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Research Article

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Contact Angle & Density Measurement for Different Silicon Surfaces

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Abstract Lotus effect studies have been increased day by day with developing technology and Molecular Dynamic (MD) Simulation is the priory example of them. The wettability of the silicon surfaces studies come from the results of the MD and lotus effect. Contact angle and density are the effect of the wettability of silicon surfaces because the other parameters were taken a constant for all cases which are Si (001) - Si (110) and Si (111). From Lorentz- Berthelot mixing rule, the interaction strength between silicon and oxygen were 0,125. Macroscopic contact angle calculated with MD simulations (LAMMPS and VMD), then density calculated from the area where water molecules touch the silicon surfaces. Finally, increased in the contact angle decreases planar density with low wetting area

Keywords Wettability of silicon surfaces, contact angle, density, MD simulation

Introduction

Biomimetic that studies on development of innovations from nature and optimized biological function, structure [1]. These processes have been used variety of subjects such as nanotechnology, artificial intelligence, microchip so on and so forth.

For biomimetic, lotus plant can be given as an example from living creatures in nature. The lotus plant that grows in muddy spots is actually the cleanest plant in the world, because the lotus plant is the only plant that has the self-cleaning feature. Self-cleaning super hydrophobic products inspired by nature are ready to become important and new products in our daily life today. Some products include coatings that reduce water drag on boats, surfaces and equipment that are exposed to fresh or salt water, building materials that remain clean without any maintenance and building materials that are better protected against abrasion and paint, and should remain dry when soaked in water. Thanks to the surface texture of the lotus plant leaf, water accumulates on the leaf in droplets [2]. Basically, water is cylindrical or spherical on the lotus plant due to the micro and Nano structures on it. Then, droplets fall down by the reason of gravitational. Some industrial companies attempted new innovation materials with using properties of lotus plant like hydrophobic. For example, a German firm ISPO manufactured house paint for self- cleaning with silicon base [3].

As determined above paragraph it can be said shortly that lotus effect based on biomimetic studies and contacts with super hydrophobicity, contact angle, roughness or self-cleaning. *Lee and Michielsen* [4] studied that rough surface compared with the smooth surfaces for wetting behavior and they studied contact angle hysteresis on super hydrophobic surface. *Patankar* [5] examined that double roughness structure or slender pillars are suitable surfaces as geometric shape for improving self-cleaning surfaces. Besides, composite drop showed that high contact angle drop was observed with low hysteresis.

Lotus effect studies that came up to the day have been made using many different materials from graphite to silicon. *Nakajima et al.* [6] used titanium dioxide coating for super hydrophobic thin films. *Zhai et al.* [7] used creating a semi fluorinated silane–coated polyelectrolyte multilayer surface to contact super hydrophobic

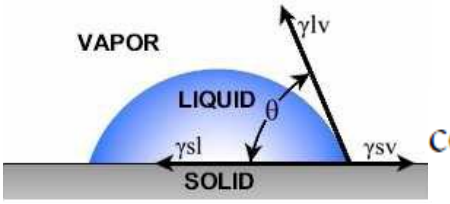
behavior of lotus leaf structure. *Han et al.* [8] used block copolymer and silica nanoparticles. *Alvarado et al.* [9] used graphene- coated silicon for which is potential applications of material.

Molecular dynamics (MD) simulations have been important role with developing nanotechnology studies, because some physical and chemical events can be easily observed with the aid of simulations. In this connection silicon is usually selected to do MD simulations as the most common material. *Barisik and Beskok* [10] matched experimental measured macroscopic contact angle with microscopic contact angle (MD) by using silicon surface. Silicon – water model was used for this working and the aim of them is to determined wetting behavior of silicon surface. *Martinez* [11] studied contact angles with using different materials which are etched and etched + hexamethyldisilazane (HMDS) were used for silicon surfaces. Contact angle of etched + HMDS Si was a little bit higher than etched Si and the value of it was nearly 93 degree. *Hermansson et al.* [12] investigated 14 different surfaces which content both etched silica and modified. They calculated contact angles that were from 5 to 96 degree and showed that hydrophobic surfaces were stronger than hydrophilic surfaces with respect to interaction between atoms and molecules. *Alvarado et al.* [9] examined contact angles of Si (100) and Si (111) with different wettability conditions and found macroscopic contact angle of 64.4°. Interestingly, *Isaiev et al.* [13] examined contact angle of two different shapes which are cylindrical and spherical on silicon surface (001). From coming results, cylindrical droplets are more efficient according to parameters of the interaction potentials.

In this article, Molecular Dynamic (MD) Simulations were applied for different silicon surfaces as (001), (110) and (111). Then, silicon surfaces that results compared with previous studies. Thanks to the different surfaces, wettability was observed and water molecules were placed on the silicon surface as cylindrical droplets. After MD Simulation contact angle of surfaces were calculated and connect interaction strength, density. The aim to find out wettability of different silicon surfaces from this study.

Model Part and Methods

To understand interaction strength and contact angle, it is the priority of this study, because studies show that interaction strength decreases with increased contact angle as determined introduction part. Contact angle is property of wettability between liquids and solids, so it can be measured from geometry (Fig. 1) and using Young's equation to calculate as below;



$$\cos\theta_{Young} = \frac{\gamma_{vs} - \gamma_{ls}}{\gamma_{vl}}$$

Figure 1: Measured method of contact angle from geometry

Some different water molecules can be tried on the silicon surfaces. *Makaremi et al.* [15] generated different water molecules as 800, 1200, 3200 and 6400 with periodic boundary conditions. Water molecules include two hydrogen atoms and one oxygen atom and angle between O-H is 109.5 degree and length 1 A°. The size and molecules of water is 45.996 × 32.0 × 38.50 A° and 5184 atoms, respectively.

Silicon is a member of group of 14 in periodic table and it is most common preferred molecular dynamic simulation studies with different format such as etched silicon, silicon dioxide etc. Besides, another reason why silicon is preferred is that its semiconductor character. In this study, Si (011), Si (110) and Si (111) surfaces were used and total size and atoms of them were given (Table 1)

Table 1: Dimensions and number of atoms of different silicon surfaces

	Size (A°)	Atoms
Si (001)	152.66×45.16×100	5280
Si (110)	149.745×43.44×100	7680
Si (111)	159.6×46.08×100	7056

Snapshots of water molecule on the different surfaces which are (001)- (110)- (111) were modelled (Fig. 2), respectively. These figures were given different directions to provide periodicity and water molecules were located at middle of the x direction. Besides, water molecules were occured as rectangular shape to observe cylindrical droplet.

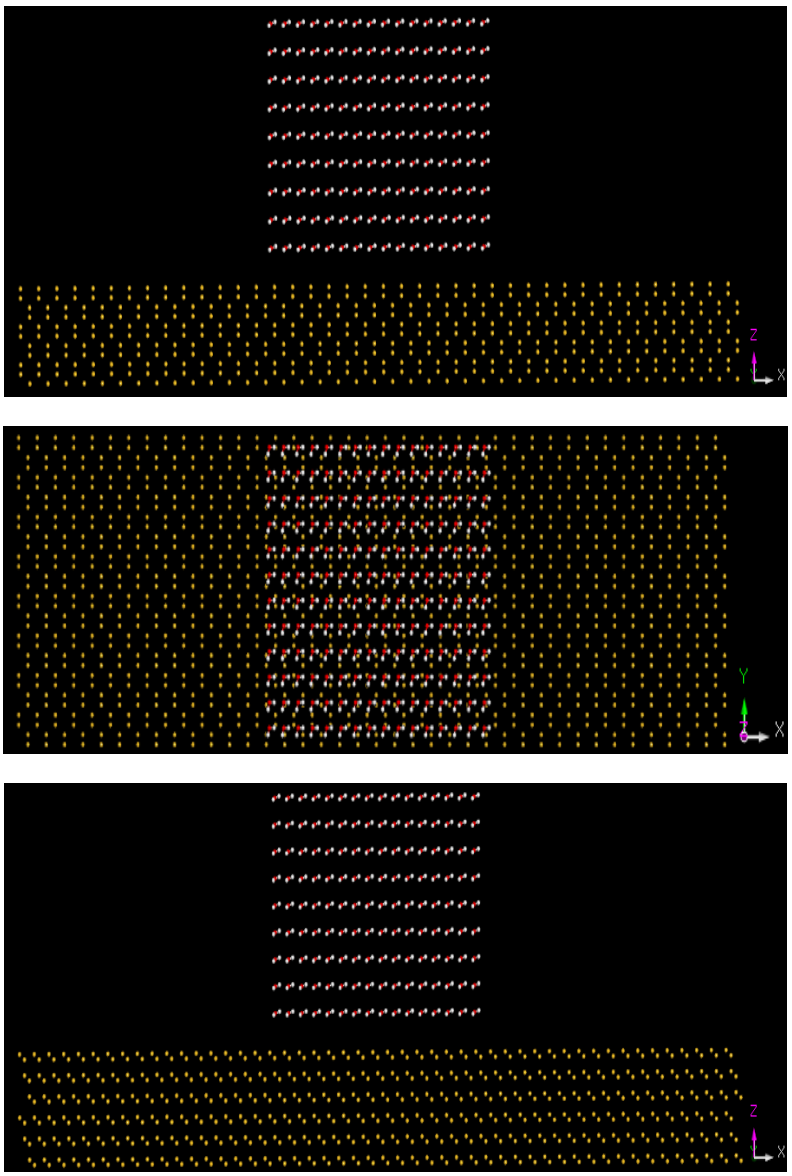


Figure 2: Snapshots of water molecules on silicon surfaces (001)- (110) and (111), respectively

Results and Discussion

First of all, density of surfaces were calculated for three cases and these results were similarly to theoretical results (Table 2). They can give how wettability on the surfaces and besides, the similarity of these results with the theoretic results indicates that the periodicity of the surface is provided.

Table 2: Compared with planar density and theoretical density for three surfaces

	Area (cm^2)	**# of Atoms**	**Density (Atoms/ cm^2)**	**Theoretical Density (Atoms/ cm^2)**
Sİ (001)	7.072E-13	480	6.788E+14	6.79E+14
Si (110)	1.001E-12	960	9.59E+14	9.59E+14
Si (111)	7.53E-13	588	7.81E+14	7.83E+14

Next step, water molecules that placed on the surface after being formed in a rectangular shape formed an interaction in MD model. Figure 3 shows the snapshots of droplets that taking the shape of cylindrical to calculate contact angle for three cases. Water molecules were together on surface in Figure 3(a,b) in spite of that water molecules could not observed together in Figure (c) due to interaction strength. According to Lorentz-Berthelot mixing rule, interaction strength decreased with increased contact angle and minimum contact angle was found for Si (110) as seen in Table 3. From results, hydrophobic wettability characterization based on Si (011)> Si (111)> Si (110) but, *Yen* [16] studied on Si (100)- (110) and (111) and found that based on Si (100)> (110)> (111) with $\varepsilon_{wf}/\varepsilon$=2. Then, *Yen* compared to $\varepsilon_{wf}/\varepsilon$=1.6 with previous value and observed same that interaction strength decreased with increased contact angle. *Barisik and Beskok* [10] were tried from 0,05 to 1 for $\varepsilon_{Si\text{-}O}/\varepsilon^*_{Si\text{-}O}$ and found that contact angle decreased with increased interaction strength. However, $\varepsilon_{Si\text{-}O}/\varepsilon^*_{Si\text{-}O}$=0,125 was used for this project and interactions can be observed precision with different values of Si-O interaction strength. In Figure (c) water molecules can be observed on the surface together using different rate of interaction parameter.

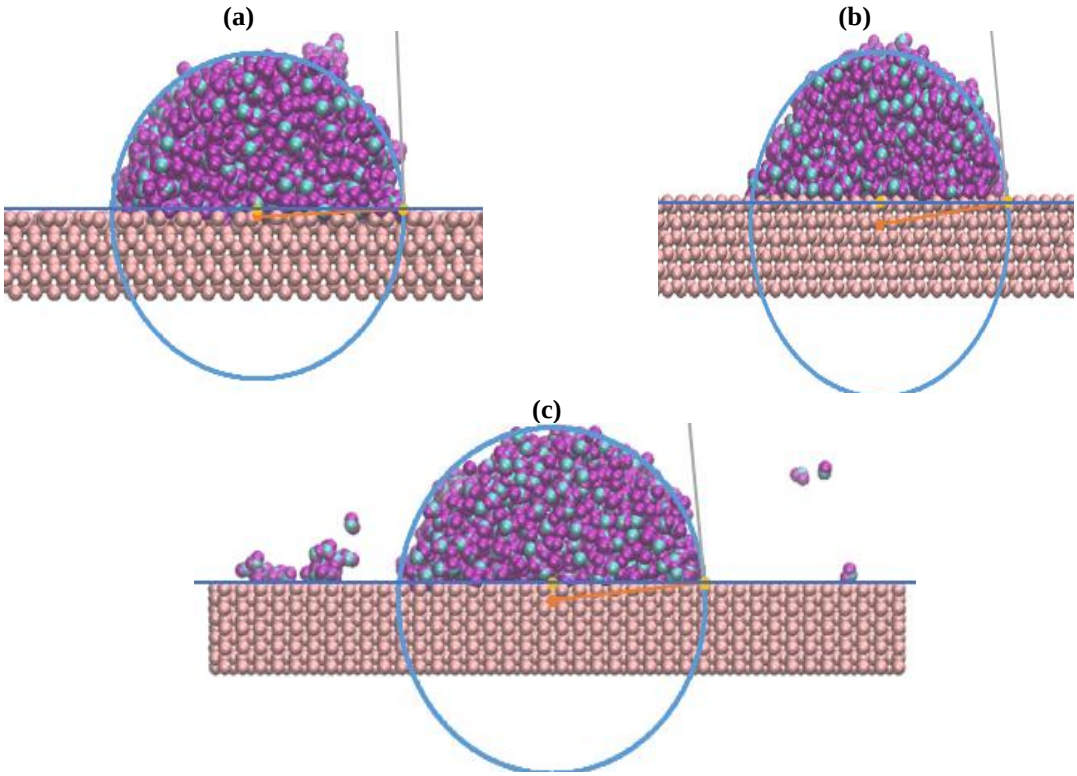


Figure 3: Snapshots of water contact angle on (a) Si (001), (b) Si (111) and (c) Si (110)

Nanoscale results can converted to macroscale results with using MD simulation to obtain contact angle and the values of them are 86°, 79° and 83° (Fig. 3). Calculated planar density compared with theoretical density (Table 2) and contact angle increased with decreased density (Table 3).

Alvarado [9] calculated nearly 85° for contact angle of Si (111) at the same interaction strength. To increase contact angle of Si (111) for this project, interaction strength are decreased but, 83° contact angle were calculated with the optimum interaction parameter.

Table 3: Compare to contact angle with density

	Contact Angle(θ)	**Density (Atoms/ cm^2)**
Si (001)	86	6.79E+14
Si (110)	79	9.59E+14
Si (111)	83	7.81E+14

Contact angle can be changed with different some methods for instance, the size of droplet effect on this parameter and *Makaremi et al.* [15] studied with 4 different number of water molecules which were 800, 1200, 3200 and 6400. The number of water molecule increased with decreased contact angle. However, *Barisik and*

Beskok [10] studied different value of interaction parameters as determined at the begin of result & discussion part and obtained that contact angle increased with increasing droplet size for only $0{,}4\times\varepsilon^{*}_{Si\text{-}O}$ case. In fact, smaller droplet generally causes lower contact angle on the high wetting surface due to cohesive forces.

Conclusion

Wettability of silicon surfaces have been investigated with using MD simulations and in the project, contact angle and density parameter compared to different silicon surfaces. The main purpose to observe changeability contact angle with different silicon surfaces which were Si (001)- Si (110) and Si (111). These three surfaces were preferred for this project due to that planar density of them could be calculated easily and compared to theoretical densities. In other words, these surfaces are common used for MD studies. Then, calculated density and theoretical density showed that the periodicity of surfaces were ensured for all cases.

Contact angle of water molecules in the same properties (size and number of atoms) placed on different silicon surfaces that were calculated with converting nano scale to macro scale and MD simulations are used for Nano/micro studies. Using the same interaction parameter ($\varepsilon_{Si\text{-}O}/\varepsilon^{*}_{Si\text{-}O}=0{,}125$) contact angles were found from 79° to 86° and if generalization was made, contact angle increased with decreased density. Then, it is necessary to change the parameters so that a surface is at the desired contact angle and this parameter is interaction strength. For this project, same interaction strength value was used and the interaction of the surface with higher contact angle at the same parameter value appeared at a higher value.

More accurate results can be obtained and improved if some parameters like different droplet size, interactions are added for the continuation of this study.

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