Atomic-Scale Ultralow Friction
– Simulation of Superlubricity of C_{60} Molecular Bearing

Naruo Sasaki^{1,3}, Noriaki Itamura^{1} and Kouji Miura^{2}

^{1} Department of Materials and Life Science, Faculty of Science and Technology, Seikei University, 3-3-1 Kichijoji-Kitamachi, Musashino-shi, Tokyo 180-8633, Japan
^{2} Department of Physics, Aichi University of Education, Hirosawa 1, Igayacho, Kariya-shi, Aichi 448-8542, Japan

Abstract. Simulation of superlubricity of C_{60} molecular bearing is performed based on molecular mechanics. Atomic-scale frictional feature along [0 1 10] direction of the graphite/C_{60}/graphite interface is numerically investigated compared with that of the graphite/graphite/graphite interface. Simulated interlayer distances of about 1.3nm are in good agreement with previous experimental results [1-3]. Atomic-scale friction coefficient of graphite/C_{60}/graphite interface decreases to about 30% of that of the graphite/graphite/graphite interface. It is clarified that three-dimensional degree of freedom of intercalated C_{60} motion is one of origins of ultralow friction of graphite/C_{60}/graphite interface along [0 1 10] direction.

1. Introduction
To control ultralow friction or superlubricity [4] is one of the most practical problems of mechanical and material engineering. Ultralow friction has been so far studied on well-defined substrate surfaces such as mica [5], Si [6], MoS_{2} [7,8], graphite [9-12] and NaCl [13] by using scanning probe microscopy. Recently, artificial carbon hybrid materials - C_{60} sandwiched graphite [14,15], which we call “C_{60} molecular bearing,” and fullerene intercalated graphite [1-3], have been successfully developed to achieve ultralow friction on an atomic scale. Since then ultralow friction of fullerene molecular bearings have attracted many attentions [16-19]. However the origin of ultralow friction and the merit as lubricant of the fullerene intercalated graphite are yet to be known from theoretical standpoints. Therefore, in this paper, atomic-scale ultralow friction of the graphite/C_{60}/graphite interface [Fig.1(a)], which can be thought to play a major role in ultralow friction of C_{60} intercalated graphite, is numerically studied compared with that of graphite/graphite/graphite interface in order to understand excellent ultralow friction of C_{60} intercalated graphite. The load dependence of graphite/C_{60}/graphite interface is studied. It has been clarified that three-dimensional degree of freedom of C_{60} motion is one of origins of excellent ultralow friction of graphite/C_{60}/graphite interface along [0 1 10] direction.

2. Model and Methods
As a model of the graphite/C_{60}/graphite interface, the close-packed C_{60} monolayer inserted between two rigid graphite sheets is used as shown in Figs.1(b) and 1(c). It should be noted that each graphite sheet is modeled by one rigid layer. Here the Tersoff potential function V_{cov} [20] and the modified
Lennard-Jones potential function $V_{vdW}$[21,22] are used as the covalent bonding and non-bonding energies, respectively. The periodic boundary condition within the (0001) plane is applied to the $1 \times 1$ ($2 \times 2$) unit cell comprised of two graphite sheets and one (four) C$_{60}$ molecule(s) surrounded by the parallelogram[Fig.1(b)]. The initial orientation between two graphite sheets is set as AA stacking.

**Figure 1.** In (a) Schematic illustration of C$_{60}$ intercalated graphite comprised of graphite/C$_{60}$/graphite interface. (b) The dotted and broken parallelograms show the $1 \times 1$ and $2 \times 2$ unit cells, respectively. (c) For the fixed graphite interlayer distance $d$, the lateral force $F_L$ and the loading force $F_z$ per $1 \times 1$ unit cell are calculated.

First, the upper rigid graphite sheet is moved to change the graphite interlayer distance $d$ along [0001] direction. Next, for each fixed $d$ (=1.4, 1.3 and 1.2 nm), the upper rigid graphite is scanned to change the lateral positions $L$ along [1010] direction [Figs.1(b) and 1(c)]. Finally, for each $d$ and $L$, the metastable structure of the graphite/C$_{60}$/graphite interface is calculated by minimizing the total energy $V_{total} = V_{cov} + V_{vdW}$, using the structural optimization, Polak-Rebiere-type conjugate gradient (CG) method[23]. Here the convergence criterion is set so that the maximum of absolute value of all the forces acting on the movable atoms, becomes lower than $1.6 \times 10^{-4}$ nN. Thus the vertical loading force acting on the upper graphite $F_z$ and lateral force opposite to the scan direction $F_L$ are obtained per $1 \times 1$ unit cell.

Here atomic-scale frictional feature observed by AFM and scanning process of AFM can be approximately described in the static limit of temperature $T \to 0$ and scan velocity $v \to 0$. Here the following adiabatic theorem holds good as the 0th order approximation that, for each scanning position of the AFM tip, all the atoms are instantaneously relaxed and the system is always located at local energy minimum. The static simulation[4,9,12] has successfully reproduced frictional force maps observed by atomic-force microscopy under the experimental condition of a scan velocity of $v \approx 100$ nm/s [1-3, 8, 9, 14, 15].

### 3. Stable structure of Graphite/C$_{60}$/Graphite interface

First, when the initial structures of graphite/C$_{60}$/graphite interface with various orientations of C$_{60}$ molecules for $d = 1.3$nm are optimized assuming that the upper and lower graphite sheets are located as AA stacking, three different types of metastable orientations of C$_{60}$ molecule are obtained. As illustrated in Fig.2(a), each type where six-membered rings, single carbon bonds, and single carbon atoms of C$_{60}$ molecules face to the upper and lower graphite sheets, is called 'AB stacking type (AB)', 'Bond stacking type (B)', and 'On top stacking type (OT)', respectively. For B type, C$_{60}$ molecule tilts by several degrees from [0001] axis. OT type is the same as 'frustrated AB stacking' obtained by
Legoas et al.[16] using structural optimization. The most stable interface is OT type for graphite interlayer distance $d \geq 1.29$nm, and AB type for $d \leq 1.29$nm [Fig.2(b)]. AB, B and OT types give the stable interlayer distances $d = 1.313, 1.320$ and $1.320$ nm, respectively, any of which reproduce well $d \approx 1.3$ nm observed in our previous TEM measurements[1,2].

As a comparison graphite/graphite/graphite interface and its total energy as a function of $d$ are also shown in Fig.2(a). The stable interlayer distance of graphite/graphite/graphite interface is calculated as $d = 0.68$ nm.

Fig.2(c) indicates that the upper graphite sheet is completely peeled from the C$_{60}$/lower graphite system for $d = 1.40, 1.41$ and $1.41$nm for AB, B and OT types, respectively. This means that the graphite/C$_{60}$/graphite interface is stable only for $d \leq 1.4$nm.

**Figure 2.** (a) Three different kinds of metastable orientations of C$_{60}$ molecules: 'AB stacking (AB)', 'Bond stacking (B)', and 'On top stacking (OT)' types. Graphite/Graphite/Graphite interface and its total energy as a function of $d$ are also shown. (b) Total energy as a function of the graphite interlayer distance $d$ for AB, B and OT types. Observed TEM image indicates interlayer distance of 1.3nm[1,2]. (c) Distances between C$_{60}$ molecule and the upper and lower graphite sheets, $d_u$ (dashed lines) and $d_l$ (solid lines), as a function of $d$.

### 4. Load dependence of Graphite/C$_{60}$/Graphite interface

Next the upper graphite sheet is scanned along [10\bar{1}0] and its opposite directions. Fig.3 shows the mean lateral force $<F_L>$ as a function of the mean loading force $<F_z>$ for AB-, B- and OT type of graphite/C$_{60}$/graphite interfaces and graphite/graphite/graphite interface. Here the mean lateral force
\[ F_L = \frac{1}{2L} \int F_1 \, dl \] is calculated as a function of the mean loading force \[ F_z = \frac{1}{2L} \int F_z \, dl \] corresponding to \( d = 1.4, 1.3 \) and 1.2nm for AB, B and OT types, respectively, where \( 2L \) denotes the scan length. The dissipation energy \( \Delta E_L = \int F_1 \, dl \) during the total scan is also plotted. As a comparison, the load dependence of the graphite/graphite/graphite interface is also plotted, where the mean loading forces \( \langle F_z \rangle \) corresponding to \( d = 0.70, 0.67 \) and 0.62nm are calculated. Please note again that the interlayer distance \( d \) is kept constant during the scan, where the variations of load \( F_z \) range from 0.011nN to 0.17nN for graphite/C\textsubscript{60}/graphite interface, and from 0.095nN to 0.71nN for graphite/graphite/graphite interface, respectively.

**Figure 3.** (a) The mean lateral forces \( \langle F_L \rangle \) as a function of the mean loading force \( \langle F_z \rangle \) for AB-, B- and OT types of graphite/C\textsubscript{60}/graphite interface corresponding to \( d = 1.4, 1.3 \) and 1.2nm, and for graphite/graphite/graphite interface corresponding to \( d = 0.70, 0.67 \) and 0.62nm, are plotted. Dissipation energy \( \Delta E_L \) during the total scan is also indicated. Simulated results using both \( 1 \times 1 \) and \( 2 \times 2 \) unit cells are shown.

The graphite/C\textsubscript{60}/graphite interface clearly exhibits smaller mean lateral force \( \langle F_L \rangle \) or dissipation energy \( \Delta E_L \) than the graphite/graphite/graphite interface. As shown in Fig.3, simulated results of AB and OT types for \( 1 \times 1 \) unit cell are just the same as those for \( 2 \times 2 \) unit cell except for the case \( d = 1.2 \) nm of OT type. Therefore, in this paper, C\textsubscript{60} dynamics obtained by using \( 1 \times 1 \) unit cell is discussed.

If the linear fitting \( \langle F_L \rangle = \mu \langle F_z \rangle + F_{L0} \) is performed, the friction coefficient of the graphite/graphite/graphite interface is obtained as \( \mu_{GGG} = 0.0082 \), which is a little smaller than the previous experiment \( \mu = 0.012 \) by Mate et al.[24] and the molecular dynamics simulation \( \mu = 0.013 \) along [10\textsubscript{T0}] direction by Matsushita et al.[25] Friction coefficients for AB and B types of graphite/C\textsubscript{60}/graphite interface, \( \mu_{GGG} = 0.0023 \) and 0.0025, respectively, are reduced to about 30% of \( \mu_{GGG} \). On the other hand OT type exhibits quite different behavior. \( \langle F_L \rangle \) increases at first as the load \( \langle F_z \rangle \) increases. However, at higher loading force of \( \langle F_z \rangle \approx 5.7 \)nN, \( \langle F_L \rangle \) decreases to about 5pN, which is smaller than \( \langle F_L \rangle \) for AB and B types. Thus Fig.3 points out difference of ultralow frictional mechanisms between AB (or B) and OT types.
5. Atomic-scale dynamics of intercalated C\textsubscript{60} molecule

Therefore each atomic-scale dynamics of intercalated C\textsubscript{60} molecule for AB, B and OT types during scan is analyzed.

5.1 AB stacking type

For AB type, as shown in Fig. 4(a-1), frictional loop with periodicity of 0.44nm along [10\textsubscript{T}0] direction of graphite lattice, is comprised of sinusoidal part with little hysteresis and saw-tooth wave part with large hysteresis. Qualitative feature of the frictional loop pattern does not change even if the load increases [Fig.4(a-2)], which can be explained mainly by the atomic-scale sliding of C\textsubscript{60} molecule. Here AB stacking registry between the upper (lower) six-membered ring of C\textsubscript{60} molecule and the upper (lower) graphite sheet is basically conserved during the scan [Fig.4(a-3)]. Scan positions 1→2→3→3′→1’ are also indicated on frictional loop. At the process 3→3’, C\textsubscript{60} molecule discretely slips to the nearest AB stacking site, which contributes to the sawtooth behavior of the force loop. C\textsubscript{60} molecule also takes a small tilting oscillation along the scan direction.

5.2 Bond stacking type

For B type, frictional loop exhibits sawtooth wave pattern for $<F_z> = 0.38nN$, which reflects oscillation of upper and lower carbon bonds of C\textsubscript{60} molecule with occasional sliding [Fig.4(b-1)]. Since the tilting angle $\phi$ of C\textsubscript{60} from [0001] axis oscillates within about a few degrees, the projection of the upper and lower carbon bonds onto the lateral plane do not match to each other [Fig.4(b-3)]. However, for the larger load of $<F_z> = 5.8nN$, B type becomes unstable after the initial scan, which induces the transition from B type to AB type around the position indicated by an arrow on frictional loop [Fig.4(b-2)].

5.3 On Top stacking type

For OT type, it should be noted that the frictional loop shows the remarkable load dependence. For the lower load of $<F_z> = 0.41nN$, frictional loop exhibits typical sawtooth behavior [Fig.4(c-1)]. Here C\textsubscript{60} molecule mainly oscillates with occasional sliding. The lower and upper on-top atoms of C\textsubscript{60} take stick-slip motion within a certain six-membered ring of the lower graphite sheet, and across the nearest neighboring six-membered rings of the upper graphite sheet, respectively [Fig.4(c-3)]. 2→2’ and 3→3’ correspond to slip motions. However, for the higher load of $<F_z> = 5.7nN$, completely different frictional loop with the periodicity of 2.56( = 0.44×6) nm appears [Fig.4(c-4)]. Here C\textsubscript{60} molecule rolls along the scan direction, which significantly reduces the mean lateral force $<F_L>$ [27]. The trajectory of the contact point between the C\textsubscript{60} molecule and the graphite sheet indicates that C\textsubscript{60} molecule rolls by $\theta = 2\pi/3$ per one period of scan of 2.56nm, with discrete rotations indicated by arrows 1-4 [Fig.4(c-4)]. Another type of rolling mode also appears in the case of $2\times2$ unit cell for a little higher $<F_z>$ as illustrated in Fig.3.

5.4 Graphite/graphite/graphite interface

The frictional loop of graphite/graphite/graphite interface [Fig.4(d)] is qualitatively similar to that of AB type [Fig.4(a)]. Because both intercalated graphite sheet and C\textsubscript{60} molecule slide to conserve AB stacking registry with the upper and lower graphite sheets, respectively. Structural difference between graphite and AB type interfaces is the number of six-membered rings involved in the contact area, although C\textsubscript{60} oscillation also contributes to the difference. Here the number of six-membered rings closest to the upper graphite sheet within the unit cell of graphite/C\textsubscript{60}/graphite interface is 16 (32 carbon atoms) for graphite interface [Fig.2(d)]. On the other hand, it is only one (6 carbon atoms) for AB type interface [Fig.2(a)]. This difference induces difference of degree of freedom of motion discussed in chapter 6.
Figures 4(a), 4(b). Frictional force loops along [1010] direction (solid curve) and its opposite direction (dotted curve) for (a-1),(a-2) AB, and (b-1),(b-2) B types of graphite/C$_{60}$/graphite interface. All the cases correspond to the $1 \times 1$ unit cell. (a-3) and (b-3) indicate dynamics of upper six-membered ring (AB type) and upper and lower carbon bonds (B type) of intercalated C$_{60}$ molecule, corresponding to (a-2) and (b-1), respectively.
Figures 4(c), 4(d). Frictional force loops along [10\overline{1}0] direction (solid curve) and its opposite direction (dotted curve) for (c-1),(c-2) OT type of graphite/C\(_{60}\)/graphite interface and (d-1),(d-2) graphite/graphite/graphite interface. All the cases correspond to the 1\times1 unit cell. (c-3) and (c-4) indicate trajectories of on-top atoms of C\(_{60}\) molecule and contact point, respectively. Contact point is plotted on the plane onto which C\(_{60}\) carbon network is projected as a function of the rolling angle \(\theta\).

6. Mechanism of ultralow friction of graphite/C\(_{60}\)/graphite interface
Comparison of graphite interface with AB type interface gives us one of scenarios of atomic-scale ultralow friction as follows. The frictional loop of graphite interface for \(\langle F_z \rangle = 5.9\) nN [Fig.4(d-2)] is qualitatively similar to that of AB type interface for \(\langle F_z \rangle = 5.8\) nN [Fig.4(a-2)]. Both the frictional loops have periodicity of 0.44nm along [10\overline{1}0] direction of graphite lattice, and are comprised of sinusoidal part with little hysteresis and saw-tooth wave part with large hysteresis. However \(\langle F_L \rangle\) of AB type interface becomes smaller than that of graphite interface due to the following reasons:

In the case of graphite/graphite/graphite interface, internal graphite sheet has a degree of freedom of mainly two-dimensional translational motion, "sliding", within [0001] plane. On the other hand, in
the case of graphite/C$_{60}$/graphite interface, intercalated C$_{60}$ molecule has a degree of freedom of three-dimensional motion.

Fig.5 shows analysis of the process during 3→3'. Within a plane including [0001] axis, C$_{60}$ molecule slightly tilts along the scan direction of the upper graphite sheet at the position 3, and then slips to the neighboring stable position and small tilting vanishes at the position 3' [Fig.5]. Here "small tilting" reduces the energy barrier and opens the energy path to the neighboring minimum position as shown in the interaction energy map of C$_{60}$ molecule plotted as a function of center position of C$_{60}$ within (0001) plane[Fig.5]. Here, intercalated C$_{60}$ molecule slides to conserve AB stacking registry with the upper and lower graphite sheets within (0001) plane similar to internal graphite sheet [Fig.5]. Thus three dimensional degree of freedom of intercalated C$_{60}$ motion, "small tilting", is one of the origin of ultralow friction of graphite/C$_{60}$/graphite interface along $[0\ 1\ 1\ 0]$ direction. Another example of three-dimensional degree of freedom of C$_{60}$ motion is "rolling", for OT type for $<F_z> = 5.7\text{nN}$ as shown in Fig.4(c-2) [27].

![Figure 5. Analysis of effect of small tilting of C$_{60}$ molecule. Dynamics of intercalated C$_{60}$ molecule for AB type interface within a plane along [0001] axis (leftmost figure) and within (0001) plane (center figure). Interaction energy map of a C$_{60}$ molecule as a function of center position of C$_{60}$ within (0001) plane (rightmost figure).](image)

**7. Conclusion**
In this paper we present our molecular mechanics study of C$_{60}$ molecular bearing. It is clarified that the graphite/C$_{60}$/graphite interface exhibits much more excellent ultralow friction along $[10\bar{1}0]$ direction than the graphite/graphite/graphite interface. It is revealed that three dimensional degree of freedom of intercalated C$_{60}$ motions, ex. "small tilting" and "rolling motion", is one of origins of ultralow friction of the graphite/C$_{60}$/graphite interface along $[10\bar{1}0]$ direction. Although, in the present paper, the model including one C$_{60}$ molecule within $1\times1$ unit cell is used, detailed study using a model larger than $2\times2$ unit cell is required.

Now, based on the above present simulated results, we would like to discuss several important factors which play major roles in superlubricity.

**7.1 Ultralow friction force on the order of pN**
It should be noted that, since all the forces calculated in the present simulation are in the order of magnitude of less than several tens of pN, high resolution Atomic Force Microscopy technique[10,13] can accelerate works of ultralow friction or superlubricity in the future.
7.2 Temperature
Present results are obtained by the molecular-mechanics simulation with the scan along [10\bar{1}0] direction at T\rightarrow 0K. At finite temperature, there is possibility that sliding, oscillation, rolling and other modes would be coupled to induce remarkable progress of ultralow friction. Furthermore, since the maximum energy difference \Delta among each metastable structure is very small (ex. \Delta \approx 45\text{meV} for \text{d}=1.3\text{nm} [see inset of Fig.2(b)]), structural transition among AB, B and OT types can quite easily occur. It is also shown that the order-disorder phase transition occurs on the single C_{60} crystal surfaces around T \approx 260K, which might change C_{60} rotational dynamics and gives rise to an abrupt change in friction and adhesion [26]. Thus there is possibility that ultralow friction of graphite/C_{60}/graphite interface can be controlled by temperature, which is closely related to C_{60} dynamics and its structure.

7.3 Scan direction
Please note the scan along [10\bar{1}0] direction corresponds to the commensurate contact between the intercalated C_{60} molecules (or internal graphite sheet) and the upper and lower graphite sheets. However the scan direction other than [10\bar{1}0] direction induces incommensurate contact at the interface, which possibly leads to the remarkable change of the relation of ultralow friction between graphite/C_{60}/graphite and graphite/graphite/graphite interfaces. Since graphite/graphite interface exhibits a remarkable scan directional dependence[10], comparison of scan directional dependence between graphite/C_{60} and graphite/graphite interfaces is now being studied by our group.

7.4 Elasticity of C_{60} molecule
Effect of elasticity of C_{60} molecule appears especially for the larger loading condition. Deformation of C_{60} molecule induces larger contact area between graphite/C_{60} interface, which enhances superlubricity in some cases, and decreases in other cases. If graphite/C_{60}/graphite interface is regarded as series of effective lateral springs derived from graphite-C_{60} interaction and shear elasticity of C_{60}, we can grasp the essential picture of superlubricity of fullerene molecular bearing.

7.5 Effect of packing of C_{60} molecule
Numerical simulation by other group has shown that jamming of smooth rolling of C_{60} occurs in the close-packed structure[19]. Therefore it is quite important to explore the best packing condition to induce C_{60} bearing, which is now being investigated theoretically and experimentally by our group.

7.6 “C_{60} molecular bearing” can be realized?
In this paper we found unique superlubric dynamic modes of C_{60} molecule, “rolling motion” along [10\bar{1}0] direction for OT type (\text{z}=1.2\text{nm}) [27]. This result indicates that control of the scan direction leads to achieve quite excellent superlubricity. This C_{60} rolling motion is directly linked to the macroscopic concept of “bearing”. Other types of rolling motion have been also numerically obtained for other systems of C_{60} intercalated square lattice sheets [17]. However it has been experimentally reported that nanobearing-induced superlubricity is difficult to be observed in the system of C_{60} adsorbed on metal surfaces [28]. Thus the combination of the C_{60} and surrounded substrate species is quite important to induce C_{60}-bearing superlubricity.

Thus simulation on many kinds of effects mentioned above, which are closely interacted with each other, can give us clues to understanding atomic-scale ultralow friction of intercalated C_{60} graphite, leading to the understanding of macroscopic ultralow friction.

Acknowledgements
This research was supported by a Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science (No.17760030 and No.18340087), "Practical Application Research, Science and
Technology Incubation Program in Advanced Regions, "JST, "High-Tech Research Center" Project for Private Universities, and JGC-S Scholarship Foundation.

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