第76回応用物理学会秋季学術講演会 講演予稿集 (2015 名古屋国際会議場)

Molecular Dynamics Simulation on Penetration of Fullerene in Thin-Film Ionic Liquid-Assisted Vacuum Deposition Process

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Thin-film (TF) ionic liquid (IL)-assisted vacuum deposition is a promising technique to produce higher quality crystal of fullerene (C_{60}) [1]. In the TF-IL vacuum deposition, C_{60} bombards the surface of the IL, diffuses into the IL, and nucleates on a substrate. To clarify the crystallization of C_{60} in the IL, it is important to understand the penetration of C_{60} into the IL. Thus, the purpose of this study is to clarify the penetration process of C_{60} into a TF-IL by using coarse-grained (CG) molecular dynamics simulation.

All simulations were performed at 400 K under the NVT ensemble with a 2 fs time step and a relaxation time of 400 ps. 1-butyl-3methylimidazolium tetrafluoroborate ([Bmim][BF_4]) IL was used, where $[Bmim]^+$ is the cation and $[BF_4]^-$ is the anion. Graphite was used as the substrate. Detail of the CG models are shown in Fig. 1. All of parameters were taken from Refs. [2] and [3]. At the first step, we simulated the penetration of C_{60} into 3 and 4 nm TF-IL as shown in Fig. 2. One C_{60} is bombarded every 20 ps with a kinetic energy of 7.5 eV. The penetration depths of C_{60} in 3 and 4 nm TF-IL are 1.5 and 2.4 nm, respectively. In addition, C_{60} is effectively stopped at 1.5 and 1.6 nm above the substrate in 3 and 4 nm TF-IL, respectively. Thus, the penetration of C_{60} is limited in a region around 1.5 nm above the substrate. To reveal the reason of the limited penetration in that region, we analyzed the structure of 3 nm TF-IL before the bombardment. We observed a layered structure as shown in Fig. 3a which was suggested by the experiment [4]. Fig. 3b shows the distribution of anion along z direction in 3 nm TF-IL. The layered structure is formed approximately from 0.2 until 2.2 nm above the substrate. We suggest that the penetration of C_{60} is limited when it reaches the layered structure. Finally, we successfully simulate the penetration of C_{60} into a TF-IL and find that the penetration of C_{60} is limited by the layered structure.

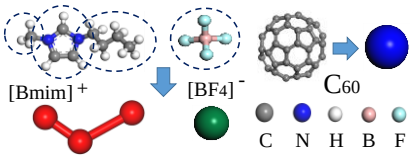

Fig. 1 Coarse-grained models.

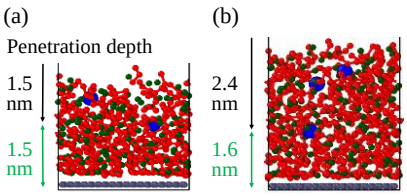

Fig. 2 Penetration of C_{60} in (a) 3 nm and (b) 4 nm TF-IL.

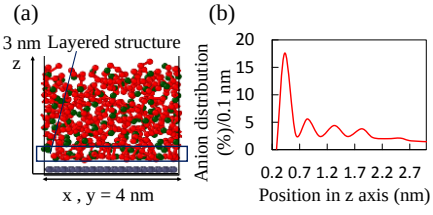

Fig. 3 (a) Layered structure in 3 nm TF-IL and (b) distribution of anion along z direction in 3 nm TF-IL.

[References]

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