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Modeling Vapor Deposition Polymerization: Kinetic Monte Carlo Approach SAIRAM TANGIRALA, YIPING ZHAO, DAVID P. LANDAU, The University of Georgia, USA — A Kinetic Monte Carlo method is employed to model vapor deposition of growing, linear-polymer thin films which have applications ranging from microelectronic interconnects to biotechnology. Our 1+1 dimensional lattice model [1] implements various dynamical processes that occur during the film-growth, including random-angle deposition, monomer adsorption, free-monomer diffusion, and polymer-end flips. The temperature (T) is parametrized using the diffusion coefficient ($D = \exp(-\Delta E_a/k_B T)$), where ΔE_a is the activation energy for surface diffusion. The diffusion coefficient (D) and the deposition rate (F) play an important role in the growth process through the ratio G ($= D/F$). We study the polymer chain length distribution, average polymer-chain length, film density, film height, surface-width, and radius of gyration as a function of G, system size (L), and time. Since polymers have much more complicated structures and interactions than those of organic materials, we find novel behaviors that are different from inorganic thin film growth. [1] W. Bowie and Y.-P. Zhao, *Surf. Sci. Lett.* **563**, L245 (2004).

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