Mechanism of low friction of graphene in ambient air condition

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Molecular dynamics simulation is used to explain the low friction of graphite in ambient air condition. In the room temperature, thermal escape motion which explain the low friction is not found in a vacuum condition. Addition of water molecules in this system, the thermal escape motion is reproduced in the room temperature. The motion is reproduced in both hydrogen and hydroxyl termination system. This is due to the hydrophobic interaction which stabilize the transfer graphene layers.

Keywords: graphite, water, molecular dynamics, superlubricity

1. Introduction

The origin of low friction of graphite in practical use, such as pencil, is not explained yet. The concept of superlubricity in incommensurate surface (the ratio of the lattice constants of two solids is rational number) [1] can not be applied since the friction of graphite occur between graphite surface and a transfer layer, which should be faced in the commensurate state in equillibrium condition which shows large friction in principle [2]. Using a coarse-grained plate model of graphene, we found a specific mode of kinetic motion which escapes the potential barrier of two graphene sheets, and the motion is named thermal escape motion (Fig. 1, [3]). Although this theory is persuasive, an experimental evidence is still being waiting, which might be difficult. Then this motion is confirmed by all-atom molecular dynamics (MD) [4]. In the MD simulation, however, at room temperature, the thermal motion of graphene made instable structure and the thermal escape motion only reproduced in low temperature of 100 K. In this paper we take into account of the effect of water molecules, which exists in ambient air condition.

2. Methods

Reactive force field is used to simulate the polarization in the graphene sheet with surrounding atmosphere correctly. Two type of functional groups in prepared for graphene sheets. The sliding is adopted by moving the topmost graphene layer (Fig. 2a, 2b).

3. Results and Discussion

At the hydrogen termination case and in vacuum and in low temperature of 50 K, the thermal escape motion which is found in previous studies [3, 4] is reproduced (Fig. 2c). In the hydroxyl group termination system in vacuum, the thermal escape motion is inhibited by the interaction between functional groups. On the other hand, the thermal escape motion is reproduced by surrounding these inhibited systems with water molecules in a room temperature. Thus, it is found for the first time that the low friction of graphite is greatly affected by the surrounding water molecules in both hydrogen termination and hydroxyl termination case. This is due to the hydrophobic interaction which stabilize the edge of transfer graphene.

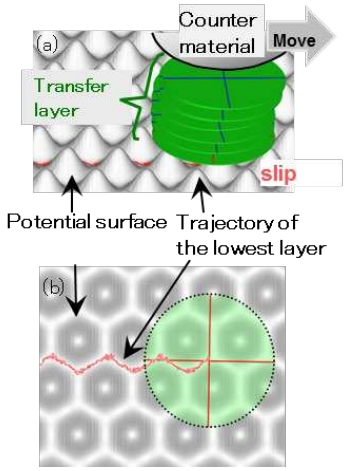

Figure 1: Thermal escape motion which is found by coarse-grained molecular simulation [3].

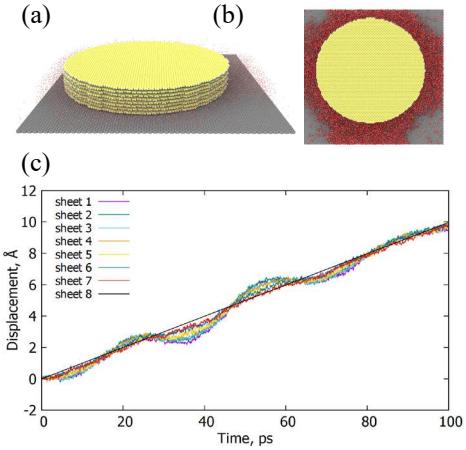

Figure 2: Snapshot of the MD simulation (a, b) and displacement of graphene sheets.

4. References

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