Research Article

Analysis of Surface Texturization of Solar Cells by Molecular Dynamics Simulations

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The purpose of this paper is to develop a simple new model, based on the classic molecular dynamics simulation (MD), alternative to complex electron-photon interactions to analyze the surface texturization of solar cells. This methodology can easily propose the absorptance differences between texturing and nontexturing solar cells. To verify model feasibility, this study simulates square, pyramidal, and semicircular texturization surfaces. Simulations show that surface texturization effectively increases the absorptance of incident light for solar cells, and this paper presents optimal texturization shapes. The MD model can also be potentially used to predict the efficiency promotion in any optical reflection-absorption cases.

1. INTRODUCTION

Achieving higher efficiency in solar cells is one of the most important issues in recent studies on the topic, and researchers have examined many methods for achieving this goal. Surface texturing of solar cells is a common approach to reduce incident light reflection and, consequently, increase solar cell efficiency.

Dry etching and wet etching are commonly used to apply surface texturization to solar cells. Dry etching means texturing without wet solutions. A plasma texturing technique using reactive ion etching, with advantages of low cost consumption and independence from crystallographic orientation, was previously proposed [1, 2]. A selective surface texturing technique using lasers recently gained some interest. Tan et al. [3] performed femtosecond pulsed laser induced forward transfer on a quartz substrate. A trench-like texturing was ablated on the donor substrate using a pulsed laser. This method exhibits good controls on the depth and width of ablated trenches.

Wet etching means surface texturing with chemical solutions. In a general surface texturing process on crystalline silicon, alkaline solutions form pyramids. This pyramidal surface shape occurs because alkaline solutions etch silicon along crystallographic orientations.

Some researchers use acid solutions to produce surface texturization. Due to the character of acid solutions, the etching rates in the different orientations are similar. Thus a semicircular structure is formed [4].

Most texturing studies focus on wet etching processes. Hylton et al. [5] conducted many experiments to compare the efficiency increase of saw-damage etching and texture etching processes using alkaline solutions on multicrystalline silicon wafers. That paper also explained the geometrical paths of incident light which defined the absorption and reflection on the pyramid structures. Nishimoto and Namba [6] developed a low-cost wet etching manufacturing process and reported the texturization of a monocrystalline silicon surface with low-cost alkaline solutions, Na_2CO_3. Recently, Gangopadhyay and his colleagues [7] further developed a new texturing method with tribasic sodium phosphate solution, claiming it was superior to the conventional method because it used less isopropyl alcohol for texturing.

The most previous studies focused on the manufacturing process. However, if we can simulate the behaviors of absorption and reflection before fabricating a new surface texturizaion on a solar cell, it is helpful to reduce the time and fabricating wastes. Therefore, it is necessary to develop a simulation methodology to govern this issue.

Molecular dynamics simulation is a technique well suited to nanoscale phenomena and mechanical behaviors. However, few studies use MD to examine solar-cell issues. One such study [8] explores the photo-induced electron-transfer phenomena on a dye-sensitized titanium solar cell with nonadiabatic MD simulations, which is based on the *ab-initio* functional theory. The study found that approximately 20% of the acceptor state was located on a titanium atom of the first surface layer. This simulation also predicted a complex non-single-exponential time-dependence of the electron-transfer process. However, many unknown factors in photon-electron interactions prevent studies from being conducted on the issue of photon absorption.

This paper presents a simple photon-atomic model with molecular dynamics simulations to explore the effects of three shapes of solar cell surface texturization. This paper also includes an estimation of the optimum texturization.

2. METHODOLOGY

First of all, if the de Broglie wavelength of a photon and an atom is smaller, we can make assumption that the absorption and reflection are closely represented as a series of collision behaviors between photons and atoms.

To avoid complications in photon-electron transformation, a rough and simple MD model was devised to govern this problem. In the classic mechanical MD simulations, a two-body attractive-repulsive potential model governs the interaction between two particles. For one particle, short-range repulsive forces rebound the too close particles from itself, and long-range attraction catches other particles closer to itself in attractive force field. Assuming that the force field between an atom and photon is spherical, the 12-6 Lennard-Jones potential model with an undetermined parameter k, which is a short-range multiple, is adopted,

$$U(r) = 4\left[k\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6} \right]. \qquad (1)$$

When photons reach the substrate, attraction and repulsion behaviors occur between silicon's atoms and photons. Figure 1 shows the mechanism of photon-atom interactions. When a photon enters the attractive field of an atom, the photon should be attracted to the center of the atom. But the repulsive force pushes the photon off center if the photon is too close to the atom center. The substrate is maintained as an NVE model (fixing particle numbers, system's volume, and total energy) in the heat-transfer process, so the photons which enter the substrate are constrained because of forces among atoms and decay of motive energy of themselves. Due to the actions of attractive and repulsive forces and the photon energy dissipation, the velocity of a photon which enters the substrate deeply tends toward zero. This behavior is considered photon absorption in a solar cell. However, some photons are repulsed at the substrate surface due to the repulsive force. This is considered reflection. The photons whose velocity decreases to zero were removed to avoid the increasing of particle numbers, and then affect the system energy.
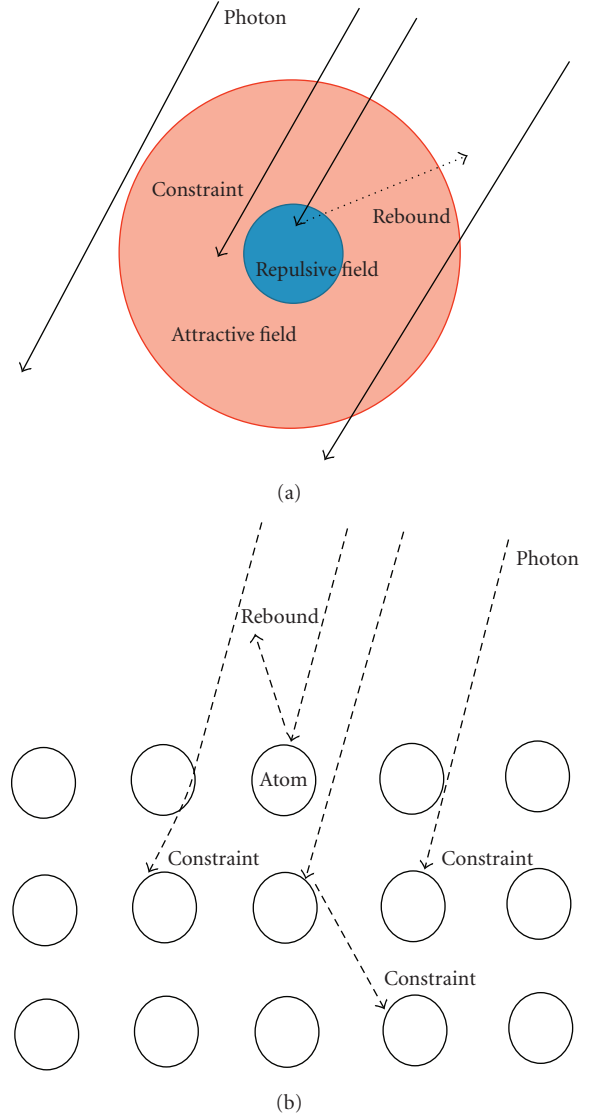

(a)

(b)

FIGURE 1: Illustrations of attractive and repulsive interaction of atoms and photons. (a) The photons move toward repulsive force field is probably rebound out, and the other photons move through attractive field is constrained or decelerated. (b) The rebounded behavior is as same as reflection. The constraint behavior is as same as absorption.

Note that the efficiency of monocrystalline silicon is, at most, 24.7% [9]. This study attempts to make a model with an absorptance reaching 24.7% in a smooth, nontextured substrate by simply adjusting k. In our simulation, k is determined to be 3.86. After this calculation, simulations of varying surface texturization with this potential model can proceed. The smooth surface model is a reference, and the other texturing models in this paper, which are simulated with the same conditions, can then be compared with the reference model. This methodology not only reasonably avoids the complexity of photon-atom interaction but also achieves the goal of trying to evaluate the efficiency of two models with different surface texturization.
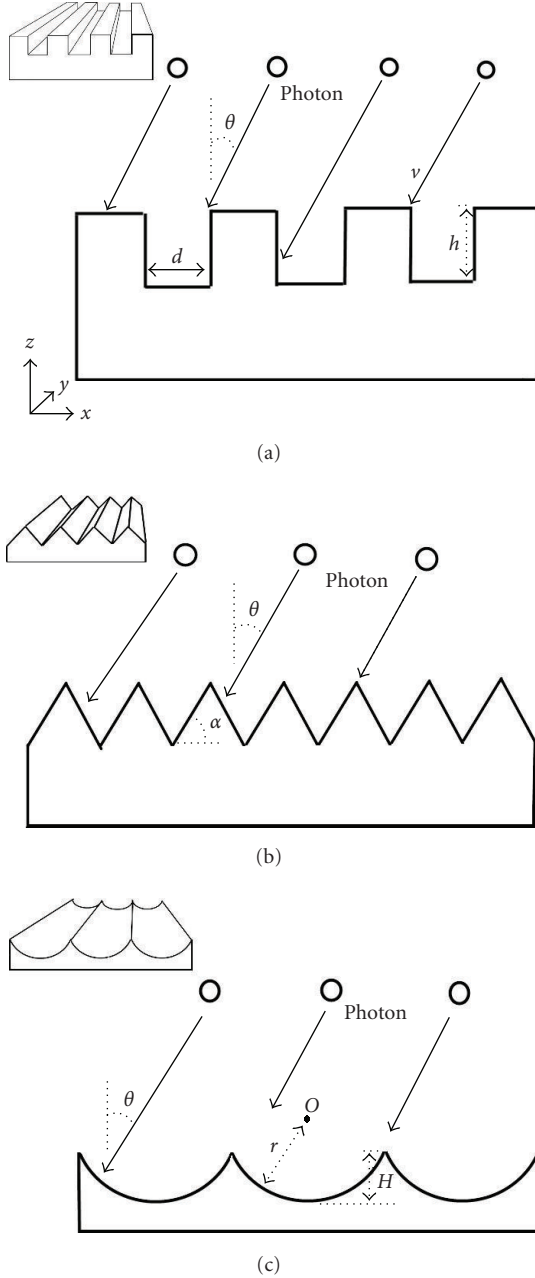
(a)

(b)

(c)

Figure 2: Physical model (a) square (b) pyramid (c) semicircle, the geometric variables are also shown in this figure.

Following this concept, monocrystalline silicon was selected as the solar cell material. This is because silicon is the most common material in all types of solar cells, and its structure is simpler for using with an MD model. The results and conclusions of this study can also be extended to other solar cells, GaAs, InGaAs, InGaP, and so forth. According to the reviews of previous studies, square, pyramidal, and semicircular texturing were demonstrated. Figure 2 shows the physical models of the three samples in this paper. A single silicon cell has a diamond structure with 8 atoms. Under the texturing surface, three layers absorb the motion

Table 1: Parameters.

Fundamental quantities	
Mass	4.65×10^{-23} g/atom in silicon
Length α	5.431 Å
Energy ε	1.792×10^{-19} J
Time t	1.77×10^{-3} ps/step
Normalized quantities	
Light speed (photon's speed) $c*$	4.8×10^6
Temperature $T*$	0.0231
Mass $m*$	0.54

energy of photons. To avoid the effects of different lengths in the x- and y-directions, the substrate of solar cells is set as a square. Periodic boundary conditions are imposed in the x- and y-directions. Due to the periodic texturing shapes, different period lengths lead to different numbers of atoms. In the case of different intervals of square texturization, at least six periods are chosen. So in the case of distance $d = 1$ cell, the number of silicon atoms is 144352. The longer the distance, the more atoms are present in the substrate. The photon incident angle varies at x-z plane. The system temperature keeps at 300 K. Table 1 shows the physical parameters of this model.

3. RESULTS AND DISCUSSION

Figure 3 shows the relationship between the height of square texturing and absorptance for the square surface case. When $h = 0$, the surface of solar cells is smooth, and the absorptance is 0.247 at an incident angle of 0 degrees. When surface texturing exists, the specimen with a greater square height has higher absorptance. However, the rate of increase becomes smaller as the height increases. Photons can easily drop into the holes with higher walls, so the substrate absorbs more photons. If the incident angle of photons increases, the absorptance lessens because more photons rebound.

Figure 4 shows how the various distances affect the absorptance. As the distance increases, the absorptance obviously decreases when the square height is 2.31 Å. As in Figure 3, the absorptance decreases as the incident angle of the photons increases. The absorptance decreases slowly when the distance surpasses 6.94 Å. In other words, the effect decreases as the distance increases.

The next example simulates a pyramidal surface. Figure 5 shows the influence of the facet tilt angle α. In this figure, the absorptance increases as the tilt angle α increases. Moreover, the rate rises quickly when α is more than 30 degrees. This result indicates that a more acute pyramid structure causes a decrease in reflection. Hylton et al. [5] discussed the possible path of light incident upon geometrically textured surface in air and concluded that a blunter facet tilted angle (sharp pyramid) facilitates light double-bounce incidence, thereby reducing surface reflection. Our results agree with that conclusion. However, the current results are totally contrary to the research by Xi et al. [4]. This is because the present study assumes the pyramid to be isosceles; thus, the
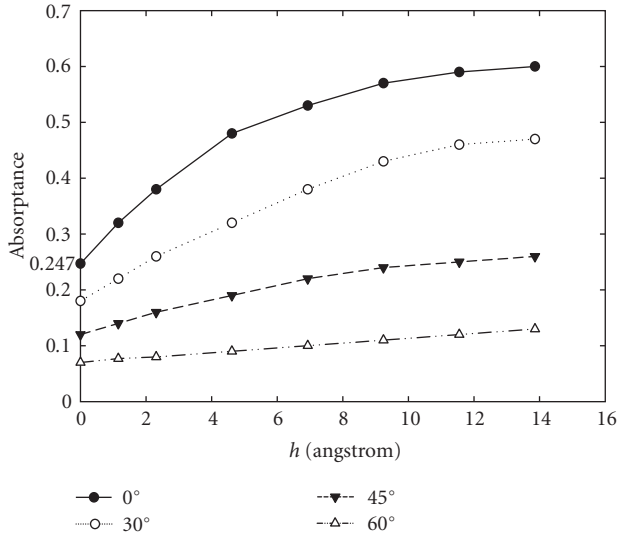
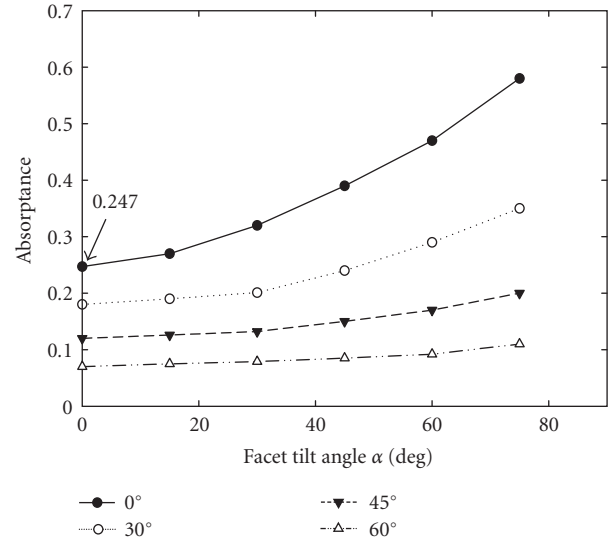Figure 3: The relation among absorptance, h and photon's incidence angle θ.

Figure 5: The relation among absorptance, facet tilted angle α, and photon's incidence angle θ.
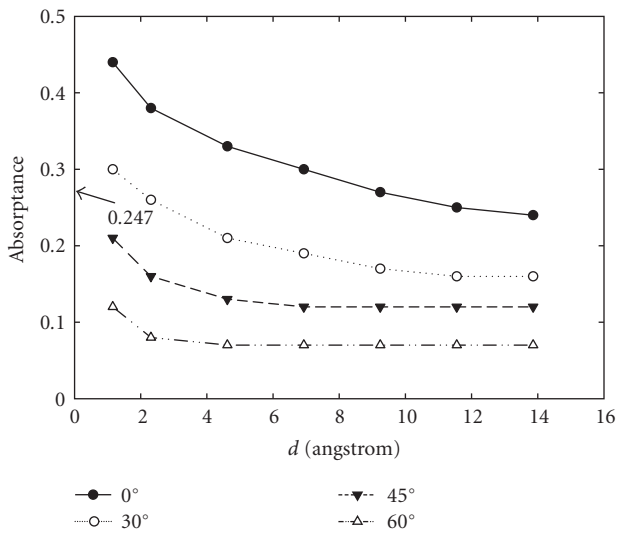

Figure 4: The relation among absorptance, distance and photon's incidence angle θ.
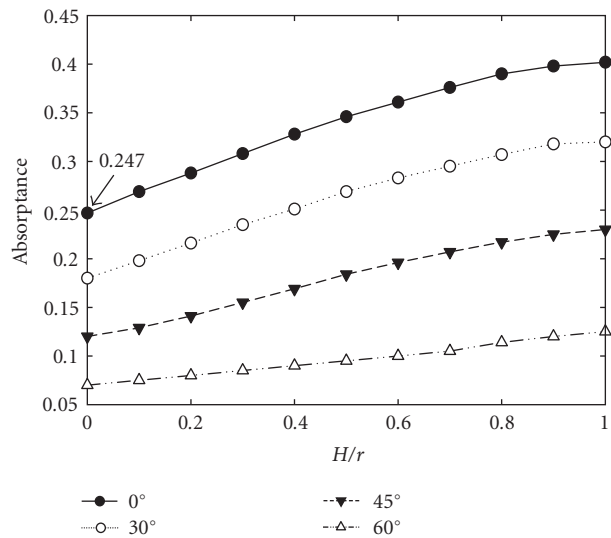

Figure 6: The dependence of absorptance on H/r in the case of semicircular texturing surface.

pyramids become sharper and taller with increasing α. This supposition leads to this phenomenon. As expected, a larger incident angle causes lower absorptance. Figure 5 shows this result.

Finally, Figure 6 shows the case of a semicircular surface. Varying the ratio of H/r, the absorptance shows a clear rising trend from 0.247 at $H/r = 0$, at which the surface of substrate is smooth, to a semicircular hole, $H/r = 1$, if vertical light meets the substrate. Obviously, the increasing rate of absorptance decreases if H/r rises. The same trend occurs at 30, 45, and 60 degrees of the incident angle, but the magnitude of absorptance is lower than that exposed by vertical light. This trend of absorption agrees well with the findings of Xi et al. [4].

4. CONCLUSION

In conclusion, this study proposes a new and simple MD model alternative to complex electron-photon interactions in quantum scale to analyze surface texturization of solar cells. Three surface texturization shapes are simulated with various angles of incident light. This methodology can easily determine the absorptance differences of various surface texturizations, and suggest better texturization shapes. Increasing the trench depth, shortening the distance between two trenches, sharpening pyramids, and adding more circling to the semicircular structure all help improve the efficiency of solar cells.

In this study, we ignore the wave behavior of photons and atoms. In fact, according to the wave-particle duality, the wave behaviors affect, either more or less, the absorption and reflection of solar cells. However, this study is a beginning to simulate the absorption by molecular dynamics. Our results also agree well with previous studies. This MD model can potentially be used to predict the efficiency promotion in any optical reflection-absorption cases.

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