2012

Nanoscale surface roughness affects low Reynolds number flow: Experiments and modeling

Robert Jaeger  
_Iowa State University_, jaeger.rob@gmail.com

Jing Ren  
_Iowa State University_, jren@iastate.edu

Yu Xie  
_Iowa State University_, yuxie@iastate.edu

Sriram Sundararajan  
_Iowa State University_, srirams@iastate.edu

Michael G. Olsen  
_Iowa State University_, mgolsen@iastate.edu

See next page for additional authors
Follow this and additional works at: [http://lib.dr.iastate.edu/me_pubs](http://lib.dr.iastate.edu/me_pubs)

Part of the [Nanoscience and Nanotechnology Commons](http://lib.dr.iastate.edu/me_pubs/74) and the [Tribology Commons](http://lib.dr.iastate.edu/me_pubs/74)

The complete bibliographic information for this item can be found at [http://lib.dr.iastate.edu/me_pubs/74](http://lib.dr.iastate.edu/me_pubs/74). For information on how to cite this item, please visit [http://lib.dr.iastate.edu/howtocite.html](http://lib.dr.iastate.edu/howtocite.html).

This Article is brought to you for free and open access by the Mechanical Engineering at Iowa State University Digital Repository. It has been accepted for inclusion in Mechanical Engineering Publications by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.
Nanoscale surface roughness affects low Reynolds number flow: Experiments and modeling

Abstract
Most micro-channel fabrication strategies generate nano-to-micro-scale, stochastic surface roughness. This inherent stochasticity can potentially be harnessed to direct microfluidic operations such as self-cleaning behavior and localized mixing. This work investigates the effect of stochastic nanoscale roughness on low to moderate Reynolds number Newtonian flow using concurrent modeling and experiments. We fabricate a microscopic channel with tailored hydrofluoric-acid-etched rough surfaces. Optical profilometry and micro-particle-image-velocimetry (micro-PIV) are used to characterize the surface roughness and flow field and is integrated with direct numerical simulation that resolves effects of nanoscale roughness. Results indicate that nanoscale roughness causes flow perturbations that extend up to the mid-plane and is insensitive to flow-rates.

Keywords
Etching, Microscale flows, Surface measurements, Rough surfaces, Flow simulations, Velocimetry, Nanoscale flows, Spectrum analysis, Polymers, Surface dynamics

Disciplines
Nanoscience and Nanotechnology | Tribology

Comments

Rights
Copyright 2012 American Institute of Physics. This article may be downloaded for personal use only. Any other use requires prior permission of the author and the American Institute of Physics.

Authors
Robert Jaeger, Jing Ren, Yu Xie, Sriram Sundararajan, Michael G. Olsen, and Baskar Ganapathysubramanian

This article is available at Iowa State University Digital Repository: http://lib.dr.iastate.edu/me_pubs/74
Nanoscale surface roughness affects low Reynolds number flow: Experiments and modeling

R. Jaeger, J. Ren, Y. Xie, S. Sundararajan, M. G. Olsen, and B. Ganapathysubramanian

Citation: Applied Physics Letters 101, 184102 (2012); doi: 10.1063/1.4764293
View online: http://dx.doi.org/10.1063/1.4764293
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/101/18?ver=pdfcov
Published by the AIP Publishing
Nanoscale surface roughness affects low Reynolds number flow: Experiments and modeling

R. Jaeger, a) J. Ren, a) Y. Xie, a) S. Sundararajan, M. G. Olsen, and B. Ganapathysubramanian b)

Department of Mechanical Engineering, Iowa State University, Ames, Iowa 50010, USA

(Received 30 July 2012; accepted 12 October 2012; published online 29 October 2012)

Most micro-channel fabrication strategies generate nano-to-micro-scale, stochastic surface roughness. This inherent stochasticity can potentially be harnessed to direct microfluidic operations such as self-cleaning behavior and localized mixing. This work investigates the effect of stochastic nanoscale roughness on low to moderate Reynolds number Newtonian flow using concurrent modeling and experiments. We fabricate a microscopic channel with tailored hydrofluoric-acid-etched rough surfaces. Optical profilometry and micro-particle-image-velocimetry (micro-PIV) are used to characterize the surface roughness and flow field and is integrated with direct numerical simulation that resolves effects of nanoscale roughness. Results indicate that nanoscale roughness causes flow perturbations that extend up to the mid-plane and is insensitive to flow-rates. © 2012 American Institute of Physics.

Soft lithography using SU-8 photoresist and poly(dimethylsiloxane) (PDMS) is a commonly used technique to fabricate microchannels. This method in conjunction with hydrofluoric acid (HF) etching is an effective rapid prototype microfabrication process of microchannels.1–3 A byproduct of such fabrication is an inherent, stochastic surface roughness.4 The surface roughness can exhibit variations in root-mean-squared roughness from microns to nanometers. Interestingly, surface roughness at these scales has been shown to lead to hydrophobicity, which can result in self-cleaning surfaces.35 which is especially useful for biological analysis and separation, biomedical testing, and nanomanufacturing applications.36 Furthermore, stochastic roughness (or texturing) in micro-channels can be harnessed for multi-functional properties like anti-reflectivity and optical transparency.34 Recent work has shown that this roughness can be “tailored” by tuning the fabrication process4,34 and open up promising avenues to enhance microfluidic applications. These promising developments necessitate a thorough understanding of the flow characteristics of fluids in rough microchannels and has been the focus of recent studies.5–7

The effect of micro-scale surface roughness ($\gamma = 1.6\%$, where $\gamma = 100\% \times$ roughness height/$D_H$, and $D_H$ is the hydraulic diameter of the channel) was examined experimentally by using micro-PIV and comparing with a smooth computational fluid dynamics (CFD) simulation of a channel of the same geometry. Flow effects in relation to periodic micro-scale obstructions in height have also been investigated using CFD by various authors.9–11 These analyses usually focus on periodic roughness and are invariably limited to 2D.12,13,15,16 In one study, Valdes et al.14 used pyramidal shapes in a 3-dimensional domain that were randomly placed throughout the channel surface in accordance to data acquired from an actual surface. However, the CFD surface did not mimic the actual surface exactly. Instead, relative roughness and peak density values were acquired from the actual surface to generate the CFD surface. As a result, the true effect of a tangible surface was not investigated. Recently, Liu et al.12 analyzed three-dimensional surface roughness using molecular dynamics in nanochannels with $\gamma = 3\%$ and found that random roughness had a greater effect on flow than periodic obstructions. While molecular dynamics simulations are exceedingly useful in gaining insight into the mechanics involved, they are limited to very small domains and time-scales due to their prohibitive computational cost.

We focus on two key issues that have not been addressed by previous investigations on roughness effects: We directly model realistic surface roughness which is extracted using optical profilometry. This is made possible by using high resolution direct numerical simulation (DNS) analysis (that is validated using concurrent micro-PIV experiments) which allows us to link nano-scale roughness to far-field flow features. We also focus on flows at low Reynolds number where viscous forces dominate, which is common for microfluidic devices, and extensively characterize the effect of varying surface roughness.

The experimental microchannel in this study was fabricated using PDMS and glass. The PDMS part was a replica made from an SU-8 mold and forms three walls of the microchannel. The PDMS part and a glass substrate (slide) were then oxygen-plasma bonded together, creating a completely enclosed microchannel for fluid transport, with the glass forming the fourth (bottom) wall of the channel. We implemented HF etching to create a surface roughness on the glass substrate that is reproducible and characterizable as a function of etching time.4 A desired stochastic surface roughness can be fabricated according to the etching time and solution concentration.4

In this study, we used an unetched glass and a roughened glass obtained as follows. A glass slide (25 mm × 75 mm, Erie Scientific Company, Portsmouth, NH) was etched in buffered HF (6:1 volume ratio of 40% NH4F in water to 49% HF in water; etch rate calibrated to 72 nm/min) for 30 min and

---

a)R. Jaeger, J. Ren, and Y. Xie contributed equally to this work.

b)Author to whom correspondence should be addressed. Electronic mail: baskarg@iastate.edu.
immediately rinsed in deionized water for 5 min. After rinsing, the etched-glass slide was dried using nitrogen gas before being oxygen-plasma bonded to the PDMS replica. Etching time was limited below 40 min since longer etching times compromised the glass transparency necessary for micro-PIV measurements. The 30-min etched glass is referred to simply as “etched glass” from here onward.

The microchannel’s surface topography was obtained using a 3D Optical Surface Profiler (NewView™ 71000, Zygo Corporation, Middlefield, CT). The optical profilometer provided a scan area of 470 μm × 350 μm, with a lateral resolution of 0.73 μm and height resolution of 0.1 nm. The surface data obtained by the optical profilometer was directly used to model the surface roughness on the bottom surface of the CFD microchannel at the same spatial resolution.

In our experiments, micro-PIV visualization of microfluidic flow was realized with a microscopic imaging system that visualizes a small area within the microchannel. In this micro-PIV experiment, the working fluid, deionized water, was seeded with 1 μm diameter nile-red fluorescent carboxylate-modified microspheres (FluoSpheres, Invitrogen Corporation) as flow-tracing particles at a concentration of 0.04%. The seed particles were illuminated using a double-pulsed Nd:YAG laser. Images of the illuminated tracing particles were captured using a CCD camera. A 40 × 0.6 NA objective lens paired with a 0.45× coupling, resulted in a total magnification of 18× and a depth of correlation of 7.8 μm.17 Further details of the micro-PIV system can be found in Li and Olsen.18 The overlapped area of adjacent interrogation windows was 50% resulting in an in-plane velocity vector spacing of 1.5 μm. In total, 1500 micro-PIV image pairs were captured at each depth and analyzed using the sum-of-correlation algorithm19–21 to obtain the velocity field.

The surface data obtained by the optical profilometer was used to model the surface roughness on the bottom surface of the CFD microchannel at the same spatial resolution. This ensured that the surface roughness used for CFD simulations was experimentally derived and non-periodic. Figure 1 shows the computational domain. The trapezoidal shape of the micro-PIV experimental microchannel (caused by the fabrication process) has identical cross-sectional dimensions as the CFD microchannel. The length of the channel was 350 μm (this is more than 10 times the surface roughness autocorrelation length (12.9 μm for the etched surface)). The channel is 390 μm wide on the top and 470 μm on the bottom. The height of the channel is 51.03 μm. The grid was composed of 12.3 × 10⁶ hexahedral elements. The elements were concentrated near the walls to accurately capture the effect of the surface roughness and boundary layers. The clustering of hexahedral elements was greater near the rough surface. For the etched glass, the roughness of the glass is one order of magnitude larger than the roughness of the PDMS. Since we expect the effect of PDMS roughness to be small in comparison with the glass roughness (this hypothesis is validated via comparison between CFD and PIV data) the PDMS surface roughness is neglected and we assume a smooth top surface for the CFD simulations.27

The full Navier-Stokes equations were solved assuming incompressible flow and constant temperature. We utilized a highly scalable implementation of an incompressible flow solver using the finite element method that incorporates streamline-upwind/Petrov-Galerkin (SUPG)22 and pressure-stabilizing/Petrov-Galerkin (PSPG)23 terms for numerical stabilization. The applicability of the Navier-Stokes equation (validity of the continuum hypothesis) is ensured due to the fact that the Knudsen number calculated on the smallest element (2.7 × 10⁻⁶) was less than 10⁻².24 We applied no-slip boundary conditions on the walls. Zhu et al.25 showed that for a microchannel with hydrophilic surfaces and a hydraulic diameter larger than 30 μm, the no-slip boundary condition is valid. In addition to PDMS being hydrophilic, the etched glass is also hydrophilic.26 Both surfaces underwent an oxygen plasma treatment during the fabrication process, which is known to increase hydrophilicity.27 Water contact angle measurements on etched glass yielded a value of 29.5°, confirming its hydrophilicity. Potential micro-sized air bubbles will also have no effect on slip.28,29 A pressure drop boundary condition between inlet and outlet was maintained. An initial guess for the pressure drop was to match the experimentally determined flow rate using the Hagen-Poiseuille flow equation (which is for a circular channel), ΔP = ƒ̇LQ/πD³, where L is the length of the channel, μ is the dynamic viscosity, Q is the volumetric flow rate, and D is the hydraulic diameter. We analyzed cases using flow rates of 0.001 ml/min, 0.01 ml/min, 0.1 ml/min which corresponds to a Reynolds number of 0.065, 0.65, and 6.5, respectively.

The effect of surface roughness was investigated by looking at the fluid structures that evolve from the rough surface. We focused on fluid structures consisting of velocity perturbations caused by the roughness itself. In order to characterize these velocity perturbations, we used autocorrelation analysis, energy spectrum analysis, and visual analysis. By examining the fluid structure characteristics as a function of height from the rough surface, a zone of influence from the rough surface was established.

The autocorrelation function, C(τ), was estimated for a velocity field in a plane to find β*, the autocorrelation length. The autocorrelation length is defined as the lag distance where the autocorrelation function decays to 1/e. Autocorrelation analysis was performed on velocity fields as slices in the xy-plane, highlighted in Fig. 1, at increasing heights from the rough surface, in order to extract the influence of surface roughness as a function of height. Note that the

---

**FIG. 1.** The geometry and mesh detail of the computational microchannel domain. The roughness height on the zoomed-in section is exaggerated for clarity. The width of the channel is 460 μm at the rough surface.
autocorrelation is calculated using the velocity-component deviations from ideal flow (perturbations). The interrogation region was taken toward the center of the microchannel away from the side-walls and entrance/exit to eliminate the side-wall boundary layer and boundary condition effects. The autocorrelation lengths (ACL) of the v-velocity perturbations was used for validation between experiments and computational results. Figure 2 shows the ACL as a function of height from the rough surface for both etched and unetched surfaces at all flow rates, Q [ml/min].

While the autocorrelation length gives valuable information about the fluid structures, an energy spectra analysis can reveal the energy cascading effects of the surface roughness. Energy spectra analysis has been used successfully for velocity field analysis in a variety of fluid phenomena. The energy spectrum is denoted as $E(k)$, where $\hat{u}$ is the discrete Fourier transform of the velocity field on a structured mesh with $n \times m$ points, where $\hat{E}(k) = \frac{1}{4} |\hat{u}(k, t)|^2$.

$$E(k) = \sum_{k-\Delta k \leq k \leq k+\Delta k} \hat{E}(k_x, k_y).$$

Figure 3 shows the energy spectra of the total velocity perturbations. Figure 3(a) reveals that the energy cascade across wavelengths has a very similar structure throughout the spectrum of flow rates over etched glass, again supporting the notion of insensitivity of effect of surface roughness as a function of flow rate, at small flow rates. Clearly, the energy spectra in Figure 3(b) reveal that larger amounts of energy in the form of velocity perturbations are produced by etched glass. Also, Fig. 3(b) shows that the energy produced by etched glass persists higher into the microchannel compared to unetched glass. There is a greater decay in the energy for unetched glass as the height from the rough surface increases, whereas the energy from the etched glass tends to persist. This is clearly seen in the slope of the energy spectra. For the etched and unetched surfaces this is approximately $-4.75$ and $-8.64$, respectively. Not only is the perturbation energy larger for etched glass, but the larger slope for etched glass compared to unetched glass means there is a greater transfer of energy for etched glass. Table I also compares the energy spectra slope ratios between experiments and simulations. The ratio is defined as the energy spectra slope ratios between experiments and computational results.

Finally, we utilized visual representation of the velocity to investigate the fluid structure away from the surface by plotting velocity contours in the $xz$-plane. Note the dramatic effects due to roughness as seen in Figs. 4(a)–4(d) which shows the v-velocity contours for both unetched and etched glass at multiple flow rates. There are large velocity plumes that originate from the rough surface and erupt to the mid-plane of the microchannel. The $R_{rms}$ of the etched glass ($\sim 19$ nm) is slightly more than an order of magnitude greater than the un-etched glass ($\sim 1$ nm), and not surprisingly, there

**TABLE I. Comparison of experimental and DNS metrics at 25 $\mu$m from rough surface ($\mu$m).**

<table>
<thead>
<tr>
<th>Flow rate (ml/min)</th>
<th>Surface type</th>
<th>ACL</th>
<th>Energy spectra slope ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Exp.</td>
<td>DNS</td>
</tr>
<tr>
<td>0.1 ($Re = 6.5$)</td>
<td>Etched</td>
<td>17.4 ± 1.7</td>
<td>17.3 ± 0.6</td>
</tr>
<tr>
<td></td>
<td>Unetched</td>
<td>14.2 ± 3.4</td>
<td>15.0 ± 2.7</td>
</tr>
<tr>
<td>0.01 ($Re = 0.6$)</td>
<td>Etched</td>
<td>16.7 ± 1.6</td>
<td>17.5 ± 1.2</td>
</tr>
<tr>
<td></td>
<td>Unetched</td>
<td>16.8 ± 1.4</td>
<td>15.0 ± 2.9</td>
</tr>
</tbody>
</table>
is an order of magnitude increase in the velocity fluctuations between the etched and unetched surfaces. What is interesting is that the small perturbations originating from the rough surface seem to combine and merge into larger structures as the height from the surface increases. These combinations give rise to the velocity plumes seen in Fig. 4.

We have shown that the effect of stochastic nano-scale surface roughness on microfluidic flow can be studied using computational fluid dynamic DNS simulations. Additionally, we have shown that validation between micro-PIV experiments and a large DNS simulation is possible using autocorrelation and energy spectra. CFD analysis lends to a deeper understanding of the characterization of the fluid flow within the microchannel, and the highly resolved DNS simulations reveal the flow to be characterizable. We show that for a range of flow rates that are diffusion dominated, the energy transfer is consistently characterizable. Autocorrelation and velocity contour analyses showed that the nano-scale surface roughness produced small structures that combine and persist well above the rough surface. In addition, the energy spectra analyses show the small eddies produced by the etched surface give rise to higher energy eddies that decay more slowly than eddies produced by the unetched surface.

The chemical etching surface treatment and other stochastic rough surfaces, even at the nano-scale, can be characterized and potentially be harnessed across a range of fluid flow rates. Devices that use microchannels such as lab-on-a-chip medical devices can potentially be tuned and further optimized for their respective applications such as reagent mixing, bubble creation and transport, fluid transport, cell manipulation by leveraging the effects of stochastic surface roughness. We envision this effect to be particularly useful in non-Newtonian fluids, which are frequently encountered in lab-on-a-chip medical devices.

Micro-sized air bubbles have been known to create an effective slip at the wall by forming an immiscible fluid layer where the slip increases. However, if the capillary pressure is great enough to force the air out of the surface features, then the no-slip boundary condition is again valid, as proved by Barrat and Bocquet (Ref. 29). The minimum pressure required to force fluid into a parallel slit of width $h$ is:

$$P_c = \frac{2}{\pi c LS} C_0 c SV$$

which is smaller than the pressure gradient applied in these experiments.


37. All the data analysis (for both experimental and CFD) is done on regions far from the entrance, exit, and side walls, and thus effects of entrance, exit, and side-walls can be safely neglected.