

Abstract Submitted
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Possible explanation of polymer surface diffusion anomaly DE-BASHISH MUKHERJI, Department of Physics and Astronomy, The University of Western Ontario, London, Ontario N6A 3K7, Canada, MARTIN H. MUSER, Department of Applied Mathematics, The University of Western Ontario, London, Ontario N6A 5B7, Canada — Surface diffusion of polymer is studied with molecular dynamics simulation. Our simulation result shows the non-monotonic behavior of the polymer surface-diffusion coefficient D as a function of surface coverage. D first increased with increasing polymer surface concentration, then suddenly drops at a critical value. This finding shows striking similarities with the experimental result [1]. We found that the strong reduction of D above the threshold concentration is related to the spontaneous formation of double-layered structures, whose bottom layers manage to lock into the registry of the substrate much better than the single-layer pancakes that form at smaller concentration. This increases the barriers for lateral diffusion and is thus consistent with small values of D at larger concentration.

[1] J. Zhao and S. Granick, *J. Am. Chem. Soc.* 126, 6242 (2004).

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