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Polymer Thin Films and Interfaces; a Layer-by-Layer Approach[1]
RONALD WHITE, JANE LIPSON, Dartmouth College — In this talk we discuss new ways to model polymer films and interfaces, including properties such as density and concentration gradients, interfacial tension, and surface enrichment. We build on recent work where we developed a very simple equation of state approach for polymer thin films, and successfully applied it to determine thermodynamic properties and even to make predictions for the thickness-dependent depression of the thin film glass transition temperature. In that very simplified mean field model, the film properties across the entire interface region were treated as a "whole sample" average. Here, we take the next step, and develop a layer-by-layer equation of state model wherein details of the interface region are captured by allowing properties to vary from one discretized layer (within which properties are uniform) to the next. The model can be solved by imposing hydrostatic equilibrium in each layer, which then leads to predictions for the corresponding density gradient and other key interface properties.

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