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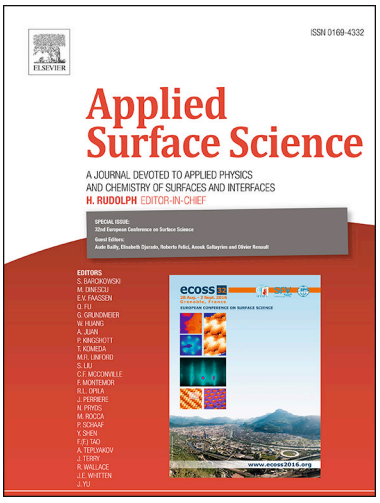

Full Length Article

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Influence of Surface Morphology on Adsorption of Potassium Stearate Molecules on Diamond-like Carbon substrate: A Molecular Dynamics Study

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Abstract: Molecular dynamics (MD) simulations were used to provide insights into the influence of nano-scale surface morphology on adsorptive behavior of Potassium stearate molecules on diamond-like carbon (DLC) substrates. Particular focus was given to explain that how the distinctive geometric properties of different surface morphologies affect the equilibrium structures and substrate-molecules interactions of monolayers, which was achieved through adsorptive analysis methods including adsorptive process, density profile, density distribution and surface potential energy. Analysis on surface potential energy demonstrated that the adsorptivity of amorphous smooth substrate is uniformly distributed over the surface, while DLC substrates with different surface morphologies appear to be more potentially corrugated, which improves the adsorptivity significantly. Because of the large distance of molecules from carbon atoms located at the square groove bottom, substrate-molecules interactions vanish significantly, and thus potassium stearate molecules cannot penetrate completely into the square groove. It can be observed that the equilibrium substrate-molecules interactions of triangle groove and semi-circle groove are much more powerful than that of square groove due to geometrically advantageous properties. These findings provided key information of optimally design of solid substrates with controllable adsorptivity.

Keywords: potassium stearate; diamond-like carbon; molecular adsorption; surface morphology

1. Introduction

In the past decades, organic monolayers adsorbed on solid substrates have received much attention because of its promising applications in reducing wear and friction, such as self-assembled monolayers (SAMs) and Langmuir-Blodgett (LB) films [1-3]. Experimentally, preparation of LB films can be achieved