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論文題目	Numerical Study of Droplet Impingement on Surfaces with Micro-scale Structures （マイクロ構造をもつ固体表面への液滴衝突の数値解析）		

（論文内容の要旨）

In this thesis, the dynamics of droplet impingement on surfaces with micro-scale structures are investigated by means of a direct numerical simulation (DNS). This thesis consists of 7 chapters, as follows.

Chapter 1 presents the background, motivation, objectives, and outline of this thesis.

In Chapter 2, the numerical methods, the examination of grid resolution, and the numerical validation are described. A coupled level set and volume of fluid (CLSVOF) method to track the gas-liquid interface and the strategy for implementing the contact angle into the boundary condition are explained in detail. An assessment of the domain size, followed by an examination of the grid resolution are conducted. Then, the validity of the numerical methods is examined by comparing the numerical results of droplet impingement on flat and textured surfaces with the results of existing experiments. The numerical methods and conditions validated in this chapter are used as the bases in the subsequent chapters.

Chapter 3 presents the relationship between the surface hydrophobicity and the groove structures. The dynamics of an impinging droplet on surfaces with different groove widths and impinging velocities are discussed. On these textured surfaces, the droplet spreads freely in the parallel groove direction, however, it jumps from the attaching ridge to the next ridge in the perpendicular groove direction (called a “jump-stick”), leading to an elliptical droplet as per the top-view. In comparison with the cases of flat surface and surfaces with small groove widths, where droplets display non-bouncing behaviors upon impingement, surfaces with large groove widths result in droplets completely bouncing off upon impingement, thereby revealing enhanced surface hydrophobicity. As the groove width increases, the droplet exhibits a smaller spreading factor, which is defined as the ratio between the diameter of the wetted area of the surface and the original diameter of the droplet, and shorter contact time between droplet and substrate, indicating that the surface hydrophobicity is gradually enhanced. However, it is suppressed with a further increase in the groove width and impact velocity, because the wetting transition from the Cassie state where only the outermost tops of the structures are wetted to the Wenzel state where the surface is fully wetted is obtained. This result suggests that the surface hydrophobicity is weakened in the Wenzel state. Finally, two phase diagrams summarizing the droplet bouncing states with respect to the surfaces and wetting state are provided.

Chapter 4 describes the behavior of an impinging droplet on a surface with a roughness gradient. The roughness gradient is created by gradually varying the groove width based on the results conveyed in Chapter 3. The effects of the Weber number, groove width, and groove depth on the rebound direction of a droplet are studied. Three types of rebound behaviors, namely, vertical rebound, rebound following, or rebound against the roughness gradient, are observed, which are dominated by both the unbalanced Young’s force and wetting state. Droplets remain in the Cassie state and rebound following the roughness gradient for a small impact velocity, small groove width, and larger groove depth. In contrast, when the combined Cassie and Wenzel states present, the droplets are partially arrested by the grooves, thus rebounding against the roughness gradient. On the contrary, vertical rebounding behaviors are obtained at small and critical impact velocities. Finally, a phase diagram, illustrating the distinct areas of the rebound direction, is presented. These results provide important

insight into the design of wettability gradient surfaces for controlling droplet transport with no external energy input.

Chapter 5 presents a novel type of surface to amplify the surface hydrophobicity as far as possible and simultaneously prevent the liquid from penetrating the grooves, as described in Chapters 3 and 4. This textured surface is fabricated via decoration with primary structures (higher) used to enhance the hydrophobicity and secondary structures (shorter) to prevent the Cassie-to-Wenzel wetting transition. The deformation, penetration, and wetting transition of the droplets on this surface are investigated. When compared with the droplet behavior on surfaces masked with only primary structures, the secondary penetration behavior is suppressed such that a relatively stable Cassie state is obtained on surfaces with both primary and secondary ridges. With increasing the secondary structure height, the liquid penetration factor and the surface emptying time decrease, meaning that the liquid penetration is suppressed by the secondary structures. The impingement position at the primary groove or the primary ridge also plays a vital role in the wetting transition. However, under a larger impinging velocity, liquid penetration occurs in the secondary structures. This two-step liquid penetration on a novel surface is explained well via theoretical models based on the correlation of Laplace's law, Young's equation, and Gibbs extension. Inspired by these findings, a more robust hydrophobic surface with multilevel structures is proposed.

Chapter 6 describes the examination of the stability of the Cassie state on multiple hole surfaces (MHS). When compared with the multiple pillar surfaces (MPS), the MHS not only enhances the surface hydrophobicity but also greatly stabilizes the Cassie state of an impinging droplet. The varying pressure in the air pocket inhibits the depinning of the three-phase contact line (TPCL). This is the fundamental reason for a superstable Cassie state on the MHS being obtained. The robustness of the air pocket on the MHS is examined by releasing droplets with large velocities. Although an extremely large impingement velocity triggers the depinning of the TPCL in some holes, a significant number of liquid-air interfaces hang between structures, and a Wenzel state is not obtained on the MHS. Finally, a new model for predicting the maximum spreading factor, considering the air cavity at the center of the droplet and the energy loss of the TPCL depinning, is derived, which is in better agreement with the experimental and simulation results than the previously proposed models are. Overall, the findings of this study deepen our understanding of the wetting stability when droplets impact on textured surfaces with air pockets.

Chapter 7 summarizes all the investigations conducted as a part of this thesis. Moreover, it provides recommendations for possible future extensions of the present study.

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（論文審査の結果の要旨）

本論文は，マイクロ構造をもつ固体表面への液滴衝突に関する研究の結果をまとめたものであり，得られた主な成果は以下の通りである．

1. 液滴に対する固体表面の動的濡れ性を表すモデルを組み込んだ気液二相流の数値解析により，平行溝型のマイクロ構造をもつ固体表面に衝突する液滴の衝突後の液膜広がりに異方性が生じること，また，溝幅の増大に伴い，最大広がりサイズや接触時間が減少し，固体表面の疎水性（撥水性）が向上することを明らかにした．また，より大きな溝幅をもつ表面に対しては，溝内に液体が浸透せずに空隙のままとなる Cassie 状態から，空隙が完全に消失する Wenzel 状態への遷移が起こるため，接触時間が増大し，疎水性が抑制される傾向に転じることを見出した．
2. 衝突液滴の反跳方向を制御することを目的として行った，平行溝の幅が空間的に変化する固体表面への液滴衝突の数値解析により，液滴の反跳方向は，衝突速度が大きくなるにつれて，真上方向，溝が密になる（溝幅が縮小する）方向，そして溝が疎になる（溝幅が拡大する）方向へと複雑に変化することを見出した．また，この挙動は，表面の濡れ状態（Cassie 状態，Wenzel 状態）が溝幅によって大きく変わり，液滴にはたらく界面張力の非対称性が生じることに起因することを明らかにした．
3. 複雑なマイクロ構造の例として提案した階層構造をもつ溝や多孔構造に対する数値解析により，これらの構造は衝突液滴が Wenzel 状態に遷移することを効果的に妨げ，大きな液滴速度条件においても固体表面の疎水性の維持を可能とすることを明らかにした．さらに，液滴の界面エネルギーと衝突時の粘性散逸に基づいて，液滴の広がりサイズを定量的に予測可能なモデルを提案した．

以上，本論文は，マイクロ構造をもつ固体表面への液滴衝突現象を対象に，複雑形状をもつ固体表面近傍の気液二相流を高精度に予測可能な数値解析手法を確立するとともに，固体表面にマイクロ構造を施すことによって濡れ特性を制御できる可能性を明らかにしたものであり，学術上，実際上寄与するところが少なくない．よって，本論文は博士（工学）の学位論文として価値あるものと認める．また，令和３年７月１６日，論文内容とそれに関連した事項について試問を行った結果，申請者が博士後期課程学位取得基準を満たしていることを確認し，合格と認めた．