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Application of a Semi-Grand Canonical Monte Carlo (SGMC) Method for the Simulation of Non-Equilibrium Systems FREDERICK BERNARDIN, GREGORY RUTLEDGE, Massachusetts Institute of Technology — The use of the SGMC as a generalized descriptive tool for interpreting experimental data obtained from non-equilibrium systems will be summarized. The usefulness of the method will be demonstrated specifically by interpreting the orientation distribution functions (odf's) of polymer melts which have been uniaxially oriented. Using SGMC, we identify the thermodynamic variables that serve as chemical potentials in a polydisperse system of orientations, and then generate the ensemble of configurations that minimizes the free energy subject to the constraints set by the odf. In this demonstration, the axial symmetry leads to the use of Legendre polynomials as the basis set for the odf. We apply our approach to obtain molecular ensembles corresponding to different values of P_2 (the first non-zero Legendre term), which are obtainable through measurements by light scattering or birefringence. Comparisons will be made to a related method by Mavrantzas and Theodorou (Macromolecules, 31, 6310 1998).

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