

Using Trimethylsilanol for creating Hydrophobic Liner compared to other Silicon Compounds

Taehong Kim^{1*}, Leah Jin³⁺, Junehyuk Lee³⁺, Sean Lee⁴⁺, Jose Jimenez⁵⁺, Samuel Kim⁶⁺, Ho Yeon Kim⁷

***These authors contributed equally**

+These authors contributed equally

Author Info

1. 12th Grade, American Heritage High School, Plantation, Florida, taehongkim001@gmail.com
2. 9th Grade, Taylor High School, Austin, Texas, jimenj9569@g.comalisd.org
3. 10th Grade, Auburn High School, Auburn, Alabama, jjleah125@gmail.com
4. 11th Grade, Sunny Hills High School, Fullerton, California, connectstem01@gmail.com
5. 11th Grade, Canyon High School, New Braunfels, Texas, eddygtv9@gmail.com
6. 10th Grade, Diamond Bar High School, Diamond Bar, California, samuelfminjunekim@gmail.com
7. Professor, Department of Chemistry and Biochemistry, Loyola University Maryland, Baltimore, Maryland, hkim5@loyola.edu

ABSTRACT

Semiconductors are crucial to computing, healthcare, military, and transportation industries. The deposition step in semiconductors— wherein thin layers of materials are applied onto the surface— is critical, requiring a liner with similar hydrophilicity to incoming materials that are required to be deposited. Without the liner, materials can flake, creating problems such as particle contamination and incomplete coverage. Several materials, such as chlorotrimethylsilane (CTS), bromotrimethylsilane (BTS), bis(trimethylsilyl)amine, and trimethylsilyl methanesulfonate, can convert hydrophilic to hydrophobic surfaces of the silica wafer. However, these materials can be cost-intensive, produce extremely strong acid by-products, or create unwanted strong and sharp odors, such as ammonia. To investigate the relationship between the acidity of reaction byproducts and the degree of liner

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hydrophobicity, we hypothesized that bromotrimethylsilane, chlorotrimethylsilane, and trimethylsilyl methanesulfonate, which produce a strong acid as a by-product, would have a lower contact angle compared to trimethylsilanol (TMS), which only creates water in the process of creating a hydrophobic liner. We found that TMS yields better hydrophobicity due to not deviating the pH of the wafer during coating. TMS only creates water in the process, which does not break the siloxane bond to reverse the reaction, unlike other chemicals that can. Thus, it follows that TMS could be an excellent choice for the deposition liner compared to other chemicals due to lowering the reverse reaction, which can lower the contact angle. The significance of these findings has the potential to lead industries to enhance uniformity and reliable adhesive properties in coatings with lower contact angles in reverse reactions.

INTRODUCTION

As digital devices become more prevalent, demand for electronics and their vital components has significantly increased. An integrated circuit (IC)— colloquially known as a “chip”— is one of the most vital components, consisting of many transistors acting as miniature electrical switches that can toggle electron flow into the system (1, 2). To make ICs, there are numerous steps in semiconductor (a material that exhibits electrical conductivity between that of a conductor and an insulator) processing, such as polishing, lithography, deposition, cleaning, packaging, and electrical testing. Each step is critical for processing to control the flow of electricity and act as amplifiers. (3). Out of these steps, we focused on deposition, a pivotal step that defines the electrical properties of a device as engineers stack desired materials over the wafer, a thin slice of semiconductor material that serves as a foundation for creating microelectronic devices (4). Semiconductor companies use many deposition materials such as titanium nitride, amorphous silicon, silicon dioxide, silicon nitride, copper, tungsten, and some rare metals including hafnium (5). In certain steps, a liner is required because incoming materials on the wafer might not pack well due to their hydrophilicity (6). Liners are placed or deposited between two different metals because different metals cannot interact well, thus inducing peeling of material can happen (**Figure 1**). If liners are deposited correctly, then the contact angle will either decrease or increase depending on the hydrophilicity of the liner (**Figure 2**).

Contact angle is the angle between a liquid and a solid surface where they meet. If the contact angle is greater than 90 degrees, then the solid surface is considered hydrophobic. Amorphous silicon and silicon nitride (SiN) liners must be hydrophobic because hydrophobic interactions create strong packing. For this reason, engineers coat their wafers according to the incoming materials (7). The most commonly used hydrophobic chemical semiconductor companies use is bis(Trimethylsilyl)amine, also known as HMDS. However, HMDS has a very distinct odor, which can be an unpleasant smell for engineers and technicians, and it requires more effort within the purification step (8). Compared to the boiling point of trimethylsilanol (99°C), the boiling point of HMDS is higher (127° Celsius), thus requiring extra energy to evaporate (8, 9). Other chemicals such as bromotrimethylsilane, chlorotrimethylsilane, and trimethylsilyl methanesulfonate are good options to convert a hydrophilic liner to hydrophobic. However, they create strong acids hydrobromic acid, hydrochloric acid, and methanesulfonic acid, respectively, which can

reverse the reaction, lowering hydrophobicity during wafer coating due to the low pH (10).

We hypothesized that chemicals that can produce strong acid as a by-product would have a lower contact angle compared to trimethylsilanol (TMS), which only creates water in the process of creating a hydrophobic liner. We tested bromotrimethylsilane, chlorotrimethylsilane, and trimethylsilyl methanesulfonate and obtained contact angles for comparison. We found that side products from the reaction can break newly formed Si O-Si bonds, resulting in a less hydrophobic surface. If the side product is a stronger acid, the contact angle is lower because of the more hydrophilic surface. Conversely, if the side product is a weaker acid, the more hydrophobic surface results in a higher contact angle. These findings can help industries improve coating uniformity and enhance adhesive reliability by promoting lower contact angles during reverse reactions.

RESULTS

Before comparing TMS with other chemicals, we tested temperature, reaction time, and the volume of the chemical to identify optimal experimental conditions for the conversion of the silica wafer surface from hydrophilic to hydrophobic. First, we determined what temperature was optimal by using 0.05 mL of TMS, without diluting with other solvents. Temperature testing is important because higher temperatures will result in faster reactions; however, there is a point at which increasing temperature does not create a noticeable change in reaction rate. We tested temperatures between 25°C and 120 °C, and found that 80°C was the optimal reaction temperature (**Table 1**). Next, we performed reaction time tests to determine the optimal time for the reaction. Reaction time is very important because we want to stop the reaction when there is no improvement in the conversion. We discovered that the optimal reaction time is 60 seconds (**Table 2**). Lastly, we looked at the impact of using different amounts of TMS in the experiments. Using more TMS will increase the reaction rate; however, we wanted to avoid wasting TMS by using too much. Therefore, we wanted to identify the amount of TMS that could give us more yield and faster time without being wasteful. We tested TMS volumes from... (**Table 3**). Overall, we found that the optimal condition to convert the hydrophilic silica surface to hydrophobic was 0.1mL TMS (without solvent) for 60 seconds at 80°C.

Using these same conditions, we then tested three different chemicals: CTS, BTS, and trimethylsilyl methanesulfonate, for their ability to convert the hydrophilic silica surface to hydrophobic. We tested the solution using a universal pH indicator to see if the wafer created a wafer surface pH of 7. We saw that CTS, BTS, and trimethylsilyl result in a wafer surface acidic, with pHs of <1, <1, and 3, respectively (**Figure 4**). Trimethylsilyl methanesulfonate yields methanesulfonic acid in the reaction, and the pH paper shows that the methanesulfonic acid-containing water is acidic. However, universal pH indicator shows that the methanesulfonic acid solution is not stronger compared to hydrochloric acid (pKa of -6.3) and hydrobromic acid (pKa of -8.3) because hydrochloric acid and hydrobromic acid are stronger than methanesulfonic acid (pKa of -1.6), which shows how hydrophobic the surface of the wafer is. TMS was the most hydrophobic, with a contact angle of 110.6°. CTS, BTS, and trimethylsilyl methanesulfonate had contact angles of 100.2°, 98.8°, and 102.1°, respectively (**Figure 3**,

Table 4). These results show that while alternatives show a comparable effect on the contact angle between the wafer and the water, and therefore how hydrophobic the wafer is, they still produce a lesser result than that of TMS. As predicted, strong acids break the siloxane bond compared to TMS, as the siloxane bond becomes more likely to be degraded or weakened.

DISCUSSION

We tested all the chemicals on the bare silica wafer because they were readily available for purchase online. First, we identified the optimal temperature for the reaction, as heat increases the reaction speed, which decreases process time. We found that 80°C was the optimal reaction temperature. Below 80°C resulted in incomplete conversion of the hydrophilic wafer into a hydrophobic one and yielded a smaller contact angle. On the other hand, above 80°C resulted in the same contact angle due to maximum conversion. We forced a reaction at 160°C to see if the reaction goes to completion; however, we did not see any increase in contact angle.

Once we found the optimal temperature, we tested various reaction times. As displayed in **Table 2**, there was no dramatic increase in contact angle. We believe this was because there are not many silanol groups left to convert to hydrophobic bonds after 60 seconds. Reaction times greater than 60 seconds showed no improvement in contact angle. Lastly, we identified the optimal amount of chemical. **Table 3** shows that 0.1 mL is the optimal amount of TMS for the reaction. Less than 0.1 mL: either not enough chemicals were used, or the reaction was not forced to completion. More than 0.1 mL: we did not achieve significantly different results. We also forced the reaction to see if there is any change; however, 0.5 mL showed no change in the contact angle.

Using these optimized conditions, we ran four different reactions to compare the conversion of the wafer surface to hydrophobic using different chemicals: TMS, chlorotrimethylsilane, bromotrimethylsilane, and trimethylsilyl methanesulfonate. We hypothesized that all the chemicals would go through an S_N2 reaction because chloride, bromide, and methanesulfonate are very good leaving groups; therefore, all other chemicals will follow the same reaction mechanism pathway. The only side product of TMS is water, and water does not impact on pH of the solution. Because water has a neutral pH, we predicted that water will not reverse the reaction compared to chlorotrimethylsilane, bromotrimethylsilane, and trimethylsilyl methanesulfonate, which produce strong acid as a by-product (11). We drew an equilibrium scheme of siloxane bond forming vs siloxane bond breaking in **Figure 5**. **Figure 4** shows the pH of each chemical after the side product is created. Some unreacted materials were not easily dissolved in the water; we saw some oil residues either floating or sinking. However, oil does not impact the pH of the solution; therefore, it should not change the outcome of the contact angle. Our results indicated that when reactions created stronger acid, the contact angle tended to be lower because strong acids reverse the back reaction. For this reason, bromotrimethylsilane had the lowest contact angle compared to others, because the hydrobromic acid was the strongest out of the two acids and water. TMS retained the highest contact angle because water is the by-product after the reaction and water does not reverse the reaction.

To ensure Table 4 results were optimized as well, we ran experiments with large amounts of each chemical, prolonged durations, and increased temperature to see the differences and recorded them in Table 5. There was a very small increase in contact angle. As a result, we concluded that increasing these variables resulted in a minimal increase in contact angle, making the changes inefficient and unnecessary. TMS is a good choice for converting the hydrophilic surface of the wafer to hydrophobic. Other chemicals might have a shorter reaction time to react on the surface of the wafer. To negate the strong acid by-product, future research can investigate putting small amounts of base, such as triethylamine, to capture the acid.

Throughout the experiment, some limitations included the equipment that was needed for deposition. If the deposition tools were available, such as chemical vapor deposition (CVD) or atomic layer deposition (ALD), we could test if incoming materials can bind with the converted surface better or worse. Furthermore, TMS is limited in the semiconductor industry because of its limited functional applications. Trimethylsilanol is at high risk of contamination and unwanted reactions if it is exposed to moisture, which is not favorable to industries, as higher chemical stability is favorable. Furthermore, because of its sensitivity to reactions, high temperatures, exposure to other chemicals, and vacuum conditions, it is often difficult to use Trimethylsilanol. There are also more cost-effective materials that can be substituted that are more stable and suited for the specific needs of the semiconductor industry, which causes the limited use of Trimethylsilanol.

Future studies could consider using a deposition tool to determine whether a changed contact angle will be stable to bind with incoming metals. Another potential avenue of study is investigating how TMS can be removed through other acids such as hydrofluoric acid, acetic acid, and phosphoric acid when the hydrophobic surface is no longer needed. Even with these limitations, engineers and semiconductor companies could benefit from lower production costs that could lead to lower costs for customers, making it more accessible. This research can ultimately provide valuable insight for industries aiming to optimize coating uniformity and adhesion performance through reduced contact angles in reverse reaction processes.

MATERIALS AND METHODS

Safety Protocol

Before any experiments, all the necessary PPE (personal protective equipment) must be followed strictly. Gas masks and goggles (AirGearPro from Amazon, B08BQNK3D) were purchased and equipped while doing any experiments. Also, nitrile gloves (Submedic from Amazon, B0CSF7XP4) were also worn throughout the experiment. Furthermore, students must wear long pants and long-sleeved shirts to minimize exposed skin. Everyone was conducting an experiment with at least one adult present with a student. All the experiments were conducted in a ventilated area such as a garage or outside of the house.

Converting the hydrophilic surface to a hydrophobic surface

We used 97.5% TMS (Aldrich #MFCD02751657) to carry out the conversion of the hydrophilic surface of a 5 mm x 5 mm, 525 μm silicon and 200 nm SiO_2 silica with P/Boron and front side polished thermal oxide layer wafer (MSE Supplies) to a hydrophobic surface. For comparison, 99.3% chlorotrimethylsilane (Aldrich, #MFCD00000502), 97% bromotrimethylsilane (Aldrich #MFCD00000048), and 97% trimethylsilyl methanesulfonate (Aldrich #MFCD00042815) were used in the rest of the experiments. For rinsing the wafers after each experiment, distilled water followed by 100% acetone was used for rinsing the wafers after each experiment. A compressed air duster (air speed $\sim 43\text{m/s}$) was used to remove any remaining residues such as water, acetone, or silicon-based oil on the wafer after rinsing with distilled water and 100% acetone. We used a scientific hotplate (Four E's, #MI0102003), which can raise the temperature of a ceramic plate to 280°C . A 1-mL capacity precision syringe (Ibis Scientific, #008131) was used to accurately measure the amount of chlorotrimethylsilane.

The optimized procedures were applied for all four chemicals: the hot plate temperature was adjusted to a predetermined target temperature of 80°C . Once the temperature was reached, we waited 10 minutes to minimize the fluctuation of the target temperature. The silica wafer was placed on the hot plate, and we waited another 10 minutes. After reaching the target temperature, 0.2 mL of silane compound was injected onto the surface of the wafer within 10 seconds. The wafer was removed from the hot plate after 60 seconds and rinsed with 10 mL of distilled water as well as 5 mL of acetone (every reaction was washed with acetone to make sure that TMS was not adhering to the surface and forming $\text{Si-O-Si}(\text{Me})_3$), then air-dried using a compressed air duster. Coated wafers were taken to an Ossila goniometer (Product code: L2004A1) for measuring contact angle. This process was repeated for each of the materials tested.

Analysis of pH of collected solution

To measure the pH of the solution after the reaction, we collected rinsed water and submerged the universal pH indicator. universal pH indicator (Amazon, Model Number: LAB-pH-14) was submerged in the solution for 1 second before being removed and examined for color change.

Analysis of the contact angle

A 5 mm x 5 mm, 525 μm silicon and 200 nm SiO_2 silica with P/Boron and front side polished thermal oxide layer wafer was centered on the test surface of a contact angle goniometer (Ossila, #L2004A1). A droplet of 10 μL water was deposited onto the silicon wafer using a 1-mL precision syringe. The water droplet was illuminated from behind through a light source, and an image was recorded by the camera. The image was analyzed using version 4.1.5 of the Ossila Contact Angle measurement analysis software, and a contact angle measurement was determined.

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Figures and Tables

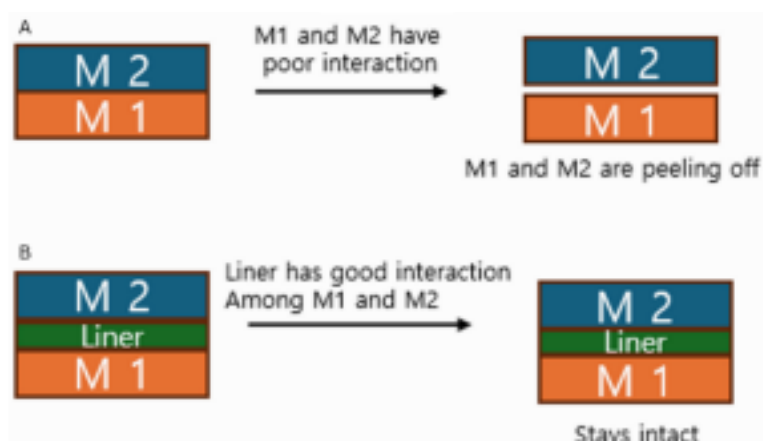


Figure 1. Deposition with and without a liner. A) If there is no liner between two different metals (M1 and M2), M1 and M2 can peel off, resulting in separation (A). B) A liner can help hold M1 and M2 together.

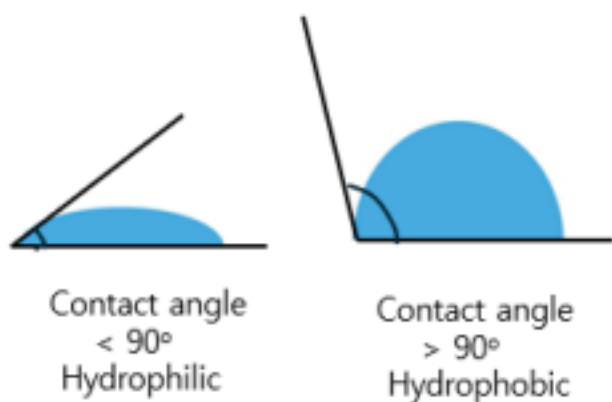


Figure 2. Diagram of contact angle delineation for hydrophobicity and hydrophilicity. The blue indicates a water droplet sitting on the surface. If the contact angle is less than 90°, the surface is considered hydrophilic. If the contact angle is greater than 90°, the surface is considered hydrophobic.

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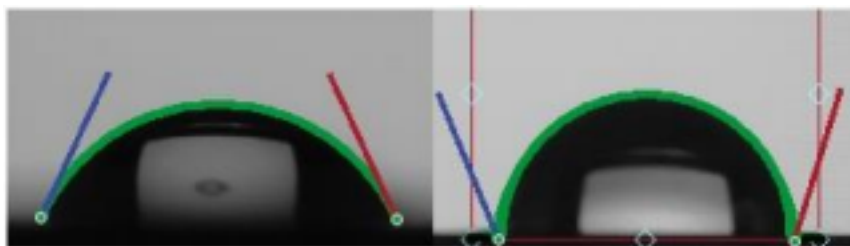


Figure 3 Surface analysis using a goniometer. The left picture shows a reference with a 64.5° contact angle, while the right picture is a TMS-treated surface with a contact angle of 110.6°.

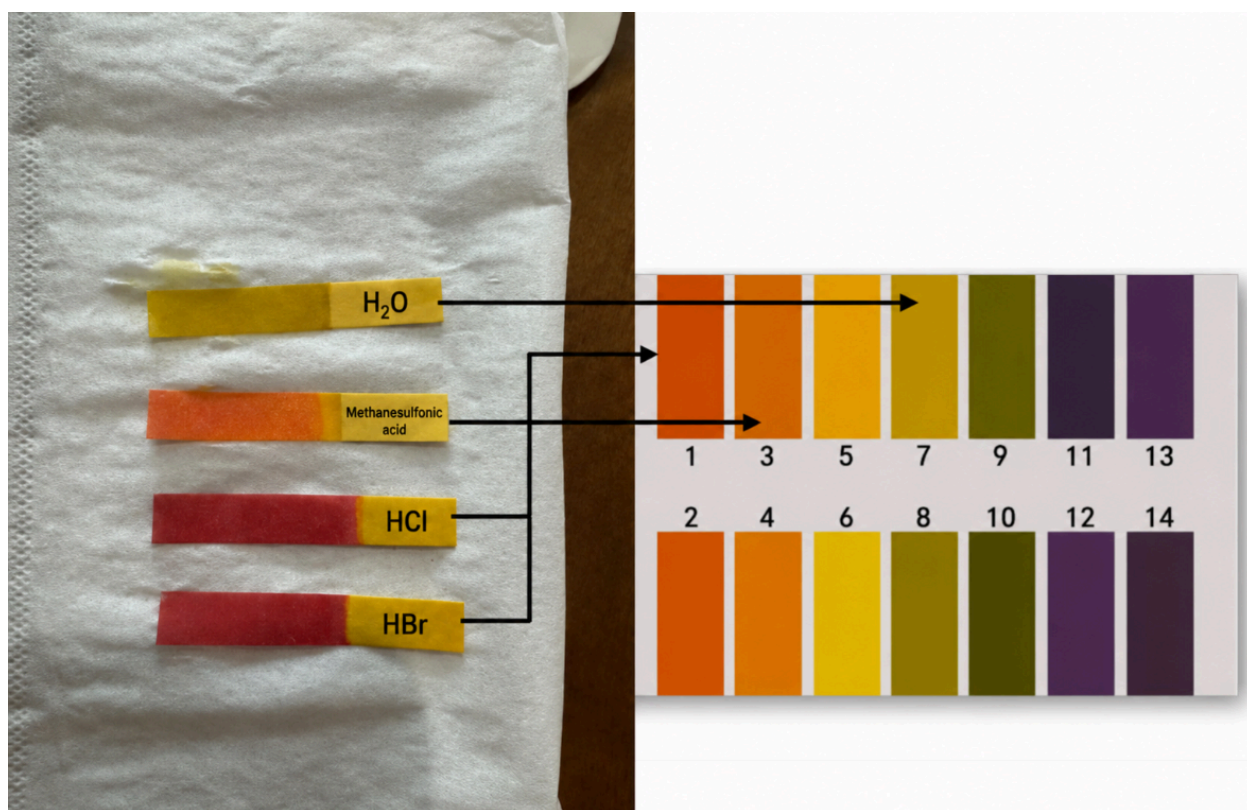


Figure 4. pH test of the solutions containing different acids. We rinsed the silicon wafer after using each chemical and collected each acid from different chemicals for testing the pH of the solutions. H₂O had a pH of 7, Sulfonic Acid had a pH of 3, HCl had a pH of <1, and HBr had a pH of <1.

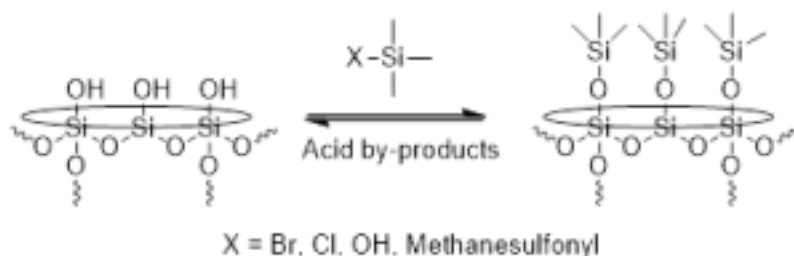


Figure 5. Equilibrium scheme of Siloxane formation. Depending on the strength of the acid, the reaction can reverse. With greater acidity, the reaction will favor breaking the siloxane bond.

TMS (mL)	Temperature (°C)	Time (second)	Contact angle (°)
Reference 0	25	60	65.4 ± 0.21
1 0.05	25	60	68.87 ± 0.35
2 0.05	40	60	75.30 ± 0.40
3 0.05	60	60	85.67 ± 0.55
4 0.05	80	60	101.13 ± 0.65
5 0.05	100	60	101.50 ± 0.20
6 0.05	120	60	101.37 ± 0.40

Table 1. Temperature optimization tests. Reaction temperature was varied to determine the optimal temperature for converting the hydrophilic surface of a silica wafer to a hydrophobic surface. 80°C was determined to be the optimal reaction temperature. Each experiment was tested three times in different wafers and averaged. Contact angle values are reported as mean ± standard deviation (SD, n = 3)

TMS (mL)	Temperature (°C)	Time (second)	Contact angle (°)
Reference 0	80	60	65.6 ± 0.22
1 0.05	80	10	70.1 ± 0.46

2 0.05	80	20	81.1 ± 0.43
3 0.05	80	40	92.9 ± 0.48
4 0.05	80	60	101.2 ± 0.50
5 0.05	80	80	101.0 ± 0.51
6 0.05	80	100	101.4 ± 0.49

Table 2: Time variation tests. This table shows how we got the optimal reaction time for converting the hydrophilic surface of a silica wafer to hydrophobic. Each experiment was tested three times in different wafers and averaged. Contact angle values are reported as mean ± standard deviation (SD, n = 3)

TMS (mL)	Temperature (°C)	Time (second)	Contact Angle (°)
Reference 0	80	60	65.3 ± 0.18
1 0.01	80	60	72.2 ± 0.47
2 0.02	80	60	82.6 ± 0.37
3 0.05	80	60	101.0 ± 0.58
4 0.08	80	60	105.7 ± 0.49
5 0.1	80	60	110.6 ± 0.44
6 0.12	80	60	110.8 ± 0.51

Table 3: Different amounts of trimethylsilanol. Different amounts of trimethylsilanol (TMS) were tested to obtain the optimal amount of trimethylsilanol. Each experiment was tested three times in different wafers and averaged. Contact angle values are reported as mean ± standard deviation (SD, n = 3)

Chemical Contact angle Reference 64.5°	pH of rinse
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	7
TMS 110.6°	7
Chlorotrimethylsilane 100.2°	<1
Bromotrimethylsilane 98.8°	<1
Trimethylsilyl methanesulfonate 102.1°	3

Table 4. Chemical comparison testing. The reaction was carried out using 0.1 mL of each chemical for 60 seconds at 80°C. Each experiment was tested three times in different wafers and averaged. Since the universal pH indicator does not give decimal values, we could not report average values.

Chemical Contact angle Reference 64.7° ± 0.24
TMS 110.6° ± 1.14
Chlorotrimethylsilane 100.7° ± 1.25
Bromotrimethylsilane 98.4° ± 1.07
Trimethylsilyl 102.1° ± 1.18 methanesulfonate

Table 5. Forced reaction test. The reaction was carried out using 0.5 mL of each chemical for 300 seconds at 160°C. Each experiment was tested three times in different wafers and averaged. TMS = Trimethylsilanol. Contact angle values are reported as mean ± standard deviation (SD, n = 3)

