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Film Formation with Reactive Hydrophobic and Polar Groups in Aqueous Solution: A Bond-Fluctuating Computer Simulation Model[1]
SHIHAI YANG, SAMUEL BATEMAN, RAS PANDEY, MAREK URBAN, University of Southern Mississippi — We study film formation with reactive hydrophobic (H) and polar (P) components in evaporating aqueous (A) solution by Monte Carlo simulation to model the polyurethane film growth. Each component is represented by mobile particles with appropriate molecular weight, interaction, and reaction functionality on a simple three-dimensional lattice $L_x \times L_y \times L_z$ with an adsorbing substrate. H and P react by forming fluctuating covalent bonds proceeding from the substrate with probability P_B. Bonds may also be formed between H and A when A is considered reactive. Growth of the film thickness (h) and surface roughness (W) are studied at a range of temperature (T). With non-reactive A, the saturated film thickness (h_s) and roughness (W_s) decay first before increasing linearly on raising the temperature. With reactive A, a fast increase of h_s at low temperature is followed by a slow increase at high temperature. W_s also shows non-monotonic dependence on temperature.

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Ras Pandey
University of Southern Mississippi

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