

Abstract Submitted  
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**Migration of a Model Lamellipodium by Actin Polymerization:  
A Molecular Dynamics Simulation Approach** JUNHWAN JEON, Department of Chemical Engineering, Vanderbilt University, Nashville, Tennessee 37235, PETER CUMMINGS, Nanomaterials Theory Institute, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 — We performed molecular dynamics simulation of a model lamellipodium with growing F-actin filaments in order to study the effect of stiffness of the F-actin filament, the G-actin monomer concentration, and the number of polymerization sites on lamellipodium motion. The lamellipodium is modeled as a two-end capped cylinder formed by triangulated particles on its surface. It is assumed that F-actin filaments are firmly attached to a lamellipodium surface where polymerization sites are located and actin polymerization takes place by connecting a G-actin monomer to a polymerization site and the first monomer of a growing F-actin filament. It is found that there is an optimal number of polymerization sites for rapid lamellipodium motion. This appearance of the maximum speed is related to the competition between the number of polymerization sites and the number of available G-actin monomers, and the degree of pulling and holding the lamellipodium surface by non-polymerized actin filaments. The model lamellipodium speed distribution is found to be Maxwellian for particles with random motion in two dimensions and is in agreement with experiment.

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