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The effect of microscopic texture on the direct plasma surface passivation of Si solar cells

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Textured silicon surfaces are widely used in manufacturing of solar cells due to increasing the light absorption probability and also the antireflection properties. However, these Si surfaces have a high density of surface defects that need to be passivated. In this study, the effect of the microscopic surface texture on the plasma surface passivation of solar cells is investigated. The movement of 10^5 H^+ ions in the texture-modified plasma sheath is studied by Monte Carlo numerical simulation. The hydrogen ions are driven by the combined electric field of the plasma sheath and the textured surface. The ion dynamics is simulated, and the relative ion distribution over the textured substrate is presented. This distribution can be used to interpret the quality of the Si dangling bonds saturation and consequently, the direct plasma surface passivation. © 2013 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4798527>]

I. INTRODUCTION

Due to the continuously increasing energy demand, renewable energy generation has become a highly topical issue. Photovoltaic (PV) solar cells are presently considered as a viable solution of these problems. Due to the dramatic reduction of manufacturing costs and the achievement of high photo-conversion efficiencies, the PV solar energy generation has been widely accepted as a competitive source of electricity.

Crystalline silicon is among the most widely used materials in the solar cell production. In crystalline silicon, recombination of charge carriers is due to several mechanisms, such as band-to-band radiative recombination, Auger recombination, and recombination on defects.^{1–5} To achieve the high efficiencies, all the recombination processes must be minimized.

Imperfections in the crystalline silicon due to impurities or crystallographic defects act as carrier traps. The bulk imperfections depend strongly on the fabrication process and are insignificant in the high solar-grade silicon. However, it is not the case for the surface. Due to the fact that the continuity of the crystal lattice is lost at the surface of any crystalline material, a large number of silicon atoms with dangling bonds are present at the surface acting as defects. The high number of these defects in silicon makes the surface recombination the dominant carrier recombination mechanism. The negative effect of the surface recombination can be minimized by decreasing the surface defect density, e.g., by surface passivation.

The surface passivation can be implemented by the field effect passivation and the direct saturation of the defects. The high amount of defects at the surface can be reduced by saturating the silicon dangling bonds.⁶ In practice, this is achieved by depositing a passivating layer over the Si surface. Amorphous silicon nitride, silicon carbide, silicon, and silicon dioxide are widely used for the passivation of crystalline silicon (c-Si) surfaces. The quality of the surface passivation depends not only on the deposited amorphous layer but also on the conditions of the crystalline silicon surface.

The silicon surfaces may either be flat or textured. Textured silicon surfaces are essential in the solar cell fabrication process for increasing the light absorption efficiency. The wet-chemistry-based approach where solar cells are textured with tetrahedral pyramids having four (111) planes is presently the state-of-the-art in surface texturing.^{7,9} This process heavily relies on toxic alkaline solutions. However, in the near future, dry, plasma-based approaches are expected to become more favorable for thinner silicon wafers. The Scanning Electron Microscopy (SEM) images of the wet- and dry-textured Si surfaces are shown in Figure 1. However, due to the fact that the textured surface area is 1.73 times larger than the flat surface and the exposed surfaces are (111) oriented,^{7–9} the surface passivation becomes more challenging. The reason is the existence of a large number of dangling bonds at the surface.

Plasma enhanced chemical vapor deposition (PECVD) is widely used for the deposition of the above mentioned passivating layers from various gaseous precursors. Since the presence of hydrogen causes the effective saturation of the dangling bonds,¹⁰ hydrogen containing gases are usually used as precursors.

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FIG. 1. SEM images of (a) wet- and (b) dry-textured Si surfaces produced in our laboratory at Plasma Sources and Application Center, Singapore. More details about the fabrication process of the textured Si surfaces can be found elsewhere.^{34–42}

In the PECVD system, the plasma bulk and the substrate are separated by a thin sheath with the width varying with the applied conditions. In the process of surface passivation, textured silicon surfaces acquire electric charge due to the balance of electron and ion fluxes onto the substrate. The equilibrium charge produces microscopic electric fields which in turn affect the ion deposition process.

Therefore, here we present the results of Monte Carlo (MC) numerical simulations in which the ion coverage in the deposition of a hydrogenated amorphous silicon (*a*-Si:H) layer is investigated. The deposition of the passivating layer onto the textured and flat crystalline silicon substrates in the plasma environment is simulated. The computed ion coverage over the surface can serve as an indicator of the probability of the dangling bond saturation in the PECVD deposition environments.

This study is based on the model, which was originally used for the simulation of the ion transport in the plasma sheath layer.^{11–15} The model is applicable for the investigation of the effect of the plasma environment on the growth of the nanostructured surfaces. This model has recently been

advanced to include the effect of the cone-like nanostructures.¹⁶ The modified model can be thus used for the simulation of the ion coverage over the textured crystalline silicon surfaces due to the presence of the cone-like structures on the surface.

It should also be noted that in many plasma-based nanostructure deposition and surface texturing processes, the ion fluxes are often comparable or even larger than the fluxes of neutral radical species. This is why the focus in this study is on the ion deposition.

The results of this study show that the presence of microscopic texture on the surface will slightly affect the uniformity of the dangling bond saturation in the plasma environment compared to the flat silicon surface. This implies that in addition to the greater surface area of the textured surfaces as well as the exposure of the (111) planes, which both increase the number of dangling bonds on the surface, the acquired charge on the surface will also affect the quality of the surface passivation through the slight reduction of the uniformity of the deposition process. The process conditions may be optimized to achieve the best uniformity. The results are applicable for the formation of the various passivating layers in the plasma deposition systems where the ions play a major role in the deposition and surface interaction processes.

II. MODEL

The ions are accelerated towards the substrate in the plasma sheath that separates the plasma bulk and the biased substrate. The minimum velocity of the ions at the sheath edge is equal to Bohm velocity, $V_b = \sqrt{K_B T_e / m_i}$, where T_e , m_i , and K_B are the electron temperature, the ion mass, and the Boltzmann constant, respectively.

Under typical experimental conditions, we have $eV_{Bias} \gg K_B T_e$, (where e and V_{Bias} are the electron charge and the substrate bias, respectively). If the above condition is fulfilled, the sheath can be considered wide. Therefore, the Child Law can be used to calculate the sheath width and the electric field across the sheath. The plasma sheath width can be estimated as

$$S = \frac{\sqrt{2}}{3} \lambda_D \left(\frac{eV_{Bias}}{K_B T_e} \right)^{3/4}, \quad (1)$$

where S and λ_D are the sheath thickness and the Debye length, respectively.¹⁷ The equation for the Debye length is as follows:

$$\lambda_D = \sqrt{\epsilon_0 K_B T_e / n_e e^2}, \quad (2)$$

where ϵ_0 and n_e are the vacuum permittivity and the electron density.

The sheath electric field acting on each ion can be calculated from¹⁷

$$\vec{E}_{Sheath} = \frac{4}{3} \frac{V_{Bias}}{S} \left(\frac{z}{S} \right)^{1/3}, \quad (3)$$

where z is the distance from the sheath edge.

As mentioned above, the textured surface (cone-like structures in Fig. 1) acquires the electric charge affected by the ion bombardment. The conical structures produce microscopic electric fields due to their surface charge. Therefore, the ions move in the combined electric field produced by the sheath and the surface texture. The electric field of the texture is calculated as the sum of the electric fields of the cone structures

$$\vec{E}(r) = \sum_{j=1}^N \int_{A_j} \frac{\sigma_j dA_j}{4\pi\epsilon_0 r^3} \vec{r} + \vec{E}_{Sheath}, \quad (4)$$

where $\vec{E}(r)$ is the total electric field at point r (the location of the ion in the sheath region). The summation in Eq. (4) is performed over the cones' surfaces; and σ_j and A_j are the surface charge density and the surface area of the cones, respectively. It should be noted that dA_j is the surface differential of A_j .

The Newton's equations of motion are used to obtain the ion trajectories in the simulation

$$\begin{cases} r(\tau) = r(0) + \int_0^\tau v(t) dt \\ v(\tau) = v(0) + \int_0^\tau a(t) dt \end{cases}, \quad (5)$$

where r , v , and a are the location, velocity, and acceleration of the ions, respectively.

III. SIMULATION

To calculate the ion coverage over the silicon textured surface, a $44 \mu\text{m} \times 44 \mu\text{m}$ substrate is considered. To include the effect of the surface texture, 100 cones with the height and diameter of $4 \mu\text{m}$ are placed on the substrate. A schematic diagram of what is used in the simulation is shown in Fig. 2 except for the bases, which are circular. This implies that the cone-like structures are used in the simulation.

As mentioned above, hydrogen atoms/ions effectively saturate the Si dangling bonds. Therefore, hydrogen-containing precursor gases are used in the deposition systems. Moreover, hydrogen can be used as a treatment step.¹⁸ Hence, to compute the ion coverage, 10^5H^+ ions are traced in the plasma sheath layer.

It should be mentioned that although other ions are present in the plasma environment of the hydrogen containing gases, their exclusion does not affect the obtained results. The reason is that the extremely small mass, very high reactivity,

FIG. 2. The schematic diagram of the array of Si microcones used in the simulations.

TABLE I. The simulation parameters.

Parameter	Notation	Value
Number of ions	N	10^5
Electron density	n_e	$5 \times 10^{18} \text{ m}^{-3}$
Electron temperature	T_e	2 eV
Substrate bias	V_{Bias}	-25 and -75 V
Sheath thickness	S	15 and 34 μm
Substrate area	A	$44 \mu\text{m} \times 44 \mu\text{m}$
Ion species	H^+	

and the high sticking probability of hydrogen make it the most favorable species for dangling bonds termination.^{18–22} It should also be noted that hydrogen can have a similar role in growth of metal oxide nanostructures.^{23–32}

The H^+ ions are randomly distributed over the simulation plane with the length and width of $44 \mu\text{m}$; this plane is located at the sheath edge and is parallel to the substrate. The initial velocities of the ions are equal to the Bohm velocity. The hydrogen ions are traced in the sheath, which is assumed collisionless. It implies that the ion-neutral collision mean free path is large compared to the sheath width. This assumption is valid under typical conditions of the Si surface treatment using low-temperature plasmas. The particles are traced till the moment of their impact on the surface.

We used the Verlet algorithm for time integration of the Newton's equations of motion (5) and executed the programs in parallel to reduce the computation time. The other simulation details can be found elsewhere.¹⁶ The simulation parameters are summarized in Table I. The presented results are valid for the textured surface at the bias of -25 and -75 V and also for the flat surface at the bias of -75 V.

IV. RESULTS

As stated above, the ions move in the sheath layer under the effect of the electric field of the sheath accompanied with the texture-produced electric field. The electric fields of the cones are due to their surface charge. The calculated charge under the bias of -25 and -75 V is shown in Fig. 3. It is clear that the total charge on each cone increases with the bias. The amount of charge is equal to 5.88×10^{-15} and 1.76×10^{-14} C for the bias of -25 and -75 V, respectively.

FIG. 3. The accumulated electric charge on the Si cones.

FIG. 4. Displacement and velocity of a typical ion for both the textured surface at the bias of -25 (a) and (b), -75 V (c) and (d), and the flat surface at the bias of -75 V (e) and (f).

The temporal distribution of the displacement and velocity of a typical H^+ ion is shown in Fig. 4. The results are presented for the textured surface at the bias of -25 and -75 V and also for the flat surface with the -75 V substrate bias.

The mentioned quantities are displayed along the Z and X axes (the changes in the Y component is similar to X). As it is seen, in the Z direction, the ion transits the sheath layer. The time of transition for the textured surface at the bias of -25 and -75 V is 0.2 and 0.25 ns, respectively. This time increases to 0.5 ns in the case of the flat surface. The sheath thickness also increases from 15 to 34 μm with increasing the applied bias.

The ion also moves along the X axis. As it is shown, the displacement increases with bias. For the textured surface, the displacement along the X axis is equal to 8 μm for the bias of -25 V, while it increases to 15 μm for the bias of -75 V. As it is clear, the particle does not move in X direction while the surface is flat.

The particle velocity in Z direction at the sheath edge is equal to Bohm velocity. This initial velocity increases with time. When the bias is -25 V [Fig. 4(b)], the velocity increases from 1.39×10^4 m/s to 1.35×10^5 m/s during the transit time. When the bias increases, the final velocity increases also. In this case, the velocity at the moment of impact is 3.73×10^5 m/s [Fig. 4(d)]. It should be mentioned that in the case of the flat surface, the final velocity is equal to 1.2×10^5 m/s [Fig. 4(f)].

As it is seen for the textured surfaces, the velocity in the X direction has the same trend as the Z direction. However, its magnitude is smaller compared to the Z-component. The final velocities for the biases of -25 and -75 V in the X direction are 9.4×10^4 and 1.44×10^5 m/s, respectively. On the other hand, when the surface is flat [Fig. 4(f)], the ions do not have a velocity along the X and Y axes, which is due to the fact that they do not move parallel to the substrate surface.

The relative ion distribution over the cone lateral surface is shown in Fig. 5. The figure displays the distribution of ion

impact points over the cone lateral surface in Z direction. The distribution implies that the H^+ ion collisions with the base parts of the cones are more frequent compared to the top sections. To better illustrate the above mentioned finding, a 3D image of the collision points is presented in Fig. 6.

This figure also suggests that the particle collisions with the base sections are more frequent. In other words, the probability of collision with the base sections increases in a textured silicon substrate. This arising non-uniformity may reduce the quality of the dangling bonds saturation, which needs further investigation.

To compare the obtained result with the flat surface, a 3D image of the particle collisions with the flat surface is also presented in Fig. 7. Considering the figure, it is clear that in the plasma surface passivation of the flat substrate, the degree of uniformity of the ion coverage is higher.

It should also be noted that although the ion collisions with the top cone sections are less probable, the surface area of these sections are smaller, and as a result, the number of dangling bonds decreases. Therefore, to obtain the correct result, the cone lateral surface is segmented into 10 sections.

FIG. 5. The relative ion distribution over the lateral surfaces of the Si cones.

FIG. 6. A 3D image of the ion coverage over the simulated micro-textured surface.

FIG. 7. A 3D image of the ion coverage over the flat Si surface.

Then, the relative number of ions along each segment (Fig. 5) is summed up. Third, the calculated number is divided by each segment area.

The obtained result is shown in Fig. 8. In this figure, the ion number density is presented for the 10 mentioned segments. As it is clear that the ion number density has a slight deviation from a straight line (flat surface), which is the

FIG. 8. The ion number density of different segments along the lateral surface of the Si cones.

indicator of an insignificant nonuniformity in saturation of the dangling bonds.

V. DISCUSSION

As briefly mentioned above, the electric charge of the textured substrate exposed to the plasma is affected by the impinging ions. This electric charge produces the electric field which in turn affects the ion dynamics. As shown in Fig. 3, the electric charge on the cones increases with the substrate bias. This result is due to the fact that the geometrical shape of the surface structures is preserved. Indeed, when the geometrical shape and consequently, the surface area are preserved, increasing the bias leads to the accumulation of a larger amount of electric charge on the textured surfaces.

Increasing the bias will also increase the sheath width. Under the wider sheath conditions, more electric charge is accumulated on the cones, and the ion dynamics is affected stronger (Fig. 3). In this case, the resulting stronger electric fields decrease the ion transit time through the plasma sheath in spite of the wider sheath.

In addition, stronger electric fields lead to the more effective acceleration of the depositing particles (Fig. 4). As a result, the ion velocity at the moment of collision with the textured surface becomes higher than under the lower substrate bias conditions.

It should be mentioned that when the surface is flat, the electric field of the plasma sheath accelerates the ions merely in the Z direction. Therefore, the electric field does not have the X or Y components; as a result, the ions do not move along these directions.

In the case of the flat surface, the ion transit time increases compared to the textured surface. The reason is the wider sheath as well as the weaker electric field due to the absence of the textured electric field. This also leads to the lower ion velocities compared with the textured surface under the same substrate bias conditions.

The ion coverage over the lateral surfaces of the cones is shown in Fig. 5. This distribution indicates that the ion collisions with the base sections of the cones prevail. This implies that for a textured silicon substrate, the ion distribution is non-uniform with the maximum located near the substrate. Although the ion coverage has a triangle-like shape, the ion number density presented in Fig. 8 suggests that the number of ions per surface area is rather uniform.

Therefore, considering the obtained results, one can state that in the case of a textured silicon surface, the uniformity of the dangling bonds saturation is affected slightly, which can be ignored or reduced by optimizing the plasma process conditions.

As mentioned, these simulations extend the previous model.¹⁶ It was previously shown that the relative ion distribution for the cones with aspect ratio of less than 10 has the same trend as in this work. Therefore, one can conclude that for different texture sizes, the quality of the surface passivation is unlikely to change. The reason is that the aspect ratio of different texture sizes is nearly ~ 1.0 . Hence, changing the texture size does not significantly affect the ion coverage pattern and consequently, the Si surface passivation. This

conclusion is consistent with the experimental results³³ where different textured silicon substrates passivated in the PECVD environment did not show different minority carrier lifetimes.

VI. CONCLUSION

To investigate the effect of texturing on the plasma surface passivation of Si-based solar cells, the transport of 10^5H^+ ions in the plasma sheath is investigated using numerical simulations. The hydrogen ions are driven by the sheath electric field as well as the microscopic electric field of the textured surface. The effect of the microscopic texture is taken into account by considering an ordered array of Si cones on the substrate. The surface charge of the cones is calculated. The ion dynamics is simulated, and the ion coverage over both the textured and the flat surfaces is obtained under different applied bias conditions representative to typical plasma-based Si surface passivation experiments.

The results of this work show that accumulation of electric charge on the textured surface in the plasma environment leads to some non-uniformity of the ion coverage on the surface. As the ion coverage represents the probability of the dangling bonds saturation on the textured surface, the ion number density (number of ions per surface area) is calculated. This quantity predicts a slight non-uniformity in the surface passivation of the textured surfaces in comparison with the flat polished surfaces.

It should be noted that the previous simulation studies^{11–16} on the plasma growth of nanostructures have shown that the ion coverage is affected by varying the process parameters. Therefore, although this non-uniformity is not significant, the experimental conditions should be adjusted to maximize the uniformity of passivation of the textured Si surfaces. The results of this study are relevant to direct plasma surface passivation of solar cells and numerous other microstructured surfaces of solid materials.

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