



## Wettability transparency and the quasiuniversal relationship between hydrodynamic slip and contact angle

Bladimir Ramos-Alvarado, Satish Kumar, and G. P. Peterson

Citation: Applied Physics Letters **108**, 074105 (2016); doi: 10.1063/1.4942400 View online: http://dx.doi.org/10.1063/1.4942400 View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/108/7?ver=pdfcov Published by the AIP Publishing

Articles you may be interested in A numerical approach for the direct computation of flows including fluid-solid interaction: Modeling contact angle, film rupture, and dewetting Phys. Fluids **28**, 062002 (2016); 10.1063/1.4949522

Wettability and friction of water on a MoS2 nanosheet Appl. Phys. Lett. **108**, 131601 (2016); 10.1063/1.4944840

Forced wetting and hydrodynamic assist Phys. Fluids **27**, 112101 (2015); 10.1063/1.4934703

Needle-free drop deposition technique for contact angle measurements of superhydrophobic surfaces J. Appl. Phys. **116**, 114903 (2014); 10.1063/1.4895779

Droplet contact angle behavior on a hybrid surface with hydrophobic and hydrophilic properties Appl. Phys. Lett. **101**, 111605 (2012); 10.1063/1.4752470



euse of AIP Publishing content is subject to the terms at: https://publishing.aip.org/authors/rights-and-permissions. Download to IP: 143.215.17.175 On: Thu, 22 Sep 201



## Wettability transparency and the quasiuniversal relationship between hydrodynamic slip and contact angle

Bladimir Ramos-Alvarado, Satish Kumar, and G. P. Peterson<sup>a)</sup>

The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

(Received 11 January 2016; accepted 7 February 2016; published online 19 February 2016)

The universality of the scaling laws that correlate the hydrodynamic slip length and static contact angle was investigated by introducing the concept of the wettability transparency of graphene-coated surfaces. Equilibrium molecular dynamics simulations of droplet wettability for Si(111), Si(100), and graphene-coated silicon surfaces were performed to determine the conditions required to obtain similar contact angles between bare and graphene-coated surfaces (wettability transparency). The hydrodynamic slip length was determined by means of equilibrium calculations for silicon and graphene-coated silicon nanochannels. The results indicate that the slip-wettability scaling laws can be used to describe the slip behavior of the bare silicon nanochannels in general terms; however, clear departures from a general universal description were observed for hydrophobic conditions. In addition, a significant difference in the hydrodynamic slippage was observed under wettability transparency conditions. Alternatively, the hydrodynamic boundary condition for silicon and graphene-coated silicon nanochannels was more accurately predicted by observing the density depletion length, posing this parameter as a better alternative than the contact angle to correlate with the slip length. © 2016 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4942400]

The solutions obtained for the Navier-Stokes equations bounded by the no-slip condition represent a fundamental basis for classical fluid dynamics and also serve as a foundation upon which other fundamental transport phenomena can be described. While the Navier-Stokes equations are derived from a physically sound model, the no-slip boundary condition is an empirical assumption not supported by any physical principles.<sup>1</sup> The early work of Navier,<sup>2</sup> first defined the slip boundary condition as

$$u_{\rm s} = L_{\rm s} \frac{\partial u}{\partial z} \Big|_{z_0},\tag{1}$$

where  $u_s$  is the slip velocity,  $\partial u/\partial z$  is the velocity gradient evaluated at the solid-liquid interface  $z_0$ , and  $L_s$  is the slip length (distance required to reach the no-slip condition after a linear extrapolation of the velocity profile).

The no-slip boundary condition is typically observed in macroscale flows; however, slip conditions have been reported, both experimentally<sup>3–5</sup> and numerically<sup>6–9</sup> for flow of nanoconfined liquids. A majority of the numerical investigations of nanochannels hydrodynamics have been focused on the determination of the nature of the boundary condition as indicated in Eq. (1), but other higher order formulations have also been reported.<sup>9</sup> The shear rate (for shear-driven flows) or driving force (for force-driven flows), confinement size, roughness, and wettability of the nanochannels walls are all among the primary parameters affecting the nature of the boundary condition ( $L_s$ ). Different responses of  $L_s$  to an increasing magnitude of the driving mechanism, such as unbounded growth,<sup>10,11</sup> bounded growth,<sup>12</sup> and decaying,<sup>13</sup>

systems, these different observations have been explained in terms of the modeling of the solid dynamics and fluid thermostating.<sup>14,15</sup> Changes are expected in the fluids properties as the size of the systems decrease due to the enhancement of the surface effects and a simple scale analysis indicates that water can maintain its bulk density down to 1 nm.<sup>16</sup> It has also been numerically demonstrated that water exhibits bulk flow behavior through carbon nanotubes as small as 1.4 nm in diameter.<sup>17</sup> Other investigations also indicate that  $L_{\rm s}$  tends to remain unaffected in confinement sizes above ten molecular diameters.<sup>18,19</sup> In the current investigation, size and shear rate affects were eliminated by using equilibrium calculations of the hydrodynamic slip (compared to non-equilibrium low-shear rate simulations) in nanochannels large enough to avoid the size-affected properties.

Previous investigations have indicated that the wettability of the nanochannels walls (solid-liquid affinity) can be correlated with the hydrodynamic slippage. A quasiuniversal relationship  $L_{\rm s} \sim (1 + \cos \theta)^{-2}$ , where  $\theta$  is the contact angle, was derived by Huang *et al.*<sup>20</sup> Additionally, they found that  $L_{\rm s}$  scaled with the interfacial liquid structure as  $L_{\rm s} \sim \delta^4$ , where  $\delta$  is the liquid density depletion length. Sendner et al.<sup>21</sup> proposed the scaling law,  $L_{\rm s} \sim (180^{\circ} - \theta)^{-2}$ , suggesting that it was more physically sound than the previous relationship due to a better interpretation of the limit  $\theta \rightarrow$ 180° in a wettability model. No noticeable difference was observed between the contact angle scaling laws when compared to the numerical calculations of  $L_s$ .<sup>21</sup> The slipwettability scaling laws were derived from a scaling analysis performed on a simple wettability model. The contact angle was found to be linearly correlated with the energy parameter ( $\epsilon$ ) of the Lennard-Jones potential used to describe the non-bonded solid-liquid interactions. However, it has been reported that not only the energy parameter but also the

euse of AIP Publishing content is subject to the terms at: https://publishing.aip.org/authors/rights-and-permissions. Download to IP: 143.215.17.175 On: Thu, 22 Sep 20:

<sup>&</sup>lt;sup>a)</sup>Electronic mail: bud.peterson@gatech.edu

length parameter ( $\sigma$ ) of the non-bonded interaction potential affect  $\theta$  and  $L_s$  as obtained from MD simulations in an opposite manner.<sup>11</sup>

The universality of the slip-wettability scaling laws can be evaluated by introducing the wettability transparency of graphene coated substrates.<sup>22</sup> By calculating  $L_s$  on two surfaces having the same contact angle, where one is coated with graphene, the robustness of these quasiuniversal relationships can be assessed. In the current investigation, equilibrium molecular dynamics (EMD) simulations were used to determine the contact angle on two silicon surfaces, Si(111)and Si(100), and the graphene-coated version of these surfaces wetted by water. The equilibrium theory of Huang and Szlufarska<sup>23</sup> was used to calculate the solid-liquid friction coefficient and L<sub>s</sub> in silicon and graphene-coated silicon nanochannels. The wettability of different silicon planes was artificially varied for comparison purposes, but unlike previous investigations, L<sub>s</sub>, was calculated in nanochannels made of different surfaces with the same contact angle as demonstrated by experiments.

The contact angle on Si(100), Si(111), and the graphenecoated version of these surfaces was calculated using EMD simulations of cylindrical droplet wettability.<sup>24</sup> Silicon and graphene-coated silicon nanochannels, having the same configuration as the wettability simulations were used for the  $L_s$  calculations. The structure of graphene was stretched no more than 4% in order to create periodic structures matching the underlying silicon substrate. The confinement size was 5 nm for every nanochannel and the area was  $5.76 \times 5.98$  nm for Si(111) and  $5.97 \times 5.97$  nm for Si(100), see Fig. S1.<sup>25</sup> The channels size was constrained by fixing the position of the outermost solid atomic layers. LAMMPS<sup>26</sup> was used to perform the simulations and VMD<sup>27</sup> for visualization. The SPC/E model<sup>28</sup> was used for modeling the water, the SHAKE<sup>29</sup> algorithm was used to enforce the rigidity of the SPC/E model, and the long-range Coulombic interactions were treated with the PPPM<sup>30</sup> algorithm with an accuracy of  $1 \times 10^{-6}$ . The nonbonded carbon-water and silicon-water interactions were modeled with truncated Lennard-Jones potentials by taking into account only the interactions with oxygen, where  $\sigma_{\rm CO} =$ 3.19 Å,  $\epsilon_{CO} = 0.4736$  kJ/mol, and a 15 Å potential cut-off  $(\theta = 64.4^{\circ})$ ;<sup>24</sup>  $\sigma_{\text{SiO}} = 2.635$  Å and  $\epsilon_{\text{SiO}}$  was varied to induce different wettability conditions. Tersoff<sup>31</sup> potential was used for modeling the Si-Si interactions in a many-body fashion. The time step for the integration of the equations of motion was 1 fs for all types of simulations.

The wettability of pristine ( $\theta_{\rm S}$ ) and graphene-coated ( $\theta_{\rm GS}$ ) silicon surfaces was theoretically and numerically investigated in order to determine the macroscopic conditions, substrate contact angle  $\theta_{\rm S}$ , required to observe wettability transparency for graphene-coated silicon. The results illustrated in Fig. 1 indicate that the theoretical model reported in Ref. 32 is sufficiently accurate to predict the wettability of graphene-coated silicon. Two different values for the equilibrium separation between graphene and silicon ( $\delta_{\rm GS}$ ) were considered, since this parameter is the only unknown in the theoretical model of wettability.<sup>32</sup> Some authors have reported values of  $\delta_{\rm GS} = 3.55$  Å, a value obtained through mixing rule approximations of the interaction potentials,<sup>33</sup> while recent experiments<sup>34,35</sup> and



FIG. 1. Wettability of pristine and graphene-coated silicon surfaces. The MD simulations results (symbols) verify the theoretical predictions (solid lines) of the wettability of graphene-coated silicon. Two different values for the equilibrium distance between graphene and silicon ( $\delta_{GS}$ ) were used for validation. The shaded region represents the wettability transparency condition with a  $\pm 2.5^{\circ}$  deviation from  $\theta_{S} = \theta_{GS}$ .

simulations<sup>36</sup> suggest that  $\delta_{\text{GS}} \approx 2.0$  Å. Hence,  $\delta_{\text{GS}} = 2.0$  Å was adopted for the remaining of this investigation. Such an equilibrium distance was enforced by defining the nonbonded Si-C interaction potential parameters as  $\sigma_{\text{SiC}} = 2.1$  Å while  $\epsilon_{\text{SiC}}$  was varied in a wide range. The results indicated no noticeable differences in the  $L_{\text{s}}$  calculations.

The nanochannel hydrodynamics simulations were conducted in such a way that similar bulk water properties were achieved for every case (for more information, see the supplementary material<sup>25</sup>). Because the wettability of the surfaces varied, the pressure required to reach the same bulk density changed as a function of the contact angle.<sup>37</sup> Hence, the number of water molecules within the 5 nm channel varied from 5776 to 5668 to cover the range from hydrophilic to hydrophobic wall conditions, respectively. The equilibrium theory proposed by Huang and Szlufarska<sup>23</sup> was used to calculate the friction coefficient  $\lambda$ , and then  $L_s = \eta/\lambda$  where  $\eta =$  $0.729 \times 10^{-3}$  Pa-s is the shear viscosity of SPC/E water.<sup>38</sup> The  $L_s$  calculation originates from the viscous law correlating the shear friction force and the slip velocity through the friction coefficient  $\lambda$ . Huang and Szlufarska<sup>23</sup> used linear response theory and the general Langevin equation to derive a relationship to accurately predict  $\lambda$  from EMD simulations. Alternatively, the molecular kinetics theory (MKT) of wetting<sup>39</sup> poses an opportunity to deepen into the relationship between wettability and slip, although the MKT was not developed for confined liquids, it could be useful for future research.

Fig. 2(a) depicts the MD calculations of  $L_s$  as a function of  $\theta$  and the curve fit of the slip-wettability scaling laws. A non-linear least-squares algorithm was used to perform the curve fittings, where only a single parameter was determined for each scaling law. The R<sup>2</sup> values were 0.74 and 0.82 for the scaling laws involving  $1 + \cos(\theta)$  and the one involving  $180^{\circ} - \theta$ , respectively. Two aspects can be highlighted regarding the bare silicon nanochannels results: (1) the simulation results seem to follow the trends predicted by both scaling laws; although,  $L_s \sim (180^{\circ} - \theta)^{-2}$  seems to be a better match for both, Si(111) and Si(100), nanochannels; (2) it is consistently observed that for  $\theta > 100^{\circ}$  the slip behavior is different, being the Si(111) surface more prone to



FIG. 2. Hydrodynamic slip behavior of silicon and graphene-coated silicon nanochannels with respect to (a) the contact angle and (b) the depletion length. The insets are close up views of the points near the *x*-axis.

hydrodynamic slippage than the Si(100) surface. When the wettability transparency condition is examined (both silicon surfaces have a contact angle of  $\sim 71^{\circ}$  for  $\delta_{GS} = 2.0$  Å, see Fig. 1), a significant departure from the slip-wettability scaling laws is observed in Fig. 2(a). These results suggest that the scaling laws that use the contact angle as a quasiuniversal parameter are not robust.

In addition to the quasiuniversal scaling laws of hydrodynamic slip, Huang *et al.*<sup>20</sup> observed the relationship  $L_{\rm s} \sim \delta^4$ , which was derived from the observed dependence of  $\delta$  on the solid-liquid interaction parameter  $\epsilon$  and the scaling performed on an equilibrium model of slip.<sup>40</sup> Fig. 2(b) illustrates  $L_{\rm s}$  as a function of  $\delta$ , obtained as

$$\delta = \int_{0}^{\infty} \left[ 1 - \frac{\rho_{\rm s}(z)}{\rho_{\rm s}^{\rm b}} - \frac{\rho_{\rm l}(z)}{\rho_{\rm l}^{\rm b}} \right] dz,\tag{2}$$

where  $\rho_s(z)$  and  $\rho_1(z)$  are the solid and liquid densities along the z-direction (height) of the nanochannel, and  $\rho_s^b$  and  $\rho_1^b$  are the bulk solid and liquid densities.  $\delta$  represents a measurement of the water depletion that exists due to the short-range repulsion between the solid and liquid atoms, see Fig. S3.<sup>25</sup> It is clearly observed that the scaling law  $L_s \sim \delta^4$  features a better prediction of the nature of the boundary condition (R<sup>2</sup>=0.97), regardless of the contact angle or the characteristics of the channel walls. Fig. 2(b) indicates that  $L_s$  is different for hydrophobic silicon nanochannels ( $\theta > 100^\circ$ ) because the depletion length is more prominent in Si(111) than Si(100) surfaces.<sup>32</sup> similar to the hydrophobic Si(111) can be explained by recognizing that both surfaces exhibit similar  $\delta$  values. Thus, Fig. 2(b) helps to reconcile the results reported in Fig. 2(a) for the three different types of nanochannels and remark the strong correlation between  $L_s$  and  $\delta$ .

During the derivation the slip-wettability quasiuniversal relationships, Huang et al.<sup>20</sup> and Sendner et al.<sup>21</sup> observed the scaling law  $1 + \cos(\theta) \sim \epsilon$  after simplifying a mean-fieldtheory-based wettability model. This expression was fundamental in the development of the slip-wettability laws and is in fact correct, as has been previously demonstrated in Ref. 21 and by others;<sup>24</sup> however, this assumption is only applicable for specific situations. The robust wettability model based on the mean-field theory, reported in Ref. 32, indicates that the contact angle depends on the  $\epsilon$  and  $\sigma$  parameters of the nonbonded solid-liquid interaction potential, the interfacial liquid structure, the planar atomic density of the solid atoms, and the underlying structure of the wetted surface, i.e., the solid structure anisotropy also plays a role in nanoscale wettability. This functional dependence is coupled and no single effect can be isolated, with the exception of  $\epsilon$  at some level. Therefore, the simplification made by Huang *et al.*<sup>20</sup> to obtain  $1 + \cos(\theta) \sim$  $\epsilon$  is valid only when the rest of the aforementioned variables are lumped into a single constant; hence, the quasiuniversal prefix of these laws is justified. Additionally, the process followed to obtain a given contact angle from MD simulations is one of calibration. The process consists of fixing one of the two non-bonded solid-liquid interaction parameters and varying the other until obtaining an objective contact angle for a given solid structure. This explains why the wettability of Si(100) is different than that of Si(111) when using the same silicon-water interaction potential,<sup>32</sup> in addition that both planes feature different density depletion when wetted, due to the anisotropy of the silicon crystal.

The hydrodynamic slip phenomenon is one of interfacial nature. Thus, a better description of  $L_s$  can be obtained when the interfacial liquid structure is considered ( $\delta$ ). The density depletion length,  $\delta$ , indicates that as the equilibrium separation between the solid and liquid atoms increases, hydrodynamic slippage is prone to occur due to the reduction of the momentum transfer between solid and liquid particles. For a nonbonded interaction, the equilibrium distance between a pair of atoms scales as  $d_{\rm eq} \sim \sigma$ . Hence, the interfacial water depletion is directly affected while the calibration process for the calculation of the contact angle is merely adjusted. Likewise, the magnitude of  $\sigma$  affects the energy corrugation of the solidliquid interaction potential, in combination with the structure of the wetted solid. For the particular systems under investigation, Fig. 3 depicts the attractive potential energy field generated between water and the first layers of solid atoms. It can be observed how the low atomic planar density Si(100) surface features a rough energy landscape with deep potential wells where liquid particles can be entrained. This explains the small values of  $\delta$ , as illustrated in Fig. 2(b) and Fig. S3.<sup>25</sup> Alternatively, the Si(111) structure features a smoother energy landscape, mainly due to the larger planar atomic density and the closely packed bilayer structure of this silicon plane. Finally, the closely packed structure of graphene in combination with a large value of the  $\sigma_{CO}$  parameter generates a flat energy landscape, above which the water molecules are only



FIG. 3. Corrugation of the solid-liquid interaction potential for (a) Si(100), (b) Si(111), and (c) graphene-coated silicon surfaces (only showing the carbon atoms). The units are kJ/mol and only the attractive potential is depicted.

affected by the magnitude of the interaction strength and not the granularity of the underlying solid substrate. This smooth energy surface helps to explain the higher values of  $L_s$  under wettability transparency conditions and the small differences observed for Si(100) and Si(111) graphene-coated channels. As it is shown in Table S1,<sup>25</sup> the silicon-water interaction strength is always greater for Si(100) than for Si(111) in order to balance the lower atomic density of the 100 plane for obtaining similar contact angles.

The wettability transparency of graphene-coated silicon surfaces was used to demonstrate the lack of generality of the hydrodynamic slip-wettability scaling laws, and the robustness of the scaling law that suggests a relationship between the interfacial liquid structure and the slip length. Because the atomistic modeling of wettability is a calibration process, the quasiuniversal relationship between the slip length and contact angle broke down when the wettability transparency phenomenon was introduced. In other words, the actual complexity of the wettability phenomenon invalidated the simple approximations used in deriving the slipwettability scaling laws. The results obtained indicate that the liquid density depletion length is a better alternative in the prediction of the hydrodynamic boundary condition in nanoconfined liquid flows. This work was supported in part by the Mexican Council on Science and Technology (CONACyT) under the scholarship 312756.

- <sup>1</sup>D. C. Tretheway and C. D. Meinhart, Phys Fluids 14, L9 (2002).
- <sup>2</sup>C. L. Navier, Mem. Acad. Sci. Inst. Fr. **6**, 389 (1823).
- <sup>3</sup>D. Lasne, A. Maali, Y. Amarouchene, L. Cognet, B. Lounis, and H. Kellay, *Phys. Rev. Lett.* **100**, 214502 (2008).
- <sup>4</sup>D. Schaeffel, S. Yordanov, M. Schmelzeisen, T. Yamamoto, M. Kappl, R. Schmitz, B. Dnweg, H.-J. Butt, and K. Koynov, Phys. Rev. E **87**, 051001(R) (2013).
- <sup>5</sup>O. I. Vinogradova, K. Koynov, A. Best, and F. Feuillebois, *Phys. Rev.* Lett. **102**, 118302 (2009).
- <sup>6</sup>C. Liu and Z. Li, Phys. Rev. E 80, 036302 (2009).
- <sup>7</sup>C. Liu and Z. Li, AIP Adv. 1, 032108 (2011).
- <sup>8</sup>H. Zhang, Z. Zhang, and H. Ye, Microfluid. Nanofluid. **12**, 107 (2011).
- <sup>9</sup>H. Zhang, Z. Zhang, Y. Zheng, and H. Ye, Phys. Rev. E **81**, 066303 (2010).
- <sup>10</sup>P. A. Thompson and S. M. Troian, Nature **389**, 360 (1997).
- <sup>11</sup>R. S. Voronov, D. V. Papavassiliou, and L. L. Lee, J. Chem. Phys. **124**, 204701 (2006).
- <sup>12</sup>A. Martini, H. Y. Hsu, N. A. Patankar, and S. Lichter, Phys. Rev. Lett. 100, 206001 (2008).
- <sup>13</sup>A. A. Pahlavan and J. B. Freund, Phys. Rev. E 83, 021602 (2011).
- <sup>14</sup>S. Bernardi, B. D. Todd, and D. J. Searles, J. Chem. Phys. **132**, 244706 (2010).
- <sup>15</sup>S. De Luca, B. D. Todd, J. S. Hansen, and P. J. Daivis, J. Chem. Phys. 140, 054502 (2014).
- <sup>16</sup>L. Bocquet and E. Charlaix, Chem. Soc. Rev. **39**, 1073 (2010).
- <sup>17</sup>J. A. Thomas and A. J. H. McGaughey, Phys. Rev. Lett. **102**, 184502 (2009).
- <sup>18</sup>J. Xu and Y. Li, Int. J. Heat Mass Transfer **50**, 2571 (2007).
- <sup>19</sup>J. A. Thomas and A. J. H. McGaughey, Nano Lett. 8, 2788 (2008).
- <sup>20</sup>D. M. Huang, C. Sendner, D. Horinek, R. R. Netz, and L. Bocquet, Phys. Rev. Lett. **101**, 226101 (2008).
- <sup>21</sup>C. Sendner, D. Horinek, L. Bocquet, and R. R. Netz, Langmuir 25, 10768 (2009).
- <sup>22</sup>J. Rafiee, X. Mi, H. Gullapalli, A. V. Thomas, F. Yavari, Y. F. Shi, P. M. Ajayan, and N. A. Koratkar, Nat. Mater. 11, 217 (2012).
- <sup>23</sup>K. Huang and I. Szlufarska, Phys. Rev. E 89, 032119 (2014).
- <sup>24</sup>B. Ramos-Alvarado, S. Kumar, and G. P. Peterson, J. Chem. Phys. 143, 044703 (2015).
- <sup>25</sup>See supplementary material at http://dx.doi.org/10.1063/1.4942400 for more information.
- <sup>26</sup>S. Plimpton, J. Comput. Phys. **117**, 1 (1995).
- <sup>27</sup>W. Humphrey, A. Dalke, and K. Schulten, J. Mol. Graphics Modell. 14, 33 (1996).
- <sup>28</sup>H. J. C. Berendsen, J. R. Grigera, and T. P. Straatsma, J. Phys. Chem. 91, 6269 (1987).
- <sup>29</sup>J.-P. Ryckaert, G. Ciccotti, and H. J. Berendsen, J. Comput. Phys. 23, 327 (1977).
- <sup>30</sup>R. W. Hockney and J. W. Eastwood, *Computer Simulation using Particles* (CRC Press, 1989), p. 540.
- <sup>31</sup>J. Tersoff, Phys. Rev. B **38**, 9902 (1988).
- <sup>32</sup>B. Ramos-Alvarado, S. Kumar, and G. Peterson, J. Chem. Phys. 144, 014701 (2016).
- <sup>33</sup>M. Shen, P. K. Schelling, and P. Keblinski, Phys. Rev. B 88, 045444 (2013).
- <sup>34</sup>O. Ochedowski, G. Begall, N. Scheuschner, M. El Kharrazi, J. Maultzsch, and M. Schleberger, Nanotechnology 23, 405708 (2012).
- <sup>35</sup>Y. Xu, K. T. He, S. W. Schmucker, Z. Guo, J. C. Koepke, J. D. Wood, J. W. Lyding, and N. R. Aluru, Nano Lett. **11**, 2735 (2011).
- <sup>36</sup>C. Tayran, Z. Zhu, M. Baldoni, D. Selli, G. Seifert, and D. Tomanek, Phys. Rev. Lett. **110**, 176805 (2013).
- <sup>37</sup>J. L. Barrat and L. Bocquet, Faraday Discuss. **112**, 119 (1999).
- <sup>38</sup>M. A. Gonzalez and J. L. F. Abascal, J. Chem. Phys. **132**, 096101 (2010).
  <sup>39</sup>E. Bertrand, T. D. Blake, V. Ledauphin, G. Ogonowski, J. De Coninck, D. Fornasiero, and J. Ralston, Langmuir **23**, 3774 (2007).
- <sup>40</sup>L. Bocquet and J. L. Barrat, Phys. Rev. E **49**, 3079 (1994).