Monte Carlo simulation of block copolymer brushes of different architecture

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A model of a film formed by grafted polymer chains was used for theoretical considerations. The linear and star-branched block heteropolymer chains were constructed on a cubic lattice. The chains were attached to an impenetrable flat surface with one arms end. The fragment of a chain attached to the surface was built of segments different from those in the remaining part. The grafted fragment of a chain was athermal while the upper one was interacting with the solvent. The computer simulations of the system were performed by means of a Monte Carlo Metropolis sampling algorithm basing on the micromodifications of local conformation. The size of the brush components and the structure of the polymer film were investigated and discussed for different chain lengths and for good and bad solvent conditions. The structure of a polymer film formed on the grafting surfaces depended strongly on the temperature and the low temperature films consisted of two separate layers showing a structure different from that formed by the interacting part of chains. It was shown that the dimensions of the chains in the brush scale in two regimes depending on the chain length. The differences in scaling exponent are caused by the crowding effect of the upper part of the brush. It was also found that the total thickness of the brush film scales linearly with the chain length.

[1] P. Romiszowski, and A. Sikorski, Int.J.Polym.Anal.Ch. **12**, 57 (2007).
[2] P. Romiszowski, and A. Sikorski, J.Non-Cryst.Solids **353**, 4591 (2007).