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Bottle-Brush Polymer Adsorption Onto Mica and Silica Surfaces. Comparison Between Experimental and Modeling Results

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Abstract: **The adsorption of a series of charged bottle-brush polymers with side chains of constant length on mica and silica surfaces is modeled using a lattice mean-field theory, and the predicted results are compared to corresponding experimental data. The bottle-brush polymers are modeled as being composed of two types of main-chain segments: charged segments and uncharged segments with an attached side chain. The composition variable *X* denotes the percentage of charged main-chain segments and ranges from *X* = 0 (uncharged bottle-brush polymer) to *X* = 100 (linear polyelectrolyte). The mica-like surface possesses a constant negative surface charge density and no non-electrostatic affinity for either the main chain or the side-chain, whereas the silica-like surface has a constant negative surface potential and a non-electrostatic affinity for the side chains of the bottle-brush polymers. The model is able to reproduce a number of experimental features characterizing the adsorption of the bottle-brush polymers for the full range of the composition variable *X* on the two surfaces, and thereby quantifying how the different nature of the two surfaces with respect to electrostatic properties and non-electrostatic affinity for the polymer affect the adsorption properties and the structure of the adsorbed layers. In particular, the surface excess displays a maximum at *X* ≈ 50 for the mica surface and at *X* ≈ 10 for the silica surface. Moreover, the thickest adsorbed layer is obtained at *X* = 10 - 25.**

Keywords: **Lattice mean-field model, bottle-brush polymer, comb polymer, mica, silica, adsorption, surface excess, density profile, non-electrostatic affinity**

I INTRODUCTION

Bottle-brush polymers that consist of a linear backbone carrying a large number of covalently attached side chains have received great interest in recent years.[1,2] A large adsorption of such polymers with hydrophilic non-ionic side chains has in several cases lead to formation of surface layers with low non-specific protein adsorption.[3-6] Such layers may also generate strongly repulsive steric interactions that provide excellent colloidal stability,[7,8] and favorable lubrication properties,[9,10] with friction coefficients as low as achievable with efficient biochemical lubricants such as mucin.[11] A prerequisite for the successful use of physisorbed bottle-brush polymer layers in applications is a good understanding of their adsorption properties and how these are affected by the nature of the surface, the polymer architecture, solution composition, and interference by surfactants and other polymers present in solution. All these aspects have been investigated experimentally[7,10,12-17] using bottle-brush polymers synthesized from poly(ethylene oxide) methyl ethyl methacrylate (PEO_{45}MEMA) and methacryloxyethlyl trimethylammonimum chlorid (METAC). The former monomer contains a 45 unit long oligo(ethylene oxide) chain and the latter a permanently charged cationic group. These polymers are referred to as PEO_{45}MEMA:METAC-X, where *X* stands for the mol% of charged segments.

The adsorption of PEO_{45}MEMA:METAC-X polymers to silica surfaces is very sensitive to changes in pH and ionic strength, and this has been suggested to be primarily due to variations in the non-electrostatic affinity between the PEO_{45} side chains and silica.[15-17] On the other hand, the adsorption to negatively charged mica surfaces has been suggested to be driven by only electrostatic interactions.[10]

As will be discussed below, there are large differences in the adsorption properties of PEO_{45}MEMA:METAC-X polymers on mica and silica. In this report we provide some further insight into the driving forces for adsorption of this type of bottle-brush polyelectrolytes onto mica-like and silica-like surfaces, and further details can be found in the article by Linse and Claesson.[18] In particular, the following aspects are illustrated: (i) the effects of polymer segment sequence, (ii) the influence of non-electrostatic interactions, and (iii) the role of surface charge density. The model approach utilizes a self-consistent lattice mean-field theory to describe the adsorbed polymer layer, which provides detailed information on surface excess and adsorbed layer structure. It facilitates a systematic variation of important parameters such as segment sequence, non-specific surface affinity, and surface charge density that is not easily varied in experiments. Thus, we are able to draw important conclusions on how these properties affect adsorption and polymer layer structure, and we are also able to suggest polymer structures with potentially useful properties.

II THEORETICAL MODEL

The adsorption of bottle-brush polymers onto planar and negatively charged surfaces was modeled on the basis of a self-consistent-field theory, initially developed by Scheutjens and Fleer[19,20] and later extended to polyelectrolytes [see e.g. [21] and references given therein] and branched polymers.[22] The extensions of electrostatic interactions and of branched polymers enter essentially independently into the theory, and hence bring no additional considerations.

Briefly, the space adjacent to a planar surface is divided into layers, and each layer is further divided into lattice cells of equal size. Within each layer the Bragg-Williams approximation of random mixing is applied, and thus all sites in a layer are equivalent. One lattice cell contains either (i) solvent, (ii) a polymer segment, (iii) a solvated cation, or (iv) a solvated anion.

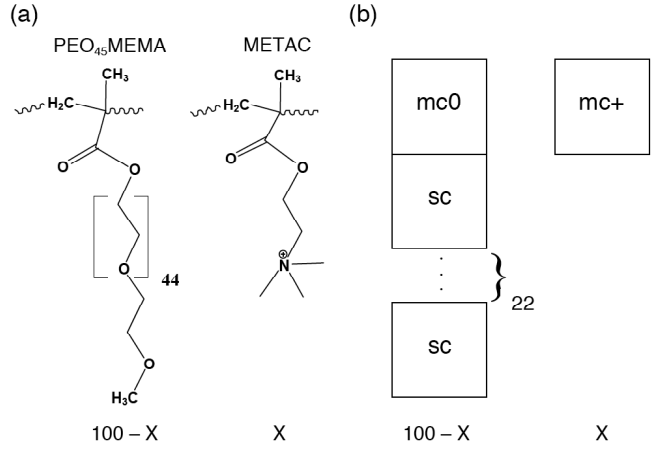

Fig. 1. a) The chemical structure of the segments in PEO_{45}MEMA:METAC-X, and b) the model of these polymers used in the lattice mean-field self-consistent field calculations

In our calculations, the polymer is composed of a main chain consisting of 200 segments of which the percentage X is positively charged and the remaining percentage $(100 - X)$ is uncharged *and* having a side chain with 22 segments. In more detail, Figure 1a shows the structure of PEO_{45}MEMA and METAC used to synthesis the PEO_{45}MEMA:METAC-X bottle-brush polymer. In our coarse-graining, Figure 1b, we represented (EO)MEMA with one uncharged segment, METAC with one charge segment, and $(EO)_2$ with one uncharged segment; hence, each chemical unit being of similar volume. The polymer is considered to be flexible, and the ordering of charged and uncharged segments of the main chain is random if nothing else is specified. When having a random sequence, for a given X the same random sequence is used, independent of other parameters. Polymers with the composition X = 0, 5, 10, 25, 50, 90, 95, and 100 are considered. The surface is modeled as having either a fixed surface charge density σ or a fixed surface potential ψ_s.

There are two different types of interactions in the model: electrostatic (charge-charge) and non-electrostatic (the rest). The non-electrostatic interaction between species in adjacent lattice sites is described by Flory-Huggins χ-parameters.[23] The same description is used for the interaction with the surface. Since only the differences of the interaction parameters involving a surface are relevant, we introduce $\Delta\chi_\alpha = \chi_{\alpha,\text{surface}} - \chi_{\text{solvent,surface}}$, α being a main-chain or a side-chain segment. The relation to the adsorption parameter χ_S is given, e.g., for the polymer by $\chi_S = -\lambda_{1,0}\Delta\chi_{\text{polymer}}$, $\lambda_{1,0}$ being the fraction of all neighbors of a site in layer 1, which resides in the surface layer. Here, $\lambda_{1,0} = 1/4$, since a hexagonal lattice was selected.

In line with the random mixing approximation, charged species (charged polymer segments and salt species) are assumed to interact with a potential of mean force, ψ_i, which depends only on the distance to the surface (layer number i). The potential of mean force is related to the charge density through Poisson's equation, $-\varepsilon_0\varepsilon_r\nabla^2\psi_i = \rho_i$, where $\varepsilon_0\varepsilon_r$ is the dielectric permittivity of the medium and ρ_i is the total charge density in layer i. The charges of the species are located to planes in the middle of each lattice layer, and the space in between the charged planes is free of charge. A uniform dielectric permittivity is used.

From the set of volume fraction profiles of the species, $\{\phi_{Ai}\}$, and the interaction parameters, a non-electrostatic potential u_{Ai} can be but species independent hard-core potential, u'_i, acting calculated for species A in layer i. There is also a layer dependent on each species. This potential is essentially the lateral pressure and is responsible for making the volume fraction in each layer sum up to one. Given the non-electrostatic potential u_{Ai} and the electrostatic energy $q_A\psi_i$ of species A in layer i as well as the hard core potential u'_i of layer i, the distribution of *unconnected* segments of type A is given by the Boltzmann weight of the sum of the three terms, $\phi_{Ai} \sim \exp[-(u_{Ai} + u'_i + q_A\psi_i)/kT]$. For polymers, the matter becomes more complex since the connectivity has to be taken into account. Finally, since $\{\phi_{Ai}\}$ depends on $\{u_{Ai}\}$ and $\{\psi_i\}$, and $\{u_{Ai}\}$ and $\{\psi_i\}$ are functions of $\{\phi_{Ai}\}$ as indicated above, $\{\phi_{Ai}\}$, $\{u_{Ai}\}$, and $\{\psi_i\}$ have to be solved self-consistently. A numerical solution of this set of implicit and nonlinear equations was carried out using up to 100 layers.

Parameters used in the model calculations of the adsorption of the bottle-brush polymers onto mica-like and silica-like surfaces are compiled in Table 1. Some of the parameters (T, ε_r, X, r_{polymer}, ϕ_{polymer}, and ϕ_{salt}) are known characteristics of the experimental systems. The values of some other parameters (d, σ, and ψ_s) are less obvious and some reasonable assignments were used. Here, we have adopted the lattice cell length d = 0.5 nm and, furthermore, σ = -0.2 (thus constant surface charge density) for the mica-like surface and ψ_s = -0.1 V (thus constant surface potential) for the silica-like surface at pH = 6. Finally, we have the remaining parameters: $\chi_{\text{main-chain,solvent}}$, $\chi_{\text{side-chain,solvent}}$, $\Delta\chi_{\text{main-chain}}$, and $\Delta\chi_{\text{side-chain}}$. First, for simplicity we assigned $\chi_{\text{main-chain,solvent}} = \Delta\chi_{\text{main-chain}} = 0$, since for low X the number of side chains grossly exceeds the number of main chains and hence the interaction involving the side chains is more important, and at high X the electrostatics dominates. Furthermore, we adopted $RT\chi_{\text{side-chain,solvent}}$ = 1.3 kJ/mol as being a reasonable value for the EO–water interaction.[24] Finally, we used $RT\Delta\chi_{\text{side-chain}} = 0$ for describing the EO–mica interaction and $RT\Delta\chi_{\text{side-chain}}$ = -10 kJ/mol (fitted) for the EO–silica interaction at pH = 6. Experimentally it is known that uncharged PEO brush polymers does not adsorb onto mica,[7] whereas it strongly adsorbs onto silica at pH = 6.[15]

On the basis of the volume fraction profiles $\{\phi_{Ai}\}$, the adsorbed amount of species A expressed as the surface excess of species A is evaluated according to $\Gamma_{\text{exe,A}} = \sum_i(\phi_{Ai} - \phi_{\text{A,bulk}})$, where the summation extends over all lattice layers. The polymer surface excess is given by $\Gamma_{\text{exe}} = \Gamma_{\text{exe, main-chain}} + \Gamma_{\text{exe, side-chain}}$.

TABLE 1

MODEL PARAMETERS

quantity		value
temperature	T	= 298 K
relative dielectric permittivity	e_r	= 80
lattice spacing	d	= 0.5 nm
degree of polymerization (main chain	$r_{main-chain}$	= 200
degree of polymerization (side-chain)	$r_{side-chain}$	= 22
bulk polymer volume fraction	$f_{polymer}$	= $1 \cdot 10^{-4}$
bulk salt volume fraction	$f_+ = f_-$	= $3 \cdot 10^{-4}$
surface charge density [a]	s	= -0.2 (mica-like surface)
surface potential	y_s	= -0.1 V (silica-like surface)
interaction parameters [b]		
$RTc_{side-chain,water}$	=	1.3 kJ/mol
$RTDc_{side-chain}$		= 0 kJ/mol (mica-like surface)
		= -10 kJ/mol (silica-like surface)
Conversion factors [c]		
C_{salt}/M		= $13.3 f_{salt}$

[a] Number of elementary charges per d^2.
[b] Other interaction parameters are zero.
[c] Obtained from the size of a lattice cell.

III RESULTS

The adsorption of the PEO_{45}MEMA:METAC-X polymers to silica surfaces have been investigated by reflectometry and by QCM-D,[15,17] and the adsorption of these polymers to mica surfaces have been investigated by ellipsometry.[7] The results obtained at low ionic strength (≤ 0.1 mM) and neutral pH (≈6) are illustrated in Figure 2. On mica, the low charge density bottle-brush polyelectrolytes ($X \leq 2$) do not adsorb at all. The maximum adsorption is achieved for PEO_{45}MEMA:METAC-50. In contrast, on silica the uncharged bottle-brush adsorbs significantly, and the maximum adsorption is obtained in the composition range $0 < X < 10$.

Clearly, even though both substrates are negatively charged the adsorption to these two surfaces differs considerably. We note that muscovite mica is crystalline layered aluminosilicate mineral. The negative charge on this substrate originates from isomorphous substitution of Al for Si, and in the crystal these charges are compensated by interlayer cations, mainly potassium. The area per surface charge is 0.48 nm^2. When immersed in water the surface bound cations dissolve and are exchanged for other ions present in solution. The mica basal plane contains no silanol groups. In contrast, the silica surface is amorphous and contains a large number of silanol groups. It is common to distinguish between isolated, geminal and associated silanol groups. The total number of silanol groups and the relative abundance of the three categories mentioned above depend on the surface preparation method.

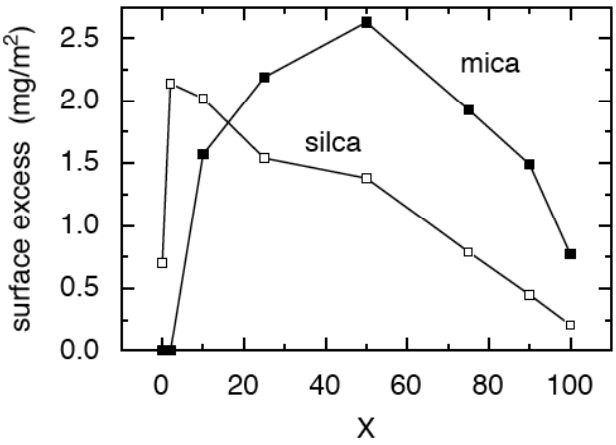

Fig. 2. Experimental surface excess of PEO_{45}MEMA:METAC-X on mica (filled symbols) and silica (open symbols) surfaces at pH = 5.5 - 6 and ionic strength ≤ 0.1 mM. Data taken from ref [7,15].

The calculated surface excess Γ_{exe} as a function of the bottle-brush composition X on the mica-like surface is illustrated in Figure 3. In these calculations the polymer has no non-electrostatic affinity for the surface.

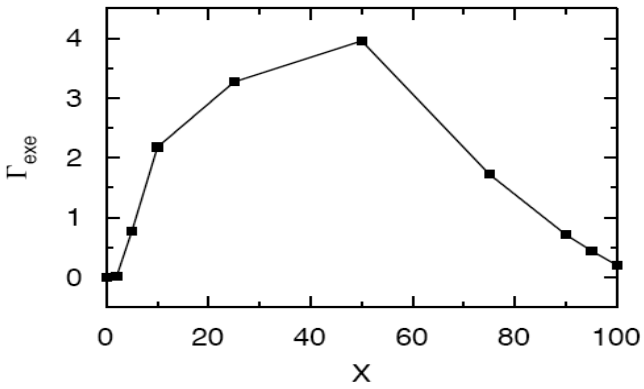

Fig. 3. Calculated surface excess as a function of polymer composition on mica-like surfaces. Parameters as given in Table 1.

We note that uncharged and very low charged ($X \leq 2$) bottle-brush polymers do not adsorb onto the mica-like surface, which is due to the lack of non-electrostatic affinity for the surface. The surface excess G_{exe} increases with increasing charge density of the bottle-brush polymer up to X = 50. At even higher X, the surface excess decreases. Qualitatively, this is in excellent agreement with the experimental findings[7] illustrated in Figure 2. In particular, both modeling and experiments show no adsorption for low charge density bottle-brush polyelectrolytes ($X \leq 2$) and an adsorption maximum at X = 50. A small discrepancy between the modeling and the experimental results is that the curvature of Γ_{exe} vs. X for $X > 50$ is different; experimentally the shape is convex but slightly concave for the modeling results.

The calculated surface excess Γ_{exe} as a function of the bottle-brush composition X on the silica-like surface is illustrated in Figure 4. In the modeling the surface potential of the silica-like surface is kept constant in order to capture the charge regulating ability of the silanol groups. The surface charge density is lower than that on the mica-like surface. In addition, there is a considerable non-electrostatic affinity between the side-chains and the surface, see Table 1.

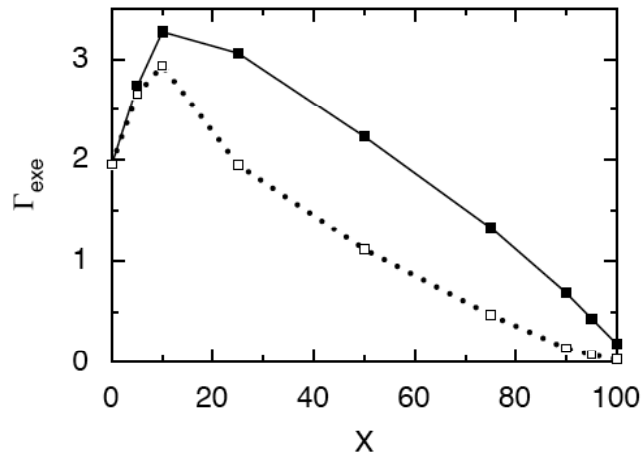

Fig. 4. Theoretical adsorption at the silica-like surface displaying surface excess Γ_{exe} as a function of the composition X (solid symbols). Parameters as given in Table 1. The corresponding data but for a surface with the constant surface charge density s = -0.02841 is also given (open symbols).

The calculated surface excess Γ_{exe} on the silica-like surface as a function of the bottle-brush composition X is given in Figure 4, whereas the corresponding experimental data on silica are shown in Figure 2. The adsorption of the uncharged bottle-brush polyelectrolyte (X = 0) on the silica-like surface is large, whereas no adsorption was found on the mica-like surface. This is a consequence of the non-electrostatic affinity between the side-chain segments and the surface and in agreement with experimental results. Introduction of a small number of charged segments increases the adsorption on the silica-like surface, and the maximal Γ_{exe} is found for X = 10, which is significantly lower than that on the mica-like surface. This is also due to the side-chain affinity to the silica-like surface. At higher X, the surface excess decreases. Experimentally, the maximal adsorption is observed at somewhat lower bottle-brush charge densities (X = 2), and introduction of a small amount of charges on the main chain has a more dramatic effect on Γ_{exe} than predicted by the modeling.

Figure 4 also shows the surface excess for a silica-like surface with the constant surface charge density σ = -0.02841; σ selected such that ψ_s = -0.1 V is obtained for a polymer solution at X = 0. For low charged bottle-brush polyelectrolytes, very similar results are obtained under constant σ and constant ψ_s conditions. On the other hand, for larger X, the charge regulating ability of the surface is important, and larger Γ_{exe} is found on the constant ψ_s-surface than on the constant σ-surface. The results obtained for the constant ψ_s silica-like surface is more consistent with experimental data than those obtained by assuming a constant σ. Thus, below we consider the constant ψ_s-surface, if not otherwise stated.

The modeling also allows calculations of the segment density profile for both main chain segments and side-chain segments. It is found that the total segment density is highest just outside the silica surface (in layer 1), but for $X \leq 75$ on the mica-like surface it is located a distance away from the surface. This is due to the lack of affinity between the side-chains and the mica-like surface. For details the interested reader is referred to the article by Linse and Claesson.[18]

Modeling has the attractive feature that it allows changes of conditions in a systematic manner, which for certain parameters is very difficult or impossible to do in experiments. For instance, for a polymer molecule with different types of segments the sequence of segments can have a large impact on surface properties. This is illustrated for the bottle-brush polymers on the silica-like surface in Figure 5.

We note the general trend that the surface excess increases with the degree of blockiness, i.e. it is largest for the diblock, and slightly larger for the random sequence than for the regular one (the same trend is observed on the mica-like surface). On the silica-like surface the maximum surface excess also moves towards a higher polymer charge density, from X = 10 for the regular sequence to X = 25 for the diblock. Interestingly, also on the mica like surface the maximum surface excess of the diblock copolymer is found for X=25.[18] Many important surface chemical characteristics such as protein repellency, good steric stabilization and low frictional forces have been found to correlate with a high PEO

concentration at the interface. This suggests that a diblock copolymer with 25 mol% of charged segments and 75 mol% of PEO_{45} side-chain containing segments may be of great value in many applications.

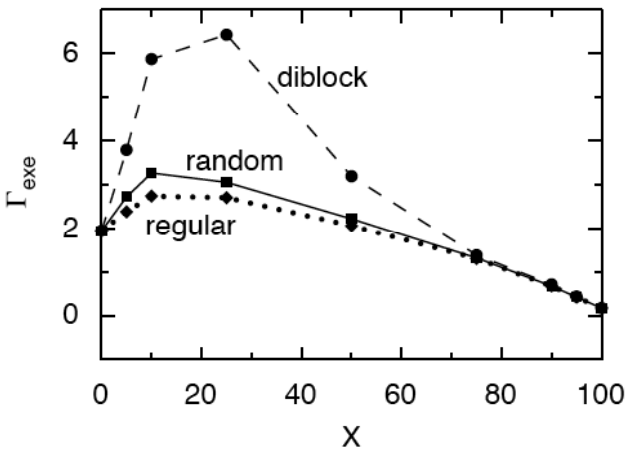

Fig. 5. Theoretical surface excess Γ_{exe} as a function of the composition *X* for the silica-like surfaces with random (squares), regular (diamonds), and diblock (circles) distributions of the uncharged and charged main-chain segments. Other parameters as given in Table 1.

We have seen that the non-electrostatic affinity between the side chains and the surface is of great importance for the adsorption and the layer structure. This is a parameter that can be expected to vary significantly for different substrates and it thus of interest to explore this further. To this end we used the mica-like surface and gradually switched on a the non-electrostatic affinity between the side chains and the surface. The results are illustrated in Figure 6.

An increase in affinity between the side chains and the surface increases the adsorption of the low charge density bottle-brush polymers, but has only a minor influence for highly charged bottle brushes where electrostatic forces control the adsorption process. We note that as the side-chain affinity is increased the polymer architecture that results in maximum adsorption shift to lower values of X, and the maximum surface excess increases. Once the interaction paramter $RT\chi_{side\text{-}chain}$ is below -10, a further increase has a limited effect, which is due to that the segment density next to the surface approaches 1 (i.e. the surface becomes saturated).

Finally, we also explore the importance of the electrostatic interactions for driving the adsorption and for limiting the adsorption. On the mica-like surface no adsorption occurs without the presence of electrostatic interactions. More interestingly, it is found that the surface excess is limited by electrostatic interactions when $X \geq 75$, i.e. adsorption proceeds until the surface charge is compensated by the charges in the adsorbed layer. However, for lower charge densities of the bottle-brush adsorption does not proceed to charge neutrality. Rather, the excluded volume repulsion between the side-chains puts a limit to the surface excess that can be reached.

On the silica-like surface the situation is more complex as illustrated in Figure 7. In this case adsorption proceeds to charge neutrality for polymer charge densities at and above X = 50, whereas excluded volume interactions limit the adsorption at lower values of X.

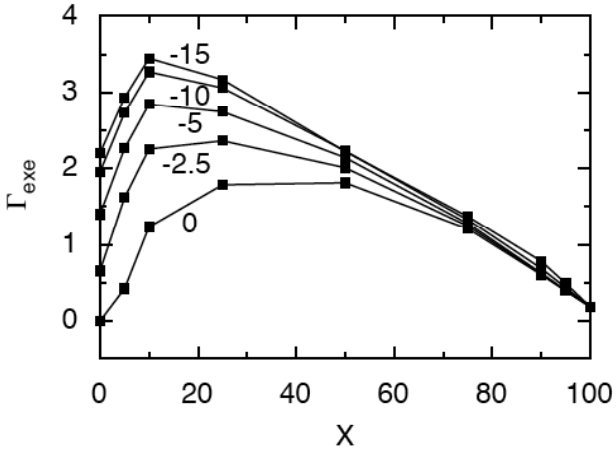

Fig. 6. Theoretical surface excess Γ_{exe} as a function of the composition *X* for the silica-like surface at indicated values of $RT\chi_{side\text{-}chain}$. Other parameters as given in Table 1.

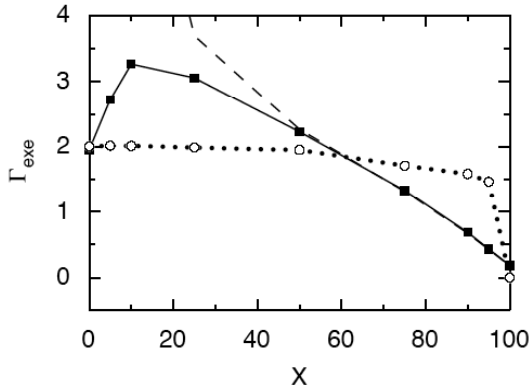

Fig. 7. Theoretical surface excess Γ_{exe} (solid curves) and corresponding data without electrostatic interaction (dotted curves) as a function of the composition *X* for the silica-like surface. Other parameters as given in Table 1. The surface excess corresponding to charge equivalence is also shown (dashed curves).

It is also interesting to note that for high values of X ($X \geq 60$) the adsorption increases as the electrostatic affinity is switched off, i.e. even though electrostatics contribute to anchoring the polymer strongly to the surface it also limits the adsorption. In contrast, at lower charge densities electrostatic interactions results in a higher adsorption than for the corresponding uncharged system.

IV CONCLUSIONS

The adsorption of charged bottle-brush polymers of various compositions onto two different oppositely charged and planar surfaces mimicking mica and silica have been investigated using a lattice mean-field approach. To obtain modeling results corresponding to experimental data, the mica surface was represented by a surface with a high constant surface charge density, whereas the silica surface was modeled as a surface with constant surface potential. Furthermore, the

polymer–mica interaction was athermal, whereas an attractive side-chain–surface interaction was assigned for the silica surface. Thus, the two surfaces differed in two important aspects.

Despite the limitations of the present model and experimental uncertainties in length and composition polydispersity, we obtained a surprisingly good representation of the surface excess and the number of adsorbed side chains per surface area as a function of polymer architecture, spanning the composition range from $X = 0$ corresponding to an uncharged bottle-brush polymer to $X = 100$ corresponding to a linear polyelectrolyte. As to the mica-like surface, the surface excess results from a balance of the attractive electrostatic polymer–surface interaction, the repulsive polymer–polymer interaction, and the repulsive conformational entropy change due to adsorption. Linear polyelectrolytes often display a maximal surface excess at $X \approx 1\text{-}5$[25-27] (in the present notation); hence, the presence of the repulsive contribution of the side chains shifts the optimal X to higher linear charge density (here $X = 50$). For the adsorption onto the silica-like surface, the effect of the non-electrostatic attractive side-chain–surface interaction becomes larger at decreasing X, and this attraction restores the appearance of the maximal surface excess to a low value of X.

We have also used the mean-field lattice model to investigate the effect of polymer segment sequence, side-chain–surface affinity, and the role of the electrostatic interactions *separately* – a task rarely feasible experimentally. We observed that the difference in surface excess between regular and random distributions is at most 20%, whereas over a 5-fold difference in excess amount between regular and block distributions was obtained. The largest difference was obtained in the polymer composition interval $10 \leq X \leq 30$. Our modeling results suggest that a maximum anchoring of PEO_{45} side-chains to both mica-like and silica-like surface can be achieved for the polymer composition PEO_{45}MEMA:METAC-25 in a diblock sequence. Such a structure is thus expected to show promising properties in applications requiring low protein adsorption, good steric stabilization and low friction forces.

From comparison with the analogous uncharged systems, we conclude that the adsorption of the bottle-brush polymers is driven by the electrostatic polymer–surface interaction at $X > 0$ for the mica-like surface, and in the interval $0 < X \leq 60$ for the silica-like surface, whereas at $X > 60$ for the silica-like surface the electrostatic repulsion between the adsorbed polymer chains limits the adsorption.

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Per M. Claesson and Per Linse. Ķemmveida polimēru adsorbcija uz vizlas un silīcija dioksīda virsmām: Salīdzinājums starp eksperimentu un modelēšanas rezultātiem

Izmantojot režģa vidējā lauka teoriju, modelēta vairāku lādētu ķemmveida polimēru polimēru ar konstanta garuma sānu ķēdēm adsorbcija uz vizlas un silīcija dioksīda virsmām, un iegūtie rezultāti salīdzināti ar atbilstošajiem eksperimentālajiem datiem. Ķemmveida polimēri modelēti kā savienojumi, kas sastāv no divu veidu skeleta ķēdes segmentiem – lādētiem segmentiem un nelādētiem segmentiem ar pievienotu sānu ķēdi. Sastāva mainīgais X raksturo lādētos skeleta ķēdes segmentus un svārstās robežās no X = 0 (nelādēts ķemmveida polimērs) līdz X = 100 (lineārs polielektrolīts). Vizlas tipa virsmām piemīt konstants negatīvs virsmas lādiņa blīvums un tam nav ne-elektrostatiskās afinitātes ne pret galveno ķēdi, ne pret sānu ķēdi, kamēr silicija dioksīda tipa virsmām ir konstants negatīvs virsmas potenciāls un neelektrostatiskā afinitāte pret

ķemmveida polimēra sānu ķēdēm. Modelis ir izmantojams, lai reproducētu virkni eksperimentālu īpatnību, kuras raksturo ķemmveida polimēru adsorbciju pilnam sastāva mainīgā X vērtību spektram uz abām virsmām, līdz ar to ļaujot kvantificēt kādā veidā divu virsmu atšķirīgā daba attiecībā pret polimēru elektrostatiskajām īpašībām un ne-elektrostatisko afinitāti ietekmē adsorbēto slāņu adsorbcijas īpašības un struktūru. Gibsa adsorbcija parāda maksimumu pie X ≈ 50 vizlas virsmām un pie X ≈ 10 silicija diopksīda virsmām. Bez tam., biezākais adsorbētais slānis iegūts pie X = 10 - 25.

Пер М. Классон и Пер Линсе. Адсорбция гребенчатых полимеров на поверхностях слюды и диоксида силиция: Сравнение эксперементальных данных и результатов моделирования.

Используя теорию средней площади, была смоделирована адсорбция гребенчатых полимеров с постоянной длиной боковых ответвлений на поверхностях слюды и диоксида силиция. Полученные данные были сравнены с экспериментальными результатами. Гребенчатые полимеры смоделированы, как соединения, основная цепь которых состоит из двух сегментов – заряженного и незаряженного сегмента с привитым боковым ответвлением. Переменная состава X описывает содержание заряженных сегментов основной цепи в диапазоне от X=0 (незаряженный гребенчатый полимер) до X=100 (линейный полиэлектролит). Поверхности типа слюды обладают постоянной негативной плотностью поверхностного заряда и не обладают неэлектростатическим сродством не с главной не с боковыми цепями, в то же время поверхности типа кремния обладают постоянным негативным поверхностным потенциалом и неэлектростатическим сродством с боковыми ответвлениями гребенчатых полимеров. Данная модель способна воспроизводить целый ряд экспериментальных признаков характерезующих адсорбцию гребенчатых полимеров в зависимости от переменной состава X и тем самым качественно охарактеризовать, как различная природа двух поверхностей по отношению к их электростатичеким свойствам и неэлектростатическому сродству влияет на адсорбционные свойства и структуру абсорбированых слоев. В частности, для поверхностей типа слюды адсорбция Гибса имеет максимум при X≈50, а для поверхностей кремния при X≈10. Кроме того, наиболее толстый абсорбированый слой получен при X=10-25.