

Molecular dynamics study of oil detachment from an amorphous silica surface in water medium

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ABSTRACT

In this paper, the mechanism of oil detachment from optical glass in water medium is studied by using molecular dynamics simulation. At the beginning, some undecane molecules are adsorbed on the amorphous silica surface to get contaminated glass. Upon addition of 6000 water molecules, most of the undecane molecules on the substrate surface can be detached from an amorphous silica surface through three stages. The formation of different directions of water channels is vital for oil detachment. The electrostatic interaction of water substrate contributes to disturbing the aggregates of undecane molecules and the H-bonding interaction between the water molecules is helpful for the oil puddle away from the substrate. However, there is still some oil molecules residue on the substrate surface after water cleaning. The simulation results showed that the specific ring potential well of amorphous silica surface will hinder the detachment of oil molecules. We also find that the formation of the specific ring potential well is related to the number of atoms and the average radius in silica atomic rings. Increasing the upward lift force, which acts on the hydrocarbon tail of oil molecules, will be benefit to clear the oil pollution residues from the glass surface.

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1. Introduction

The organic pollution on the surface of the optical element is a pressing issue that needs to be addressed. The National Ignition Facility is the world's largest optical system which contains laser glass, fused silica, KDP, DKDP, etc. [1,2] Due to the pollution of the optical element, the laser-induced damage in high-power laser system will occur [3]. The pollution of the optical element would degrade the optics damage threshold and limit system life. While macro-molecules of organic pollutants are cleaned easily, there still remain some micro-molecules [3]. The residue organic pollutants need to be further studied. So a MD simulation is conducted to investigate the detachment of oil molecules from the surface of fused quartz.

When in contact with the silica surface, the oil phase would be divided into several layers [4]. Some experiments on detachment of oil drops from silica substrate were carried out, and the mechanisms of oil detachment from substrate had been analyzed [4–10]. Recent papers [4,5] show findings that the detachment process of oil from silica surface involves three stages. In stage one, the water channel perpendicular to the silica surface was

formed, and the interaction between the water and substrate is the driving force. In stage two, because of the water diffusion along the silica surface through H-bonding between water molecules and the hydroxyl group of the silica, the water molecules destroy the first oil layer. In stage three, the buoyancy force tends to detach the drop from the substrate. These three stages showed that the substrate is cleaned completely. But it is difficult to achieve this in the actual situation. In this article, we will display the oil detachment from silica substrate in actual situations, in which there are both the horizontal water channel and vertical water channel. There are also some experiments where different organic pollution is used to do simulations. These involve the simulations about adsorption and detachment of oil on the solid surface [6–13]. The simulation objects of oil molecules include Pyridine and Alkyl Pyridine [9], dodecane [10], organic methanol [11] and so on. We select the undecane molecules as oil phase.

In addition, many authors' studies are focused on the factors of roughness about the residue oil after detachment from the silica substrate. They investigated effects of roughness about detachment of oil from the fused quartz and analyzed the mechanism of residual oil. But the mechanism is different from this research about the surface roughness [14–17]. They studied the effect of roughness on adsorption [14,15], wetting [16,17]. While the roughness they created is artificial. It is not natural. In this article, the surface

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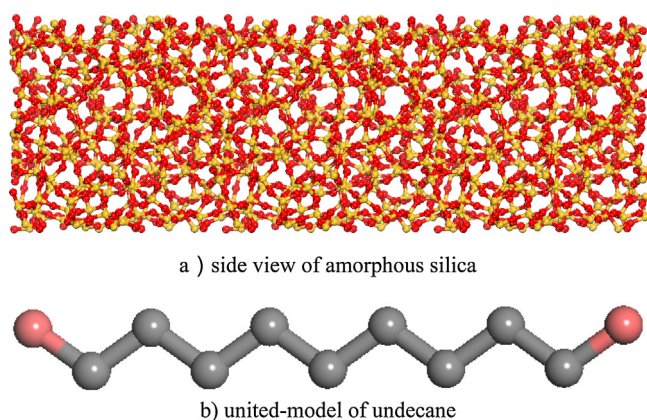


Fig. 1. Snapshots of amorphous silica and oil molecule used in the simulation.

defects of fused quartz are naturally occurring in the imitation of the natural condition.

Then some researchers devoted their research to the surface of air/water or oil/water [18–21]. Chanda et al. used the decane molecules as oil medium [18]. The hydrocarbon tails decane are more vertically oriented at the oil/water interface [18,19]. R.J.K. Udayana Ranatunga and co-workers show the behavior of surface-ligated nanoparticles in the oil/water interface [20]. It indicated effective self-assembly method of nanoparticles [21]. From their results, we can know that hydrocarbon tails are vertically oriented at the oil/water interface. In addition, some studies use the different materials of silica as the substrate. Zhang et al select the crystalline silica as the substrate [5]. From their results, the detachment of oil is complete. Yang and co-workers studied the effects of silica surface on different orientations [22]. They investigated the adsorption on (1 1 1), (2 2 0) and (3 3 1) surface on silica. Other authors also studied the amorphous silica [23–26] that is usually obtained by annealing from 8000 to 300 K. Yang's result may help to explain the effect of amorphous silica such as fused quartz on oil detachment.

In recent years, with the computer power increasing, molecular dynamics (MD) simulation has become a powerful tool to study the structural and properties of surfactant, silica substrates at the microscopic level [23]. It can also provide molecular-scale understanding of oil droplet detachment from solid surfaces, which is difficult to obtain from experiments. In our work, we would use the molecule dynamic simulations to simulate the adsorption that the optical element is polluted by oil drop and that the detachment of oil from quartz glass. We could get the information of the whole process, which is hard to obtain from experiments. The undecane is selected as the oil phase. In addition, we would analyse the mechanism of residual oil on the surface of quartz glass that is formed in the simulation of natural conditions.

2. Modeling and simulation details

2.1. Modeling

Our MD simulations were carried out using LAMMPS package (Plimpton 1995). The optic glass surface, which has a structure of

Table 1
Lennard–Jones parameters and charges for atoms and groups in our simulation system.

Atom	σ (nm)	ϵ (kJ/mol)	$q(e)$
Si	0.3795	0.5336	+1.283
O	0.270	1.912	−0.6415
CH ₂	0.393	0.3908	0
CH ₃	0.393	0.9478	0

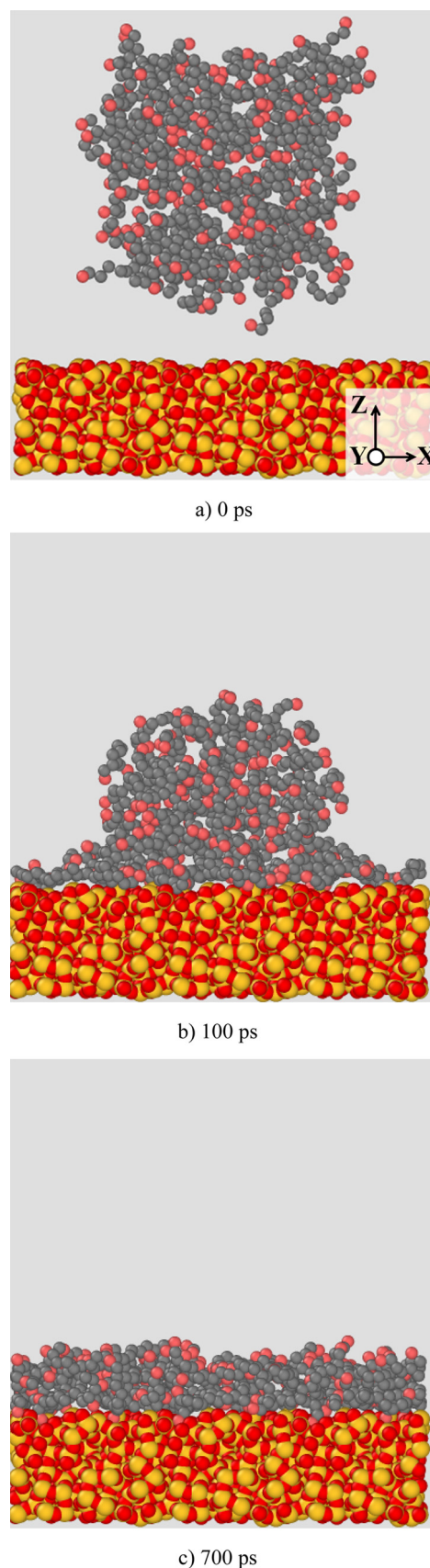


Fig. 2. Consecutive snapshots of the adsorption of the oil molecules.

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