

Conformational properties of polymers near a fractal surface

Viktoria Blavatska^a, Wolfhard Janke^b

^a*Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine*

^b*Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany*

Abstract

The conformational properties of flexible polymer macromolecules grafted to an attractive partially penetrable surface with fractal dimension $d_s^{pc} = 91/49$ are studied. Employing computer simulations based on the pruned-enriched Rosenbluth chain-growth method, estimates for the surface crossover exponent and adsorption transition temperature are found. Our results quantitatively reveal the slowing down of the adsorption process caused by the fractal self-similar structure of the underlying substrate.

Keywords: polymer, adsorption, percolation cluster, chain-growth algorithm, surface crossover exponent

1. Introduction

The study of polymers near disordered surfaces is of great importance, since most naturally occurring substrates are rough and energetically (or structurally) inhomogeneous. Surface heterogeneity has a crucial effect on polymer adsorption phenomena [1, 2, 3, 4, 5]. Since most chemical substrates are proved to be of fractal nature [6], studying the influence of a non-trivial surface geometry on polymer adsorption is of particular interest. It is established [7] that the adsorption process is enhanced (diminished) when the fractal dimension of the substrate is larger (smaller) than that of a plain Euclidean surface. A number of studies has been dedicated to polymer adsorption on a family of finitely ramified fractals [8, 9, 10]. Also of great importance is the study of polymers in the vicinity of fluctuating surfaces, such as membranes [11].

Energetical inhomogeneity arises due to the presence of various chemical compounds in the substrate, interacting with the monomers of the polymer chain in a different manner. In the language of lattice models, such surfaces can be modeled as a two-dimensional regular lattice with different types of randomly distributed sites, e.g., one type with attractive interactions with the monomers and the other one being neutral (treated as defects or impurities). In this concern, it is worthwhile to study the situation when the concentration of attractive sites on the surface is exactly at the percolation threshold and a spanning percolation cluster of attractive sites appears [12]. A percolation cluster is a fractal object with fractal dimension $d_s^{pc} = 91/49 \approx 1.89$ [13]. The neutral sites of the surface (which do not belong to the percolation cluster) could be considered as penetrable for the polymer chain, so the polymer is adsorbed on an attractive fractal with fractal dimension d_s^{pc} . This can thus model the process of polymer adsorption on an attractive, partially penetrable membrane, which could be of interest in biophysical applications.

In the present paper, we report a careful computer simulation study of polymer adsorption on a fractal substrate formed by a percolation cluster on a two-dimensional square lattice.

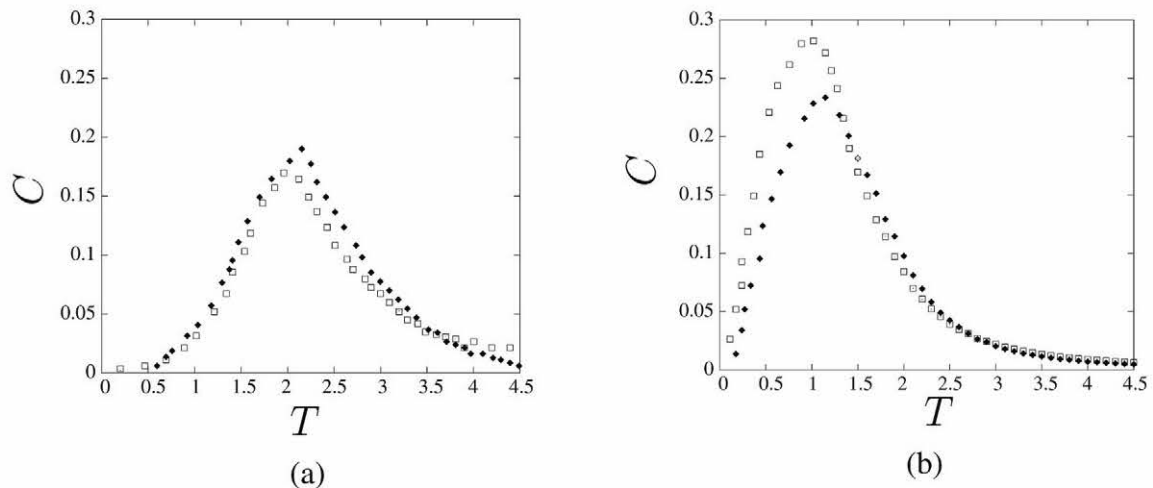


Figure 2: Specific heat per monomer as a function of temperature for a polymer chain near (a) a homogeneously attractive surface and (b) an attractive percolation cluster as a function of temperature. Squares: $N = 40$, filled diamonds: $N = 100$.

of polymer chains in three dimensions grafted with one end to the percolation cluster are studied with the pruned-enriched Rosenbluth method (PERM). Examining the peak structure of the heat capacity, we find an estimate for the surface crossover exponent, governing the scaling of the adsorption energy in the vicinity of the transition point, $\phi_s^{p_c} = 0.425 \pm 0.009$, and for the adsorption transition temperature we obtain $T_A^{p_c} = 2.64 \pm 0.02$. As expected, the adsorption is diminished, when the fractal dimension of the surface is smaller than that of the plain Euclidean surface due to the smaller number of contacts of monomers with attractive sites.

Acknowledgments

We thank Niklas Fricke for useful discussions. Work supported by Sächsische DFG Forschergruppe FOR877 under Grant No. JA 483/29-1, DFG Sonderforschungsbereich SFB/TRR 102 (Project B04), and Graduate School of Excellence GSC 185 “BuildMoNa”. V.B. is grateful for hospitality of the Sächsische DFG Forschergruppe FOR877 during an extended research stay in Leipzig.

References

- [1] M. Kawaguchi and T. Arai, *Macromolecules* 24 (1991) 889.
- [2] G. Huber and T.A. Vilgis, *Eur. Phys. J. B* 3 (1998) 217.
- [3] K. Sumithra and A. Baumgaertner, *J. Chem. Phys.* 109 (1998) 1540.
- [4] M.S. Moghaddam and S.G. Whittington, *J. Phys. A* 35 (2002) 33; M.S. Moghaddam, *J. Phys. A* 36 (2003) 939.
- [5] J. Zierbarth, Y. Wang, A. Polotsky, and M. Luo, *Macromolecules* 40 (2007) 3498.
- [6] D. Avnir, D. Farin, and P. Pfeifer, *Nature* 308 (1984) 261; *J. Chem. Phys.* 79 (1983) 3566.
- [7] E. Bouchaud and J. Vannimenus, *J. Physique (France)* 50 (1989) 2931.
- [8] S. Elesović-Hadžić, I. Živić, and S. Milošević, *J. Phys. A* 36 (2003) 1213.
- [9] V. Bujanja, M. Knežević, and J. Vannimenus, *J. Stat. Phys.* 71 (1993) 7.
- [10] S. Kumar, Y. Singh, and D. Dhar, *J. Phys. A* 26 (1993) 4835.
- [11] T. Auth and G. Gompper, *Phys. Rev. E* 68 (2003) 051801; *Phys. Rev. E* 72 (2005) 031904; S. Karalus, W. Janke, and M. Bachmann, *Phys. Rev. E* 84 (2011) 031803.
- [12] D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor and Francis, London, 1992).
- [13] S. Havlin and D. Ben Abraham, *Adv. Phys.* 36 (1987) 155.
- [14] J. Hoshen and R. Kopelman, *Phys. Rev. B* 14 (1976) 3438.
- [15] P. Grassberger, *Phys. Rev. E* 56 (1997) 3682.
- [16] E. Eisenriegler, K. Kremer, and K. Binder, *J. Chem. Phys.* 77 (1982) 6296.
- [17] P. Grassberger, *J. Phys. A* 38 (2005) 323.