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Molecular dynamics simulations of collagen adsorption onto grooved rutile surface: The effects of groove width

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ABSTRACT

The early adsorption stages of collagen onto nano-grooved rutile surface without hydroxylation were studied using molecular dynamics and steered MD simulations. On the basis of plane rutile (1 1 0), two kinds of models have been adopted: single groove and parallel grooves along [1 -1 1] crystal orientation with various width dimensions. Initially, collagens were parallel or perpendicular to the groove orientation, respectively, in order to investigate the influence of groove width on collagen adsorption. The simulation result suggests that surface grooves could exert a strong effect on collagen adsorption: when collagen was parallel to the groove direction, adsorption was favored if the groove width matched well with the dimension of collagen. However, adsorption strength may decrease as the groove width expanded. As for the condition of collagen perpendicular to the groove orientation, collagen was difficult to bend and insert into grooves in the free adsorption procedure. But the steered MD simulation results reveal that more energy was consumed for collagen to insert into narrower grooves which may be interpreted as strong barrier for adsorption. We believe that adsorption will be favored if appropriate dimension match between dimension of collagen and the groove width was approached.

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1. Introduction

Protein adsorption on solid surface has long been emphasized for its critical rule in many applications such as bio-sensing and surface modification of biomedical implants [1]. In particular, to interpret the mechanism of the cell-protein-biomaterial interaction is fundamental to evaluate the biocompatibility of biomaterials [2,3]. It has been confirmed that the surface pre-adsorbed ECMs, such as RGDS [4], fibronectin [5] and collagen [6–8], could influence cell behaviors like cell morphology, adhesion, proliferation and differentiation. Besides, many studies [9–11] have shown that the formation of contact guidance, which represents the orderly organized fibroblast cells on grooved surface, is attributed to the orderly distributed cell protrusions aroused by the surface anisotropic distributed proteins. However, the mechanism for this anisotropic distributed protein is still not fully understood. Vonrecum [10] suggested that sharp surface discontinuities on chemically homogeneous substrata, such as the edges of ridges on micro-grooved substrates, could be active sites for protein adsorption due to a local increase of the surface energy. In addition, elaborately fabricated surface topographies such as nano-metric pores [12], valleys [13] and convexities [14] were favored for protein adsorption and nucleation. Moreover, the surface roughness [15,16] could influence protein adsorption which turned out to be an important parameter in biomaterial design. Manwaring [17] found that the secreted matrix proteins became more organized as the surface roughness increased. However, the mechanism and the influence rule of surface topography on protein adsorption still remain unsolved.

Based on solving the Newton's equations of motion numerically, the classical MD simulation is employed to give insights into the natural adsorption dynamics of biomolecules on solid surface in solution at atomic level. Protein adsorption on perfect metal surface has been studied in large quantities, but a few studies have been carried out to investigate the effects of nano-topographies on protein adsorption. The simulation work of Raffaini [18] suggested that the adsorption strength depended on surface topographies and he found it was stronger on the inner concave SWNT surface than on the flat grapheme, being slightly weaker on the outer convex surface of SWNT. Heinz [19] also confirmed that the inner edges of the stepped Au surface were favored for single peptide adsorption while the adsorption strength was much weaker when interacted with small Au nanoparticles. In addition, the dimension [20] of the nanostructures also played a key point on peptide adsorption

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and the surface topography may be favored for P3HT adsorption if the curvature radius of the spherical nanocaps was greater than the average polymer chain length. However, the topographical factors on peptide adsorption still need to be investigated in detail. In this work, the adsorption of collagen-like peptide on grooved rutile (1 1 0) surface was conducted via the MD simulation. Various dimensions of the grooved substrates were modeled and their influence on collagen adsorption, especially the groove width was discussed in detail.

2. Method

2.1. Model building

Rutile (1 1 0) surface was chosen as a model system in this work since it is the most stable crystal face with a lattice dimension of $\sqrt{2}a \times c$ along the [1 -1 0] and [0 0 1] crystal direction [21], respectively. In general, frequent defects observed on the rutile (1 1 0) surface always include step edges, oxygen vacancies, line defects and impurity. The stable step edges observed on (1 1 0) surface are mainly parallel to the [1 -1 1] and [0 0 1] direction, whose stability has been identified via the STM observation [22], and DFT calculation [23].

In this work, grooved topographies with different dimensions were built in order to investigate their influence on collagen adsorption. All the grooves had a [1 -1 1] orientation, which were obtained by removing the rutile unit cells layer by layer along [1 -1 1] crystalline direction [21]. The side walls of the groove has a (2 3 1) crystal face which exposed large quantities of unsaturated Ti (4- and 5-coordinated) and O (2-coordinated) atoms. Substrates with a single groove and parallel grooves (illustrated in Fig. 1) were modeled with various groove width ranging from 16.2 Å to 37.7 Å and they were named M1–M4 and M5–M8 for short. Surface hydroxylation of rutile surface was not taken into consideration in this work.

As a major structural protein in the extracellular matrix, collagen is composed of three polypeptide chains, each with the repeating triplet amino sequences of Gly-X-Y, where X and Y are frequently proline (Pro) and 4-hydroxyproline (Hyp), respectively. The stability of collagen's triple helical structure is maintained by the inner-chain hydrogen bond between carbonyl oxygen (O_{CO}) of Pro and amino hydrogen (H_{NH}) of Gly. The collagen has excellent flexibility with a long-rod like structure of 1.5 nm in radius and about 300 nm in length. In this work, the crystal structure of collagen segment was derived from the protein data bank [24] (PDB: 2KLW), with residue sequences of (-Pro-Lys-Gly-)$_{10}$, (-Asp-Hyp-Gly-)$_{10}$ and (-Pro-Hyp-Gly-)$_{10}$ in each chain, respectively. The N- and C-terminals of the collagen were capped by Ace (—$COCH_3$) and Nme (—$NHCH_3$), respectively, to avoid the spurious end effects. Since rutile has a low ZPC of 5.3 at 35° [25], the surface could be neutral if the pH was around 5.3. Under this condition, the predominant forms of lysine [26] and aspartic acid [27] are $(COO^-)(NH_3^+)CH—(CH_2)_4—NH_3^+$ and $(COO^-)(NH_3^+)CH—CH_2—COO^-$. Therefore, we may assume that the distal hydroxyl group in Asp residue and distal amino group in Lys residue have the same ionic state with that in the aspartic acid and lysine, and Asp residue and Lys residue were negatively and positively charged, respectively. But the whole charge of the system was zero.

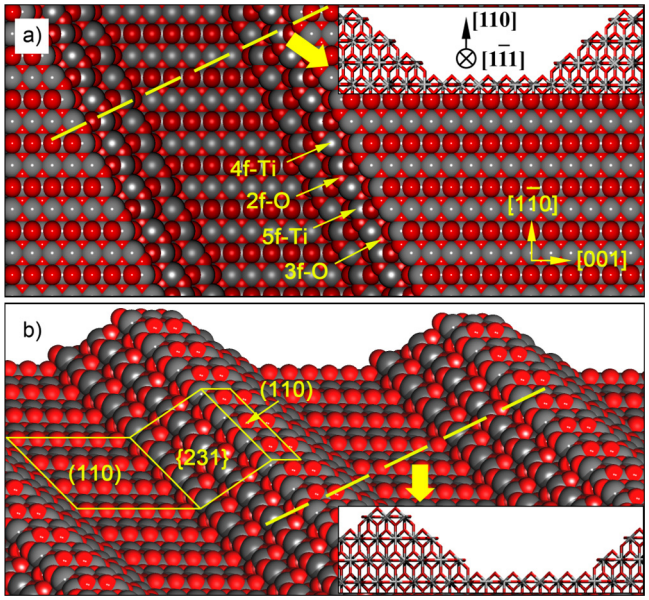

Fig. 1. Two kinds of groove models, (a) single grooved model, (b) parallel grooved model. The atoms of the surface are rendered through gray (Ti) and red balls (O). 4f-Ti represented the 4-coordinated Ti atoms located at the side of the groove wall. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In M1–M4, the collagens were inserted in the grooves with a minimum distance of 4.5 Å between the atoms of collagen and the substrate surface. All the collagens in M1–M4 had same position and initial conformation. In terms of the substrates with parallel grooves (groove width increased from 16.2 Å to 37.7 Å in M5 to M8), collagens were perpendicular to the groove orientation also with a minimum distance of 4.5 Å from the top of the grooved surface. The initial positions between collagen and the substrates and other model parameters were listed in Table 1. The initial conformations of collagen on single grooved surface (M1 as an example) and parallel grooved surface (M7 and M8) were figured out in Fig. 2, as well as the distribution of water molecules near the grooved surface.

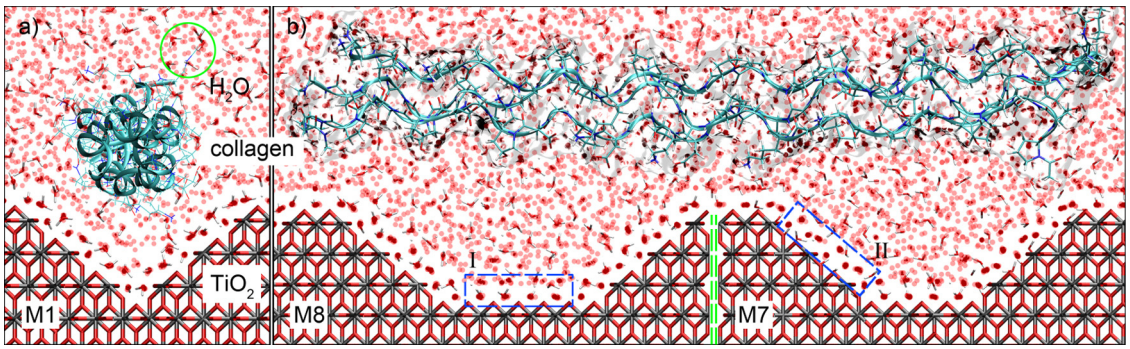

Fig. 2. Initial adsorption conformations of collagen on single grooved surface (M1 instead) (a) and parallel grooved surface (M7 and M8 instead) (b). The red dot represented water oxygen atoms on grooved surface, and deep color meant high density of water molecules. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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