Serial Pushing Model for the Self-Assembly in Dip-Pen Nanolithography

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Based on molecular dynamics simulations, we propose a diffusion model for the selfassembly in dip-pen nanolithography. A central question in such modeling is how a nascent droplet created below an AFM tip spreads out to form a self-assembled monolayer (SAM) on a substrate later. In the present model, a molecule dropping from the tip pushes a molecule on the substrate out of its original position, and the molecule pushed out in turn pushes its own neighbor. A SAM grows through such a series of push-induced movements. The initial pushing propagates all the way to the periphery where there is no molecule to push out. By implementing our model in random walk simulations, we study the structure and growth dynamics of the SAM generated by a fixed tip and the lines and characters created by a moving tip. We investigate how the SAM is influenced by the molecular dripping rate and tip scan speed. A salient feature of our model is its ability to generate various SAMs by changing the directional coherence length of the push-induced displacement. If we choose the coherence length to be zero, each push-induced displacement is random in direction to give a compact circular SAM. As the directional coherence length increases, the SAM becomes a noncircular pattern with distinct branches. In the limit of an infinite coherence length, the SAM becomes a long narrow cross due to the substrate anisotropy.