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MICROTEXTURES INVERSELY DESIGNED FOR CASSIE-BAXTER WETTABILITY

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ABSTRACT

Wettability control has numerous applications in the areas of super-hydrophobicity, anti-drag, lubrication, liquid separation, self-cleaning coatings, etc. Texture morphology together with surface free energy determines the wettability of a substrate surface. Microtextures on a substrate surface can effectively change the surface free energy and further dominate the wetting behavior. Two different wetting modes can exist on a textured solid surface; they are the Wenzel and Cassie-Baxter modes. In the Wenzel mode, the liquid completely fills the microtextures. In the Cassie-Baxter mode, vapor pockets are trapped by the liquid/vapor interface supported on the microtextures. The wetting mode can transfer from the Cassie-Baxter case to the Wenzel case, when the liquid is physically pressed with removing the vapor pockets. In this mode transition, the hydrophobicity of a solid surface is decreased, because the surface free energy decreases along with the liquid filling of the microtextures. Several artificial microtextures have been reported to derive robust Cassie-Baxter wettability on a solid surface. They are widely designed by periodically arraying circular posts, square posts and tapered cones. Before our researches, more efficient inverse design methods were deficient for those microtextures. Therefore, it is advantageous to develop inverse design methods to efficiently acquire microtextures with enhanced robustness of Cassie-Baxter wettability.

The typical configurations of microtextures are the single-/over-layered and hierarchical geometries. Single-/over-layered geometries can be fabricated by the conventional lithography processes, which are typical top-down processes in microscale. Hierarchical microtextures can be fabricated by the bottom-up processes, e.g., two-photon polymerization. In the following, those geometries are inversely designed for three different symmetric tiles of a solid surface, and the lattices for these tiles are regular triangles, quadrangles, and hexagons (Figure 1).

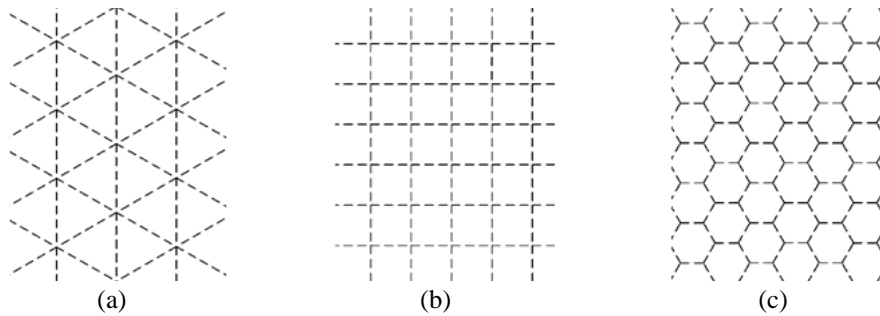


Figure 1: Demonstration of the tiling of a flat solid surface, using a regular (a) triangle, (b) quadrangle, (c) and hexagon respectively.

Among the current inverse design methods, topology optimization is the most efficient in determining the structural configurations [1-4]. The density method and level set method are two of the most widely used ones to implement the efficient gradient information-based topology optimization. Compared to the level set method, the density method has the merits of efficient and robust convergence, weak dependence on the initial guess of the design variable, and capability on dealing with multiple constraints. Therefore, density method-based topology optimization is adopted to inversely design the microtextures for Cassie-Baxter wettability.

For single-layered microtextures, robustness of the Cassie-Baxter wettability of a rough solid surface can be measured by the volume of the liquid bulges supported on the top of the microtextures. Smaller liquid-bulge volume corresponds to more robust Cassie-Baxter wettability. To minimize the liquid-bulge volume, we developed a topology optimization-based inverse design procedure for the discovery of suitable periodic microtextures, with synthetically considering the manufacturability as well as contact angle and surface-volume ratio of the liquid bulges [5]. Based on numerical calculations of the corresponding topology optimization problem, underlying effects are revealed for several factors, including the Bond number, duty ratio, feature size, and lattice constant. The effects of feature size and lattice constant provide approaches for compromisingly considering the robustness of the Cassie-Baxter mode and manufacturability of the inversely designed microtextures; the effect of the lattice constant permits the scaling properties of the derived microtextures, and this in turn provides an approach to avoid the elasto-capillary instability driven collapse of the micro/nanostructures in the derived microtextures. (Figure 2)

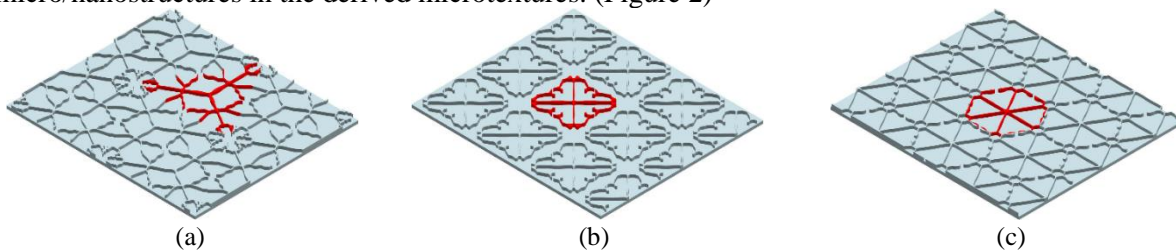


Figure 2: Inversely designed single-layered microtextures for the periodic tiles of regular triangle (a), quadrangle (b), and hexagon (c), respectively.

Overlaid microtextures are potentially more effective in ensuring the robustness of the Cassie-Baxter wetting performance, because of the layer-by-layer increase of the duty ratio and their effective approximation of the full hierarchy. By presenting a monolithic inverse design approach, composed of a series of topology optimizations, microtextures can be derived with hierarchy approximated by overlaid geometries as shown in Figure 3 [6]. In this optimization procedure, two sequential and neighboring optimization tasks are linked through the design domain of the downward layer, determined by an offset extension of the physical density representing the pattern of the upward layer. This ensures the manufacturability of the microtextures for an overlaid lithography process. Layer-by-layer robustness enhancement is thereby achieved, and the capability to anchor the three-phase contact lines after the collapse of the liquid/vapor interface supported by the upward layer.

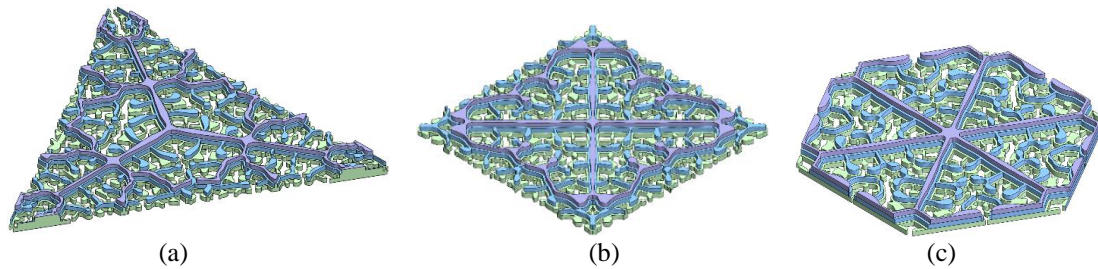


Figure 3: Inversely designed structure units for the overlaid microtextures with three layers, for the periodic tiles of regular triangle (a), quadrangle (b), and hexagon (c), respectively.

Hierarchical microtextures can be another more effective choice to achieve robust Cassie-Baxter wetting performance. They are composed of the base and secondary structures; and they can support more metastable statuses of Cassie-Baxter mode. To inversely design the hierarchical microtextures, we proposed a novel inverse design approach by using a topology optimization method combined with optimal control, where control and design variable are defined for a two-dimensional manifold corresponding to the morphology of the main structure and pattern of the secondary structure respectively. Then, the optimal match of the base-structure manifold and secondary-structure pattern is achieved on a solid surface with the three considered regular-polygon tiles. (Figure 4)

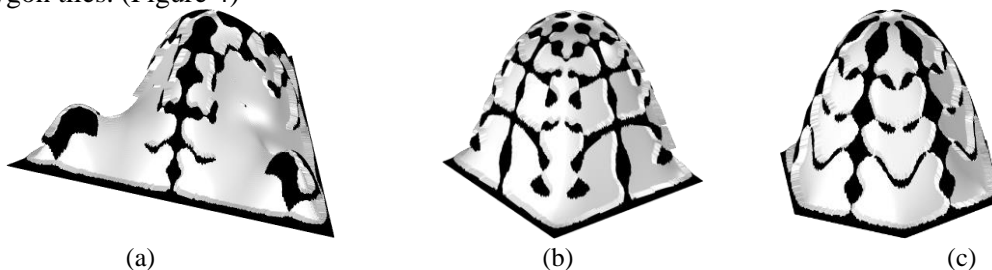


Figure 4: Inversely designed structure units for the hierarchical microtextures composed of base and secondary structures, for the periodic tiles of regular triangle(a), quadrangle(b), and hexagon(c) respectively.

In the future, we will explore the micro-/nano-fabrication of the derived hierarchical microtextures and experimentally test their wetting dynamics.

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