Molecular Mechanism for the Detachment of Degradable Antifouling Coatings

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Abstract: Degradable self-polishing antifouling coatings are expected to be the next generation of antifouling coatings due to their excellent environmental friendliness and static antifouling effect. However, the polishing process and mechanism are still unclear. In this work, steered molecular dynamics (SMD) simulations were conducted to investigate the detaching process and mechanism of the degraded main chain (DMC) and the antifouling agent, and the influence of substrate hydrolysis degree was also studied. The results show that without water scouring, the DMC and antifouling agent molecules are always adsorbed to the coating surface in a static environment due to the non-bonding interaction of the substrate. The strong interaction between the substrate and the water molecules can form a water film that hinders the detaching process. The non-bonding interactions from the substrate, the encroachment of water molecules on the hydrogen bonding sites of the clusters, and the unevenness of the substrate surface always prevent the clusters from being detached completely. This work elucidates the microscopic process and mechanism of main chain degradable self-polishing antifouling coatings in the presence of seawater and also sheds light on the direction of optimizing degradable self-polishing coatings for accelerating their commercialization application.

Keywords: Molecular dynamics simulation; Degradable self-polishing coatings; Marine antifouling; Water intrusion