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Roughness in a kinetic film growth of hydrophobic and polar components in aqueous solution - spectroscopic studies and Monte Carlo simulations OTTS DANIEL, LUIS CUEVA-PARRA, RAS PANDEY, MAREK URBAN, University of Southern Mississippi — Using Monte Carlo simulations, we investigate the film formation from mobile constituents of multi-component mixtures in order to understand the spectroscopic measurements of polyurethane thin film. The mixture consists of water (A), hydrophobic (H) and polar groups represented by particles of appropriate molecular weight and interactions on a discrete lattice. The empty sites of the host lattice matrix are used to describe effective medium for the mobile constituents. Metropolis algorithm is used to move particles. Periodic boundary condition is used along transverse directions with open top for water evaporation and impenetrable adsorbing substrate at the bottom. Stable film morphology emerges as system precipitate, equilibrate, evaporate, and covalent bonds form from the kinetic reactions. Density profile and roughness of the film are examined in detail as a function of temperature and water concentration. Increase in roughness due to phase partitioning on increasing the water concentration is found to be consistent with the experimental observations.

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