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To cite this article: N Saad et al 2012 IOP Conf. Ser.: Mater. Sci. Eng. 42 012052

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Characterization of the state of a droplet at a micro-textured silicon wafer using a finite difference time-domain (FDTD) modeling method

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Abstract. In this study, we introduce a finite difference time domain method to study the propagation and reflection of an acoustic wave on smooth and micro-textured silicon surfaces in interaction with droplets in different states. This will enable numerical investigations of interfaces composed of periodically distributed well-defined pillars. One type of transducer was modeled generating longitudinal wave. Three configurations were studied: the Cassie state, the Wenzel state and a composite state for which the droplet collapsed into the middle height of the pillars. After analysis of the displacement along y direction in the silicon wafer, we were able to show that a longitudinal wave is sensitive to the detection of the state of the droplet. The first experimental results made it possible to show a good agreement between modeling and experiments.

1. Introduction

Superhydrophobic materials hold substantial capacity for potential applications extending from selfcleaning surfaces, completely water impermeable textiles to low cost energy displacement of liquids in lab-on-chip devices. Superhydrophobic surfaces displaying high contact angle and low contact angle hysteresis also reveal a self-cleaning features and low drag for fluid flow. Lotus leaves and bird feathers are one of many surfaces that are known to be superhydrophobic due to their rough surface. So in order to modify the hydrophobic property of the surface, it is possible, not just modify its chemical composition but also its hierarchical structures by changing surface roughness.

On such surfaces a drop of water can experience two different states: suspended on a composite surface of material and air pockets (Cassie-Baxter state) or following all the contours of the rough surface (Wenzel state).



International Symposium on Ultrasound in the Control of Industrial Processes (UCIP 2012) IOP Publishing IOP Conf. Series: Materials Science and Engineering **42** (2012) 012052 doi:10.1088/1757-899X/42/1/012052

This subject is receiving much attention; several models based on theoretical calculations were developed in order to estimate the critical values (e.g. line density criterion, surface roughness height [1], drop's surface energy criteria [2], etc..) for which one can predict in advance whether the drop will collapse or be suspended by pillars. Experimentally, current measurements are done by optical means, which often are limited by technological barriers. Ultrasound, beside acoustic, are generally used either to detect and characterize defects in structures [3], or to highlight the levels of adhesion [4]. While a consistent method for characterizing textured interfaces is missing, the aim of the present work and thus its originality lies in determining the potential of acoustics to characterize the state of a droplet on microtextured surfaces.

This paper is arranged as follows. Section II presents a finite difference time domain (FDTD) model design for acoustic wave propagation through a microtextured structure in interaction with a fluid. A brief overview of the early experimental work as well as initials results are reported in section III. Finally, the last section summarizes the main findings and conclusions of this joint study.

2. Methods and Models

Figure 2 illustrates a 2D cut of the structure of different models developed in this work. In the simulation, the two-dimensional model is assumed infinite in the Z direction and finite in X and Y Cartesian coordinates (OXYZ). Every structure consists of three different regions. The first one is composed of an anisotropic single crystal silicon microtextured with different patterns. Its physical characteristics are those of an anisotropic monocrystalline silicon of mass density $\rho = 2330$ kg.m⁻³, longitudinal speed C₁ = 8433 ms⁻¹ and transverse speed C_t = 5843 ms⁻¹. Pillars of width `a`, height `h` and pitch `b`, are considered parallel to the Y axis, that is the direction of wave propagation. The second region is water of mass density $\rho = 1000$ kg m⁻³ and longitudinal speed C₁ = 1490 ms⁻¹ (Ct = 0 ms⁻¹).

The third region is a homogeneous region formed of air modeled as a fluid of mass density $\rho = 1.3$ kg.m⁻³, in which the speed is C₁ = 340 ms⁻¹.



Figure 2. 2D cross section of the FDTD model structure.

In many fields of application, the study of the propagation waves in complex media has long been an important area of interest. Sigalas et al. [5] described in details the FDTD method for acoustic and elastic wave propagation in two dimensional composites. Based on this later study, our model of acoustic propagation has been developed and results will be directly reported below.

The first set of simulations was carried out with the objective of studying the reflection of an acoustic wave on silicon surfaces. Figure 3 illustrates the results of comparing a smooth surface to a textured surface plotted in terms of the absolute values of the y displacements along the transducer in function of time. The textured surface displays the following parameters: pillar width $a = 15 \mu m$, pillar height $h = 20 \mu m$ and pitch $b = 15 \mu m$ (where the pitch defines the inter pillars distance).

Figure 3 shows the result of the first simulation: The ratio between the amplitudes of the first reflected echo on the smooth surface and that of the textured one is 50% which matches with the ratio of the reflecting surface. Concerning the second echo appearing on the curve corresponding to the textured surface, it is delayed of about 4.6 nanoseconds with the respect to the first one. The propagation delay corresponds to the acoustic propagation Δt in the pillar (c_l is the speed of the longitudinal wave in y direction).

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$$\Delta t = \frac{2 \cdot h}{c_{\star}} = \frac{2.20.10^{-6}}{8433} = 4,7.10^{-9} s = 4,7ns$$
(1)

This means that the first echo derived from the reception of the wave signal reflected on the bottom of the grooves and the second one from the reception of the wave signal reflected on the top of the pillars.

The same simulation was achieved for a second textured structure having different height and the same pillar width and pitch. The result proves our initial finding pointing that time spacing between echoes enables the height of the pillars to be assessed.





Figure 3. Absolute values of y displacement for a smooth and textured surface in function of time.

Figure 4. Absolute values of y displacement for a textured surface of height 2h in function of time.

The second set of simulations determines the wetting behavior of the above-mentioned first textured structure. Three cases were studied: The Wenzel state, the Cassie state and an intermediate state for which liquid penetrate into the middle height of the pillars.

We can clearly see for these cases the decreasing of the amplitude of the second echo with the increasing of the contact area between the solid and water. This phenomenon is explained by the fact that with the decreasing of solid/liquid interfacial area, the liquid loading is less important which means that reflection is becoming more important. For example, for the first echoes, the ratio of the amplitudes between Cassie and Wenzel is approximately 80% which is the reflection coefficient for a solid-water interface.



Figure 5. Absolute values of y displacement in function of time for a textured surface in interaction with different state of a droplet (Cassie, Composite and Wenzel).

3. Experimental Method

We limit the experimental study on a microtextured Silicon sample patterned with an array of pillars of diameter 15 μ m, height 20 μ m and pitch 30 μ m [6]. The ultrasonic emission source used in the

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experiment is an 800 MHz ZnO transducer deposited by radio frequency magnetron sputtering on the rear face of the sample as presented previously [7]. Experimental measurements were carried out by measuring the S_{11} scattering parameter identified as being the ratio of the complex amplitudes of the reflected to the incident voltage thanks to a Suss Microtech prober coupled with a Hewlett Packard 8753 Vector Network Analyser [8]. The impulse response of the system is obtained by inverse Fourier transforming the frequency domain received signal. Initial results clearly show the two echoes obtained from modeling. The time delay between them matches the propagation time in pillars. A difference in amplitude between the echoes for the different states of the droplet is even verified.



Figure 6. Experimental results for the absolute values of y displacement in function of time for a textured surface in interaction with different state of a droplet (Cassie, Composite and Wenzel).

4. Conclusion

We have presented high frequency ultrasonic method able to characterize textured surfaces. This method can be useful to evaluate pillar's height. Initial experimental results are demonstrated to be in good agreement with the simulation showing promising and exciting results of our approach.

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