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Finite-volume-method Simulations of Automatic Droplet Transportation on Gradient Structures Driven by Laplace Pressure and Wettability Gradient

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Droplet transportation on the substrate plays a crucial role in applications such as drug delivery, medical diagnosis and micro assay. Many techniques for droplet transportation have been developed by using electric field, magnetic field, vibration and irradiation, but these techniques require external power sources. We demonstrate automatic droplet transportation driven by gradient wettability and Laplace pressure through FVM (finite-volume-method) simulations. Droplets on substrate with gradient wettability move directionally, but the driving force may not be enough for long distance transportation. Conical and wedgy structures offer a considerable driving force yielded by Laplace pressure for droplets motion, and droplets move easily toward the thick end on hydrophilic conical fiber, however it slows down or even stops when located in certain specific positions. Conical tubes and wedgy grooves exhibit similar performances. Structures combined gradient shapes and gradient wettability can conquer the problems and excellent droplet transportation ability is obtained. Wedgy structures are more suitable for large scale fabrication since they can be achieved through traditional IC (integrated circuit) process.

We have achieved the free energy, free energy gradient and velocity of the drops along the symmetry axis with the data exported from the simulation results. The driving force of the Laplace pressure and gradient wettability is not proportional to the velocity of the drop because the friction varies as the drop shape changes. Thus we introduce the ratio of the free energy gradient relative to the gravity in order to evaluate the driving force. The influence of parameters, such as half-apex angle, wettability and wettability gradient, on the performance of the gradient structures is analyzed and optimized. Meanwhile the side wall and bottom wall of the wedgy grooves can be designed and fabricated in different materials, which are also investigated to further optimize the structures.

Keywords: droplet transportation; wettability gradient; finite-volume-method; free energy gradient

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拉普拉斯压力和浸润性梯度驱动的梯度结构表面液滴自动输送仿真研究

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微液滴在基底上的输送在很多领域扮演重要角色，如药物输送、医学诊断、显微分析等。通过使用电场、磁场、震动和光照等方法，已经开发出了很多微液滴的输送技术，但是这些技术都需要外部能量来驱动。在浸润性梯度和拉普拉斯压力作用下，我们通过有限体积法仿真演示了液滴的自动输送过程。液滴在浸润性梯度表面能够定向移动，但是要获得较长距离的输送，它受到的驱动力还远远不够。锥形和楔形结构通过拉普拉斯作用力可以为液滴的定向移动提供足够的驱动力。液滴在锥形光纤表面的定向移动非常容易，然而，当液滴到达一定的位置时，液滴的运动变得非常缓慢甚至停止运动。锥管和楔形沟槽的结构也表现出类似的特性。结合形状梯度和浸润性梯度的结构可以很好地解决这个问题，并且表现出非常优异的液滴输送能力。楔形结构更适合规模化制备，这是由于楔形结构跟传统的集成电路制备工艺有很好的兼容性。

我们从仿真结果中得到了液滴的自由能、自由能梯度和速度沿对称轴的分布。液滴受到的拉普拉斯压力和浸润性梯度的驱动力跟液滴的运动并不成正比，这是由于液滴的摩擦阻力会随着液滴的形状改变而变化。因此，我们引入了自由能梯度跟重力的比值用于评价驱动力的大小，研究了半锥角、浸润性及浸润性梯度等参数对结构性能的影响，并对这些参数进行了优化。同时，由于楔形沟槽的侧壁和底部材料可以不一样，我们也对不同材料构成的楔形沟槽开展了了进一步的研究和优化。

关键词：液滴输送；浸润性梯度；有限体积法；自由能梯度