Supporting information

Molecular Dynamics Simulation of Nano-Droplets Impacting Stripe Textured Surface

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Content

S1. Variation of droplet temperature against time during impact

First, the droplet temperature increases rapidly with the spreading behavior after impacting the solid surface. Then the temperature decreases as the spreading rate of the droplet decreases. When the droplet reaches the maximum spreading state, the droplet temperature reaches the lowest point at the same time. Later, the droplet starts to contract and the temperature rises slightly. Finally the temperature stabilizes as the droplet breaks away from the surface.

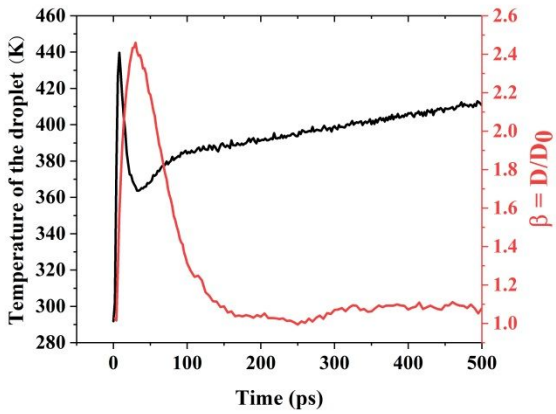

Figure S1. Variation of temperature and spreading factor β (D is the droplet diameter, D0 is the initial droplet diameter.) with time after a droplet impacting the plane at an initial velocity of 9 Å/ps.

S2. Comparison of simulation results with macroscopic experiments by normalized expansion factors and time

Here we define the contact factor $\lambda = L/D_0$, where L is the length of the contact region. We also define a characteristic time $\tau_c = (\rho d^3/\gamma_{lv})^{1/2}$ based on the free vibration period of the droplet proposed by Rayleigh [15], and dimensionless the time at different scales. According to the dimensional parameters of the texture structure in reference [20], we select the surface with ridged large period and texture bottom angle of 60 ° for comparison.

From Fig. S2 (a), we can see that the overall contact factor and the contact time obtained from our simulation are larger than those in the experiment [20]. The difference in contact factor is mainly due to the larger Weber number of simulated droplets. As can be seen in Fig. S2 (b), if dividing the contact factor by the maximum value, the trend of the spreading process of the droplets with time is basically the same. However, difference appears in the contraction process. We speculate that this is due to the difference in the size of the surface texture and the scale effect.

The size of the surface texture causes the difference in contact angle. The contact angle of the textured surface prepared in the reference [20] is 153.2° in the *x* direction and 152.5° in the *y* direction [20]. The simulated surface we used for comparison has a contact angle of 149.0° in the *x* direction and 146.27° in the *y* direction, both of which are slightly smaller than the experimental values [20]. In addition, it can be seen that although the Weber number of the nano-droplet is larger than that of the experimental droplet [20], the nano-droplet dose not produce splitting. Therefore, a significant difference from the macroscopic experiment is produced in the contraction process.

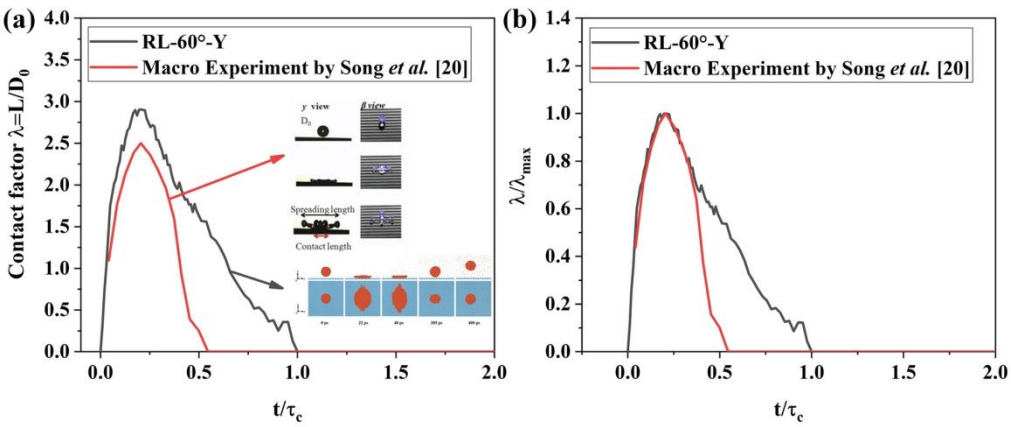

Figure S2. Validation of microscopic simulations and macroscopic experiments of droplet impact strip weaving. (a) The variation law of the contact factor $\lambda = L/D_0$ with time. (b) The variation law of the contact factor divided by the maximum value with time.