單顆液滴撞擊固體表面薄膜之分子動力學模擬探討

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摘要

本文利用分子動力模擬的方法針對不同的參數，探討真空環境下單顆液滴撞擊固體面上薄膜的行為及影響。影響液滴撞擊行為的參數主要分為液滴撞擊速度、液滴尺寸、薄膜厚度及材質(本文採用氦、氬、氙三種材質)。主要的結果利用可視化程式呈現在內容中。當撞擊速度大時，液滴在表面上會有飛濺的現象，而撞擊速度小的時候，液滴趨於圓球的形狀。不同的薄膜厚度對於液滴的後期發展有較大的影響。在不同的液滴尺寸中，較大的液滴可以快速的攤開達到欲噴灑的表面，但也伴隨著較高的王冠狀液滴發生。所以建議採用較小的液滴，可以得到較平滑的面。在模擬系統中主要採許同樣的溫度及密度，但由於三種惰性氣體在同樣溫度、密度下不是所期望的狀態，由結果可知氦在撞擊過程中已經趨於氣體的狀態，然而氙已經趨於固體狀態，故內容討論主要針對氬作液滴行為上的討論。

Molecular Dynamics Simulation of an Impinging Droplet onto Solid Wall with Thin Film

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Abstract

The behavior of single droplet impinging onto the solid wall with the thin film was investigated. It is mainly discuss the different effects such as the impact velocity of droplet, droplet size, the film thickness and the species of atoms in the study. The deformation of droplet using visualization program "pvwin" was observed. For argon, the results revealed that for the large impact velocity of the droplet, the inertia force of the droplet may overcome the surface tension of the liquid and splash takes place and for low impact velocity of the droplet, the droplet tends keep its spherical shape on the surface and it was like the spread behavior. For the low H_f, the main phenomenon of droplet is like the crown breaking up into many tiny droplets shortly after impact. The whole crown expands outwards as the shape of a bowl. In contrast, the droplet developed approximately cylinder-like crown normal to the surface for the large H_f. The molecular dynamics method is expected to be useful, for getting

insight of physico-chemical problems at atomic scale. Further problems, to change some effect factors, such as impact angle, environmental state to approach the practical condition and to apply the different potential m to deal with the different atoms and predict the behaviors such as rebound, stick, etc.