Theoretical Study of Water Contact Angle on Heterogeneous Surface via Coarse-Grained Molecular Dynamics

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Contact angle (CA) on solid surface is used to figure out the properties of materials in the various fields, due to its simple measurement. Although CA on the heterogeneous surface can be predicted by Cassie equation, it is only applicable to small pattern size compared to water droplet. However, it is hard to be applied because the size difference between water droplet and pattern is reduced due to miniaturization of materials. To resolve this issue, Cassie equation should be modified. In this study, modified Cassie equation and the morphology of water droplet were investigated via coarse-grained molecular dynamics. The model system was constructed with water droplet with 60 nm diameter on four types of heterogeneous surfaces. To apply the modified Cassie equation, contact line or contact area fraction was measured. As a result, CA from modified Cassie equation with contact area fraction was well matched with CA. Also, morphology of water droplet was confirmed that it has circular at small pattern and hexagonal at larger pattern. The cause of morphology change was explained with interaction and structure of water near the heterogeneous surface.