Quantifying the Curvature of Polymer Brushes

LUCIANO COSTA[1], CARLOS RODRIGUES[1], SERGEI SHEIKO[2]

[1]IFSC – Universidade de São Paulo, Caixa Postal 369, 13560-970, São Carlos, SP, Brasil.
{luciano,carod}@if.sc.usp.br
[2]UNC – University of North Carolina, 27599-3290, Chapel Hill, NC, USA
sergei@email.unc.edu

Abstract. This work describes a method to evaluate the curvature of backbone of polymer molecules. The algorithm for curvature is based in derivative theorem of Fourier Transform suitable for treating contours.

1. Introduction

Cylindrical brush molecules are polymer molecules that consist of a long flexible main chain (backbone) and densely grafted side chains [1]. The interest in such molecules is due to conformational effects caused by competition of the flexibility of the backbone and the flexibility of the covalently linked side chains. Here we present a study of backbone curvature of cylindrical brushes with different length of the side chains after a process of compression and expansion.

2. Experimental part

Two images of brushes with different length of the side chain are presented in figure 1. AFM images were collected in tapping mode. The curvatures of molecules were obtained by software SPIA (Scanning Probe Image Analysis) that was developed for analysis of digital images.

First, the images were segmented by using threshold methods and the resulting contours of the molecules were extracted through a contour following algorithm. The backbones were obtained through the skeletization of these contours, and were filtered in order to eliminate those cases that had more than two branches. The backbones were dilated and the contour extracted again. The curvature algorithm described in [2] was applied to the obtained contours, and one of their sides was chosen to represent the curvature of backbone. The histogram of curvature was fitted by a Gaussian, whose width was related to the conformation of the molecules.

3. Discussion

Table 1 shows the width of Gaussian distribution obtained for curvature before and after the compression.

We see that the curvature decreases with the side chain length. This is explained by steric repulsion of the side chains at the concave side of the backbone.

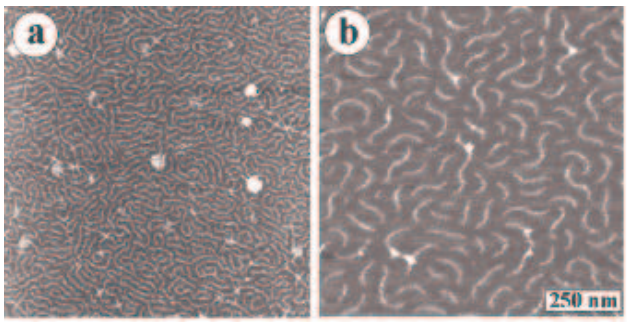

Figure 1. AFM images of PBA brushes with two lengths of side chains: (a) DP=9, (b) DP=51.

Table 1. Gaussian width.

DP[a)]	BC[b)]	AC[c)]
09	0,05	0,08
51	0,02	0,06

[a)] Degree of polymerization; [b)] Before compression.
[c)] After compression.

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3. References

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