the Langevin stochastic force and vibrations in the graphite flakes, the oscillator dynamics may be roughly described as

$$\dot{x} = v, \tag{6}$$

$$\mu\dot{v} = -\frac{\partial U(x)}{\partial x} - \gamma v + F_m \sin(\omega t + \varphi), \tag{7}$$

where μ is the mass of the movable top graphite flake, x is the displacement with respect to the fixed bottom graphite flake, v is the relative velocity, F_m is the amplitude of driving force applied to the top graphite flake with angular frequency ω and initial phase φ, γ is the friction coefficient with an imposed constant values 0.01. We suppose the initial velocity is always equal to zero. To obtain stable oscillation, the states of the oscillator and the driving force must return to the original states after one period T. So the angular frequency ω of the driving force has to be equal to the integral multiple of the natural angular frequency Ω,

$$\omega = n\Omega. \tag{8}$$

Although these frequencies are only a small subset of total possible frequencies, the conditions are absolutely necessary. Limiting the solutions to this subset is not artificial. Outside this subset, the oscillatory system can not always fully restore in one period. Nevertheless this limitation is not essential for a harmonic potential because the natural frequency Ω is not dependent on the initial displacement.

For the purpose of ensuring the complete restoration of the anharmonic oscillator and the external force in one period, the displacement, velocity and energy have strict periodicity. Once the external force is given, its period can't change. Thus the oscillator must adjust its parameters, such as displacement and phase, to make the oscillatory frequency and the driving frequency match. If the initial conditions are proper, the energy that the periodical driving force afford is equal to the dissipation of oscillation energy due to the frictional force in a period, then we have

$$\int_0^T \{F_m \sin(n\Omega t + \varphi) - \gamma v(t)\} v(t) dt = 0. \tag{9}$$

The displacement at time t is dependent on many parameters, including the shape of the potential, the initial displacement, the friction coefficient, and the frequency, initial phase and amplitude of the driving force, namely $x[t; U(x), x(0), \gamma, \omega, \varphi, F_m]$. In order to sustain the stable oscillation, the displacement and the velocity must return to the initial values after one period T. It follows that

$$x[t = T; U(x), x(0), \gamma, \omega, \varphi, F_m] = x(0), \tag{10}$$

$$v[t = T; U(x), x(0), \gamma, \omega, \varphi, F_m] = v(0). \tag{11}$$

It is very difficult to determine the conditions concerning multiple parameters operation for sustained oscillator. If the driving frequency satisfies Eq. (8), then the conditions of the stable oscillation are determined by the initial phase and the amplitude of the controlled force. Each equation of the combination gives a curve in the $\varphi - F_m$ plane. From this, we can obtain the solutions for the combination of Eqs. (10) and (11). Here the Verlet velocity algorithm and steepest descent method were used to solve them.

3 Results and discussion

3.1 Equal-length L_1 and L_2

The frequency of free oscillation of the system depends on the initial extrusion of the top graphite flake for the anharmonic oscillator. We find that, for the initial displacement $x(0) = 1$ and $x(0) = 2$ of $L_1 = L_2 = 4$, the frequencies of the oscillator in the case with the absence of the driving force and frictional force are $\Omega = 1.11048$ and $\Omega = 0.78536$, respectively.

As demonstrate above, to sustain stable oscillation, the driving frequency must be equal to the integral multiple of the oscillatory frequency once the top graphite flake is released from an initial displacement. We take the driving frequencies as $\omega = 2\Omega$ and $\omega = 3\Omega$ for $L_1 = L_2 = 4$. The curves satisfying Eqs. (10) and (11) are shown in Fig. 2, where case 1, case 2 and case 3 correspond to $x(0) = 1$, case 4 corresponds to $x(0) = 2$. There are many solutions that satisfy Eq. (10) or (11), and one initial phase φ corresponds to several amplitudes F_m, same if vice versa. However, there is only several solutions within the range $-2\pi \sim 2\pi$ for the initial phase φ. The cross points of the curves in the $\varphi - F_m$ plane are $(\varphi, F_m) = (-1.05135, 2.06287)$, and $(\varphi, F_m) = (-1.03147, 2.16222)$, $(\varphi, F_m) = (-0.05882, 0.10546)$, and $(\varphi, F_m) = (-0.08333, 0.14922)$ for case 1, case 2, case 3 and case 4, respectively. As increasing the driving frequency, the amplitude F_m of the driving force needed to sustain the stable oscillation decreases for the initial displacement $x(0) = 1$.

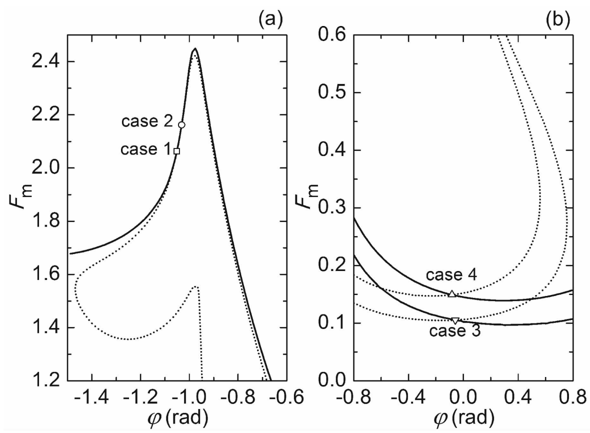

Fig. 2 Sustainable oscillation amplitude and initial phase of equal length graphite flakes for (a) $\omega = 2\Omega$ and (b) $\omega = 3\Omega$. The solid and dotted lines correspond to Eq. (10) and Eq. (11), respectively.

The analysis has been performed with reference to the phase space, examples of which are shown in Fig. 3 corresponding to cases of Fig. 2. We consider that the trajectories of interest are those that form a closed loop in one oscillation cycle, as these will show the desirable aspect for any driven oscillator system. It is found that every solution for the combination of Eqs. (10) and (11) corresponds to a closed loop. The simulation results indicate that the phase diagram of each oscillator is not a standard ellipse, but a smooth loop. Consequently the oscillator is anharmonic vibration periodically. Interestingly, the oscillation amplitude is unequal for the frequency $\omega=2\Omega$ and equal for the frequency $\omega=3\Omega$. Furthermore, the phase trajectories are asymmetric. So the choice of the driving frequency has great influence on the behavior of the considered oscillator.

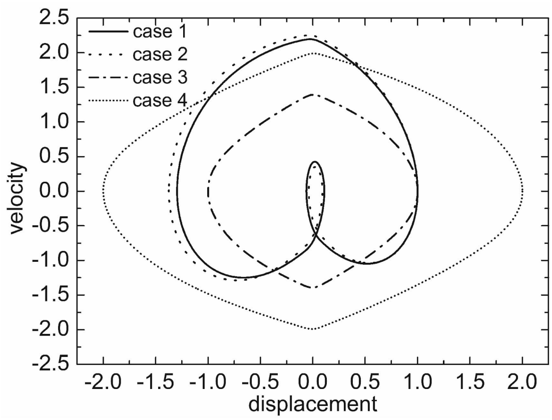

Fig. 3 The resulting phase space trajectories corresponding to cases of Fig. 2.

In order to understand the forces that contribute significantly to the oscillatory behavior, a typical result is shown in Fig. 4 for case 3. It is indicates that the driving frequency is three times that of net force, velocity and displacement. Furthermore, we found similar results in the cases of both small and large initial displacement. As are explicitly plotted in Fig. 3, the choice of the initial displacement has little influence on the behavior of the considered oscillator. Accordingly only if the driving frequency is equal to the integral multiple of the oscillatory frequency and the initial phase and amplitude of the controlled force satisfy certain conditions which are determined by the combination of Eqs. (10) and (11), we can conveniently choose different initial displacements to sustain stable oscillation.

The driving force applied on the graphite flake is periodical, the net forces are not exactly zero after a driving period T_ω, as shown in Fig. 4. With regard to the same initial displacement and different driving forces, the displacement may be positive or negative and the oscillator may even move backward at $t = T_\omega$. This state is the initial condition of next driving period, which has great effect on the following movement. Furthermore, probably the maximums of the positive and negative displacement are also unequal. Consequently the conditions to sustain the stable oscillation of graphite flakes are very rigorous.

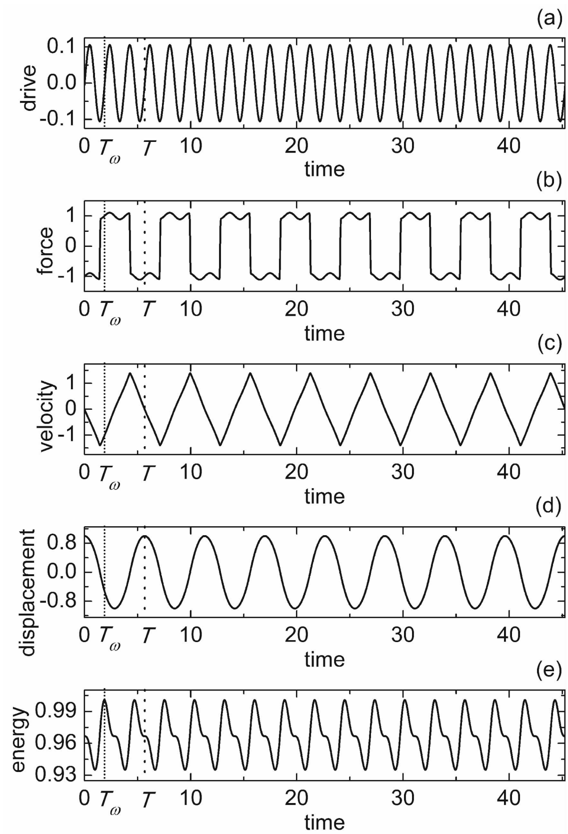

Fig. 4 (a) driving force, (b) total force, (c) velocity, (d) displacement, and (e) total energy of the moving graphite flake as a function of time for case 3. T and T_ω are oscillation period and driving period, respectively.

3.2 Unequal-length L_1 and L_2

For the initial displacement $x(0) = 2$ nm of $L_1 = 2$ and $L_2 = 4$, the frequency of the oscillator in the case with the absence of the driving force and frictional force is $\Omega=0.73618$. The curves satisfy Eq. (10) and Eq. (11), corresponding to the solid lines and the dotted lines, respectively, are shown in Fig. 5. For case 8, the cross point of the curves in the $\varphi - F_m$ plane is $(\varphi, F_m) = (-1.58486, 0.88493)$, which gives the solution that the graphite oscillator can oscillate under stable conditions. An enlarged view of case 10 is shown in (c) to emphasize the possibility of obtaining more choices to sustain persistent oscillation. In the $\varphi - F_m$ plane, we can measure the deviation that the displacement and velocity relative to the initial value after one time period with $\Delta = [x(T) - x(0)]^2 + [v(T) - v(0)]^2$. Those points drop into the region of $\Delta < 10^{-4}$, corresponding to the shaded parts, can be treat as stable oscillation approximately. So we can conveniently choose different initial phases and amplitudes of driving force to sustain stable oscillation.

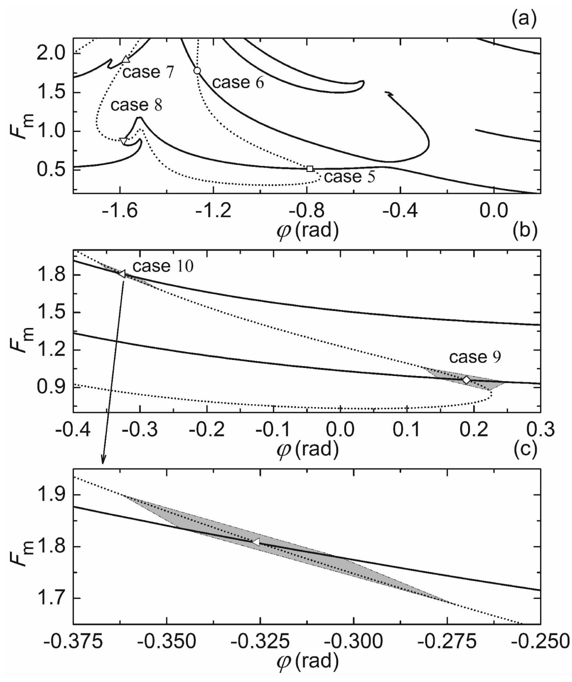

Fig. 5 Sustainable oscillation amplitude and initial phase of unequal length graphite flakes for (a) $\omega = 2\Omega$ and (b) $\omega = 3\Omega$. An enlarged view of case 10 is shown in (c) to emphasize the possibility of obtaining more choices to sustain persistent oscillation.

The calculation results of the controlled stable oscillations are presented in Fig. 6 for unequal length graphite oscillators. Comparing with the cases of equal length, we observed similar phenomena. Although the oscillation behaviors are more complicated, we can realize sustained oscillation with more choices.

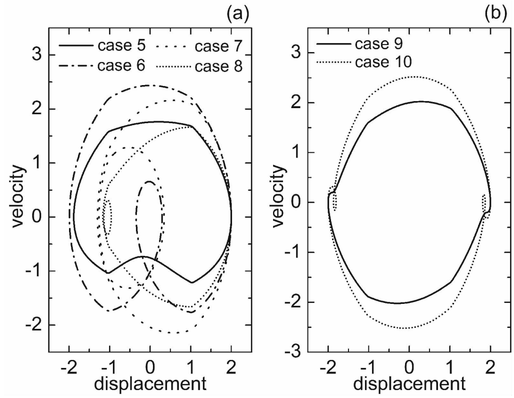

Fig. 6 The resulting phase space trajectories corresponding to cases of Fig. 5.

4 Conclusions

In this paper, we investigate the controlled conditions under which the graphite-based NEMS can realize sustained stable oscillation driven by periodical harmonic force. Our numerical calculation indicates that the use of proper driving force can be an effective and convenient approach to control and tune graphite-based oscillators. We have determined the parameters and characteristics corresponding to the controllable operating conditions for the stable oscillators. Furthermore, we find that, if we choose the amplitude and the initial phase of the periodical harmonic driving force satisfied the conditions of the combination of Eqs. (10) and (11), we can realize the stable oscillation of the graphite-based oscillator.

References:

[1] Kawai S, Benassi A, Gnecco E, *et al*. Superlubricity of graphene nanoribbors on gold surfaces[J]. Science, 2016, 351: 957.

[2] Socoliuc A, Bennewitz R, Gnecco E, *et al*. Transition from stick-slip to continuous sliding in atomic friction: Entering a new regime of ultraflow friction [J]. Phys Rev Lett, 2004, 92: 134301.

[3] Ma M, Benassi A, Vanossi A, *et al*. Critical length limiting superlow friction [J]. Phys Rev Lett, 2015, 114: 055501.

[4] Liu Y, Grey F, Zheng Q. The high-speed sliding friction of graphene and novel routes to persistent superlubricity [J]. Sci Rep, 2014, 4: 4875.

[5] 尹汤海，张红. 环形石墨烯纳米结构的等离激光激发[J]. 四川大学学报：自然科学版，2016，52：343.

[6] 陈自然，徐友辉，何展荣. 磷掺杂石墨烯的结构、光谱及电子性质[J]. 四川大学学报：自然科学版，2016，53：587.

[7] Zhao S，Lv Y，Yang X. Layer independent nanoscale electrical properties of graphene studied by conductive scanning probe microscopy [J]. Nanoscale Res Lett，2011，6：498.

[8] Novoselov K S，Jiang Z，Zhang Y，*et al*. Room-temperature quantum Hall effect in graphene [J]. Science，2007，315：1379.

[9] Zhang Y，Tan Y W，Stormer H L，*et al*. Experimental observation of the quantum Hall effect and Berry′s phase in graphene [J]. Nature，2005，438：201.

[10] Meyer J C，Geim A K，Katsnelson M I，*et al*. The structure of suspended graphene flakes [J]. Nature，2007，446：60.

[11] Rose F，Debray A，Martin P，*et al*. Suspended HOPG nanoflakes for HOPG nanoresonator engineering and new carbon nanostructure synthesis [J]. Nanotechnology，2006，17：5192.

[12] Lee C，Wei X，Kysar J W，*et al*. Measurement of the elastic properties and intrinsic strength of monolayer graphene [J]. Science，2008，321：385.

[13] Yang J，Liu Z，Grey F，*et al*. Observation of high-speed microscale superlubricity in graphite [J]. Phys Rev Lett，2013，110：255504.

[14] Zheng Q，Jiang B，Liu S，*et al*. Self-retracting motion of graphite microflakes [J]. Phys Rev Lett，2008，100：067205.

[15] Cumings J，Zettl A. Low-friction nanoscale linear bearing realized from multiwall carbon nanotubes [J]. Science，2000，289：602.

[16] Zheng Q，Jiang Q. Multiwalled carbon nanotubes as gigahertz oscillators [J]. Phys Rev Lett，2002，88：045503.

[17] Kis A，Jensen K，Aloni S，*et al*. Interlayer forces and ultralow sliding friction in multiwalled carbon nanotubes [J]. Phys Rev Lett，2006，97：025501.

[18] Schwarz U D，Zwörner O，Köster P，*et al*. Quantitative analysis of the frictional properties of solid materials at low loads. I. Carbon compounds [J]. Phys Rev B，1997，56：6987.

[19] Liu E，Blanpain B，Celis J P，*et al*. Comparative study between macrotribology and nanotribology [J]. J Appl Phys，1998，84：4859.

[20] Buzio R，Gnecco，Boragno C，*et al*. Friction force microscopy investigation of nanostructured carbon films [J]. Carbon，2002，40：883.

[21] Dienwiebel M，Pradeep N，Verhoeven G S，*et al*. Model experiments of superlubricity of graphite [J]. Surf Sci，2005，576：197.