

ad **Chun-Wei Yao,** D; a ; M;chaca E<sub>s</sub>;; s, La a U ; , B;a , TX 77710, USA Add c a c correspondence of  $d_i$  and simulations to Ping H, a **[phe@lamar.edu](mailto:phe@lamar.edu)** Add; a c ; d; c; ; ; ; Ch -W; Ya a c ao@lamar.edu  $(R, c, ; d 23 Ma 2019; acc, ; d 27 J ; 2019)$ 

# Abstract

<span id="page-1-0"></span> $p^d$ e egd, h b id surfaces. In this paper, the pseudo-line tension is incorporated into a formally developed slip boundary developed slip boundary developed slip boundary of model to capture  $\int d\theta$  surfaces with nanoscale topological and or chemical heterogeneity. The inclined  $\Gamma$ plate method is used to measure the advancing and receding and as well as well as  $\mathcal{L}$  as  $\mathcal{L}$  conditions. Continuum of conditions. Continuum of  $\mathcal{L}$ simulations have been tested for four droplet sizes ranging  $\mathcal{L}^{\mathcal{A}}(T)$  for  $\mathcal{L}^{\mathcal{A}}(T)$  $f \left( \begin{array}{ccc} 1 & 30 & L \end{array} \right)$  on  $f \left( \begin{array}{ccc} 1 & 1 \end{array} \right)$  on a flat polytetrafluoroethylene (PTFE) sub $s_{\rm tot}$  . Numerical results have been compared with experimental results have been compared with experimental results of  $\sim$ ments, and good agreements have been found.

E perimental setup<br> $\frac{1}{1}$   $\begin{array}{ccc} 1 & \frac{1}{1} & \frac{1}{1} & \frac{1}{1} \\ \frac{1}{1} & \frac{1}{1} & \frac{1}{1} \\ \frac{1}{1} & \frac{1}{1} & \frac{1}{1} \end{array}$ In this study, we examine a water droplet sitting on a  $\mathbf{r}$ or inclined flat surface at room temperature. The droplet volumes used in the 4, 10, 20, and 30 L, and are deposited in the study are deposited in the  $4, 10, 20, 30$  L, ited and measured using a manual syringe. An experimental syringe. An experimental system of  $\mathbf{A}$ system was built for the sliding-angle measurement, which consisted of a rotation stage sub-system and an image capturing  $s = s$  as shown in Supplementary Fig. S1. The dynamics  $S = s$ images of droplets were captured using a high speed camera. The PTFE substrate was used after being cleansed in an ultra-

The unbalanced Young's stress will be nonzero only when ts goes beyond the two bounds in Eq. [\(9\)](#page-1-0) if ts , (<sup>g</sup>SLV<sup>k</sup>gs) ,

- <span id="page-3-0"></span>critical roll-off angle in the simulation are found the same as in the same as in the same as in the same as in the experiment. To valid at a dvancing and recently and recently stresses in  $\mathcal{A}$ Fig. 2(e) are the unique stress pairs are tested pa in simulations, and two of them are shown in Fig. 2(c),  $(\begin{array}{cc} S_{\rm L} \end{array})^{\bullet} = 5 \quad N / \quad , (\begin{array}{cc} S_{\rm L} \end{array})^{\bullet} = -80 \quad N / \quad , \quad F \quad . \quad 2$ ( ), (  $_{SL}$  ) = 50 N/, (  $_{SL}$  ) = −10 N/ T two in Figs. 2(c) and 2(e) are two extreme conditions: (i)  $\frac{1}{\sqrt{1-\frac{1}{2}}}$ erogeneity of strong adhesion on the recent site in Fig. 2(c) and (ii) heterogeneity of strong adhesion on the advancing addition on the advancing  $\mathcal{I}$ site in Fig. 2(d). Both cases  $\mathbf{F}$  and  $\mathbf{F}$  are away far awa
- from the experiment, and both droplets do not roll of the plate  $\frac{H}{\rho}$ at the tilting angle of  $49.2^{\circ}$ . Especially, we note that when  $\mathcal{L}$  $\binom{K}{\text{SL}}$   $\binom{V}{\text{SL}}$   $\binom{V}{\text{SL}}$



A 30 µL droplet on a tilted plate A 30 L dropped has a much smaller critical roll-off angle than  $\mathcal{H}$ the 20  $L$  droplet presented in the presented in the previous subsection, because subsection, because subsection, because  $L$ the droplet weight increases  $T$  increases. The average critical roll-off angles and  $T$ is 22.6  $I^*$  30 L, and the experimental case, whose case, whose case, whose case, whose case, whose case, whose critical case, whose contract case, whose case, whose case, whose case, whose case, whose case, whose case,  $t_1$  co $2$  plent is  $0^{t-t}$ .

 $N'$ , −10  $N'$ ), (3  $N'$ , −80  $N'$ ),  $(50 N'$ ,  $-5$  N/). A<sub>lthough</sub> (14 N/m, −10 N/m) is not f to the correct stress pair, its contour plotted in red clearly deviates from the experimental shape. Supplementary Figure S7 presents the three-dimensional view of the droplet contours at  $\mathcal{I}_\text{a}$  $(10 \text{ N}/\text{N} , -14 \text{ N} /), (3 \text{ N} , -80 \text{ N} /),$  (50 N/  $m, -5$  N/m) and the contact lines.

Equilibrium, advancing and receding contact angles

The experimental and simulation results of contact angles are presented in Supplementary Fig. S8. Error bars are shown for experimental data, while our simulations do not have an obvious error, since the continuum model itself is a deterministic system. The hysteresis in the experiments of 4, 10, 20, and 30 µL droplets are 16.7°, 29.3°, 32.3°, and 21.7°, respectively. Our simulation results agree well with the experiments, and most numerical contact angles fall into the experimental ranges, except for the advancing contact angle in the 20 µL case, whose value is just slightly below the lower bound. In addition, a water droplet on a copper substrate has been studied experimentally and numerically in this paper. Experimental and simulation results of 4, 10, 20, and 30 µL water droplets are presented in Sect. 8 of the Supplementary Material. Our simulation results match well with the experiments.

Discussions on pseudo-line tensions



## Concluding remarks

A N–S<sub>t</sub><sup>t</sup></sub> slip boundary model for the contact line dynamics  $\frac{f}{1-\frac{12}{10}}$ has been developed in our previous work.  $\frac{1}{\sqrt{2}} \prod_{i=1}^{n} \frac{1}{\sqrt{2}}$ model is extended to capture  $\mathbb{C}$ AH using the advancing the advancing the advancing and advancing and advancing and and advancing and and advancing the advancing  $\mathbb{C}$ receding pseudo-line tensions, which represent either or both the topological and chemical heterogeneity in the nanoscale on a solid surface. Based on the pseudo-line tensions, the pseudo advancing and receding pseudo-line stresses are calibrated using the tilting plate method through comparisons between simulations and experiments. For dropperiments  $f \cdot 4$  to  $4$  $30 \mathrm{L}^{\prime}$  have been rigorously experimented and simulated. Good agreements have been found between  $\mathcal{F}_k$ experiments for all the contact angles and contact angles and critical roll-official roll-offic and  $\mathbf{M}^{\mathbf{t}}$  is study reveals that pseudo-line tension  $\frac{1}{\sqrt{1-\frac{1$ line tension varies at the advancing and receding modes, droplet sizes, and tilting angles. Future studies are needed to the studies of the studies are needed to the studies of the studies of the studies of the s develop a constitutive relation between pseudo-line tension and interacting model developed in this is a set of  $\mathbb{T}$ paper can be utilized to model a liquid droplet interacting with higherarchical surfaces in which the microscale roughness  $\frac{1}{2}$ is modeled as the domain boundary and nanoscale roughness is modeled using pseudo-line tensions.

## Supplementar material

The supplementary material for this article can be found at  $\mathcal{F}_{\text{in}}$  are for this article can be found at  $\mathcal{F}_{\text{in}}$ :// . . /10.1557/<sup>1</sup> .2019.92.

#### Acknowledgments

 $T$ <sub>d</sub> (REG) A<sub>rt</sub> and  $LU^{\dagger}$ <sup>2018 R</sup>esearch E G  $e^{i\theta}$  (REG) A  $e^{i\theta}$  supporting the support of supporting the support of  $f$  for support of  $f$  for  $f$ where we have  $\mathbb{C}$  supported by  $\mathbb{C}$  supported by  $\mathbb{C}$  and  $\mathbb{C}$  in  $\mathbb{C$  $M$   $M$   $A$   $\downarrow$  CAPM<sup> $\downarrow$ </sup>  $L$ <sup> $\downarrow$ </sup>  $U$ <sub> $\downarrow$ </sub>  $t_A = \frac{T_A}{f} + \frac{R}{f}$  (TACC) UT  $A = \int_{0}^{1} \left( \int_{0}^{\frac{\pi}{4}} \frac{1}{\sqrt{2}} \right) e^{-\frac{\pi}{4}} dx$  (grant #G-819854).  $\mathcal{C}$  the Center for  $\mathcal{C}$  innovation,  $\mathcal{C}$  $E_{\text{t}}$   $\begin{array}{ccc} 1 & 1 & 0 \\ 1 & 0 & 0 \end{array}$  (CICE)  $\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 0 & 0 \end{array}$  w. P.  $\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 0 & 0 \end{array}$  $A$ <sup>D. H</sup>sing-C<sub>h</sub> M. Paul L<sub>1</sub>f<sub>1</sub>f cussions and encouragement. We then  $\mathbb{E} \left[ \mathbf{I}^T \mathbf{I} \right]$  $\frac{D}{M}$ ,  $\frac{1}{C}$  for  $\frac{1}{C}$  for  $\frac{1}{C}$  for  $\frac{1}{C}$  for  $\frac{1}{C}$  $t$  M. C is  $t$  is the HPC maintenance.

#### **References**

1. H.B. Ea, D.J.C.M. 'Mannethian', and J.M. Oh: Contact angle for  $i$ , and  $j$  $r, r, r$  dant and and applications. Colloid Polym. Sci 291, 247  $(2013)$ .

- 2. R. D., M. Harno. V. Thom, R. Boh, b, and V. S, carries. 2. Gouten angle hysteresis originates original to the contract of  $a$  investigation on  $a$  investigation on  $a$
- S*oft Matter* **7**, 9380 (2011).<br>3. L.C. Gaoad T.J. McCah: Coacoa کین پنجاب and T.J. McCah: Coacoa L*angmuir* **22**, 6234 (2006).<br>4. J.W. G bb , H.A. B , ad, a d R.G. Va Na , : *The Scientific Papers of*
- J. Willard Gibbs (L<sub>og</sub>a, G;; ad Ca, N; -Yad B ba, 1906), . 288.
- 5. L. Baad A.W. N; a : G; ; a a h; cacah; ca a *. J. Chem. Phys.* **66**, 5464 (1977).<br>6. N.L. G; ነ; dad R.J. God: L; ;ad i; ;; a ac;
- for bases, by an oil details drop. Biol. 17, 246 (1967).
- 7. R.J. God and M.N. Ko: The effect of definition and  $\epsilon$ , i.d. Colloid Interface Sci. 71, 283 (1979).
- 8. J. D  $\zeta$  of a d J.D. M  $\zeta$ : Th $\zeta$ ,  $\zeta$  c ac,  $\zeta$  i,  $\zeta$  c  $\zeta$  i,  $\zeta$  c  $\zeta$  i,  $\zeta$  and  $\zeta$  i,  $\zeta$  i,  $\zeta$  and  $\zeta$  is (1992).
- 9. J. Drefich and J.D. Miller: The line of the line tension in the line of the line of the line tension in the line of the line of the line o  $t_i$  . Particul. Sci. Technol. 10, 1 (1992).