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Single chain structure in thin polymer films: corrections to Flory's and Silverberg's hypotheses A. CAVALLO, Institut für Physik, Universität Mainz, Germany, M. MÜLLER, Department of Physics, University of Wisconsin-Madison, USA, J.P. WITTMER, Institut Charles Sadron, Strasbourg, France, K. BINDER, Institut für Physik, Universität Mainz, Germany — Conformational properties of polymer melts confined between two hard structureless walls are investigated by the bond-fluctuation model. Chain extension, bond-bond correlation function and structure factor are computed and compared with recent theoretical approaches attempting to go beyond the Flory's and Silverberg's hypotheses. We demonstrate that for ultrathin films the chain size parallel to the walls diverges logarithmically, $R^2/2N \approx b^2 + d \log N$ with $c \sim 1/H$. The corresponding bond-bond correlation function decreases like a power law $C(s) = d/s^\omega$, being s the curvilinear distance between bonds and $\omega = 1$. Upon increasing H we find—at variance with Flory—the bulk exponent $\omega = 3/2$ and, more importantly, a strongly decreasing amplitude $d(H)$ that gives direct evidence of an *enhanced* self-interaction of chain segments reflected at the walls. Systematic deviations from the Kratky plateau as a function of H are found for the single chain form factor parallel to the walls in agreement with the *non-monotoneous* behavior predicted by theory. For large H the deviations are linear with the wave vector q but very weak. In contrast, for thin films, very strong corrections are found (albeit logarithmic in q) suggesting a possible experimental verification of our results.

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