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Molecular Dynamics Simulation of Thin Film Growth of Organic Semiconductors

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Abstract

Molecular dynamics simulations of thin film growth of organic semiconductors are presented. This study is intended to examine the concepts experimentally proposed by various researchers.

1. Introduction

Thin film growth of organic semiconductor molecules is critically important to fabricate high performance organic devices. Variety of techniques are now applied for the organic thin film growth including physical vapor deposition, inkjet printing and solvent vapor annealing. The atomic / molecular scale mechanisms involved in the crystal growth in these techniques have not been elucidated in detail. The factors involving the crystal growth are the van der Waals interaction between the molecules and molecules and the substrate surface, and additionally hydrogen bonding and bond rotation or twisting in some cases. Various parameters such as temperature, molecular supply flux (in the case of physical vapor deposition), solvent vapor pressure (in the case of ink jet printing and solvent vapor annealing) are very important. In order to resolve various factors involved, computer simulation is very helpful. Owing to the development of fast computers and algorisms, it is now feasible to simulate the crystal growth by molecular dynamics with classical force field.

2. Methods

In this work, molecular dynamics simulation packages Gromacs and Tinker were used with several established force field parameters. Some parameters were adjusted by using the information obtained by quantum chemical calculations.

3. Results and Discussions

We will present some of our recent results on the simulation of crystal growth, which are intended to answer the questions posed from experiments as shown in Table 1.

References

[1] A. Hoshimo, S. Isoda, H. Kurata, T. Kobayashi, J. Appl. Phys. 76, 4113-4119 (1994).

[2] H.Tada, K. Saiki, A. Koma, Jpn. J. Appl. Phys. 30 L306-L308 (1991).

[3] K. Itaka, M. Yamashiro, J. Yamaguchi, M. Haemori, S. Yaginuma, Y. Matsumoto, M. Kondo, H. Koinuma, Adv. Mater. 18, 1713- 1718(2005).

[4] S. Ikeda, K. Saiki, T. Tsutsui, Y. Edura, H. Wada, K. Miyazoe, K. Terashima, T. Inaba, T. Mitsunaga, T. Shimada, Appl. Phys. Lett. 88, 251905 (2006).

[5] T. Shimada, A. Suzuki, A. Sakurada, A. Koma, Appl. Phys. Lett. 68, 2502-2504 (1996).

[6] M. Ohtomo, Y. Tsuchida, N. Muraya, T. Yanase, S. Sakai, T. Yonezawa, T. Nagahama, T. Hasegawa, T. Shimada, J. Phys. Chem. C 117,11555 (2013).

[7] J.C. Wittmann and P. Smith, Nature 352, 414-417 (1991).

[8] M. Misaki, Y. Ueda, S. Nagamatsu, Y. Yoshida, N. Tanigaki, K. Yase, Macromolecules 37, 6926-6931 (2004).

[9] A. Kubono, Mol. Cryst. Liq. Cryst. 378, 145-161 (2002).

[10] T. Shimada, K.A.Cho, A. Koma, Phys. Rev. B 63, 153404 (2001).

[11] T.Shimada, H. Taira, A. Koma, Chem. Phys. Lett. 291,419-424 (1998).

[12] A. Suzuki, T. Shimada, A. Koma, Jpn. J. Appl. Phys. 35, L254-L256 (1996).

[13] A. L. Briseno , S. C. B. Mannsfeld , M. M. Ling , S. Liu , R. J. Tseng , C. Reese , M. E. Roberts , Y. Yang , F. Wudl, Z. Bao, Nature 444, 913-917 (2006).

[14] S. Lucas, G. Witte, C. Woll, Phys. Rev. Lett. 88, 028301 (2002).

[15] T. Shimada, Thin Solid Films 515, 1568 (2006).

concept	problem	ref.
epitaxy and crystal orientation	accurate prediction	1
polymorphism	accurate prediction	2,3
graphoepitaxy	effect of surface modification	4
surface steps	roles in thin film growth	5,6
polymer friction transfer substrate	mechanism of "epitaxy"	7,8
nucleation	kinetic control	9,10
epitaxy and lattice pressure	critical thickness	11
selective epitaxy	accurate prediction and control	12,13
electronic interaction	accurate prediction	14
solvent vaper annealing	mechanism and control	15

Table 1: Concept and problems to be solved in crystal growth of organic thin films