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Fabrication of sub-wavelength antireflective structures in solar cells by utilizing modified illumination and defocus techniques in optical lithography

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Abstract

We demonstrate a simple method, which is combining modified illumination and defocus techniques to fabricate sub-wavelength antireflective structures for solar cells. The optimum pyramid resist and silicon profiles can be obtained after exposure, development and common dry etching processes. The reflection and transmission properties are analyzed by the rigorous coupled-wave analysis in two-dimensional microstructure and find the reflectance is dramatically increased as consideration of all diffraction orders. Therefore, patterning the sub-wavelength texturing structures for eliminating the diffraction order light is important. Patterning sub-wavelength structures should use the short wavelength combining defocus exposure or using a suitable modified illumination exposure system. The optimized pyramid structures are simulated in dosage-focus matrix with different types of light source. Results show the quadrupole modified illumination system with large process latitude is suitable for patterning sub-wavelength pyramid structures.

Keywords: Antireflection structures; Modified illumination; Pyramid structures; Optical lithography; Solar cells

1. Introduction

Silicon-based solar cells are developed for a long time and will be a vital candidate in the future for the mature fabrication techniques and relative low-cost. Recently, other semiconductor materials based solar cells such as gallium arsenide, indium phosphide, and germanium are intensely investigated for their high quantum efficiency and can be easily constructed intermediate band structures [1–3]. All of these semiconductor materials have high refractive index in visible and near infrared ray (NIR) regimes that will cause the high Fresnel's reflection between the air/semiconductor interface [4,5]. Therefore, the key issue for increasing the external quantum efficiency (EQE) of semiconductor based solar cells is how to reduce the interface reflection of the solar cell working-wavelength regime.

Many researches have been reported for the reduction reflectance of silicon-based solar cell. Conventionally, the wet etching method is used to fabricate the V-groove antireflective structures on a single-crystal silicon surface by an alkaline solution such as KOH or tetra-methyl ammonium hydroxide (TMAH). By using the different etching rate between the $\langle 100\rangle$ and $\langle 111\rangle$ surfaces of silicon crystals, the V-groove profile and surface roughness can be controlled by varying the concentration of alkaline solutions [6]. In respect of multicrystalline substrates, this method is less practicable for texturing due to the various crystallographic grain orientations [7]. Reactive ion etching (RIE) based on chlorine or SF_6/O_2 was found to be an alternative method for the formation of texturing structures on multicrystalline and single-crystalline silicon substrates [8,9]. However, the surface profile of a solar cell is strongly dependent on the RIE process conditions. Imprint lithography had been used to fabricate sub-wavelength antireflective structures [10]. However, the complicated tri-layer

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resist processes would decrease throughput and reliability of the process.

Previous researches indicated that the optimum antireflection structure of solar cells was pyramid [11]. However, pure wet or dry etching processes generally resulted in a random fashion without close packed structures. In this paper, we demonstrate a simple method, which is combining modified illumination and defocus techniques in optical lithography to fabricate sub-wavelength antireflective structures for solar cells. The optimum pyramid resist and silicon profiles can be obtained after exposure, development and common dry etching processes. The reflection and transmission properties are analyzed by the rigorous coupled-wave analysis (RCWA) in two-dimensional microstructure [12–14]. Patterning the sub-wavelength texturing structures for eliminating the diffraction order light is generally desired. The sub-wavelength structures can be patterned by using a short wavelength combining defocus exposure or a suitable modified illumination exposure system. The optimized pyramid structures are simulated in dosage-focus matrix with different types of light source. By contrast with previous works, reflectance of texturing structures are affected by optical lithography processes rather than etching processes. Therefore, high performance of texturing structures in solar cells with large area and high reproducibility can be obtained by conventional optical lithography.

2. Simulation and experiment setup

In this paper, we used the rigorous couple-wave analysis to simulate the reflection and transmission properties in two-dimension microstructure. The rigorous couple-wave analysis is widely used to analyze the optical diffraction of periodic structures as shown in Fig. 1a. Maxwell's equations in a periodic medium are solved with applying the field and permittivity. As shown in Fig. 1b, the pyramid structure with period Λ and height h is divided some parts in the vertical direction with gradient size for the RCWA simulation. In order to fabricate the pyramid structure, we use the commercial optical lithography simulator (PROLITH™) to simulate the aerial images and cross-section profiles of resist under different optical source, exposure dosages, defocusing distances, and modified illumination types. Experimental parameters can be established by referring with simulation results. The optimal resist profile can be adjusted by controlling the defocus, exposure dosages, and modified illumination type of a commercial exposure system (I-line stepper, Canon, FPA-3000 i5+). In the experimental procedures, silicon wafers were coated with resist by a spin coater and development system (TEL Track, MK-8). After the optical lithography processes, the resist patterns were transferred to the substrate by the reactive ion etcher (Anelva, ECR-6001) with

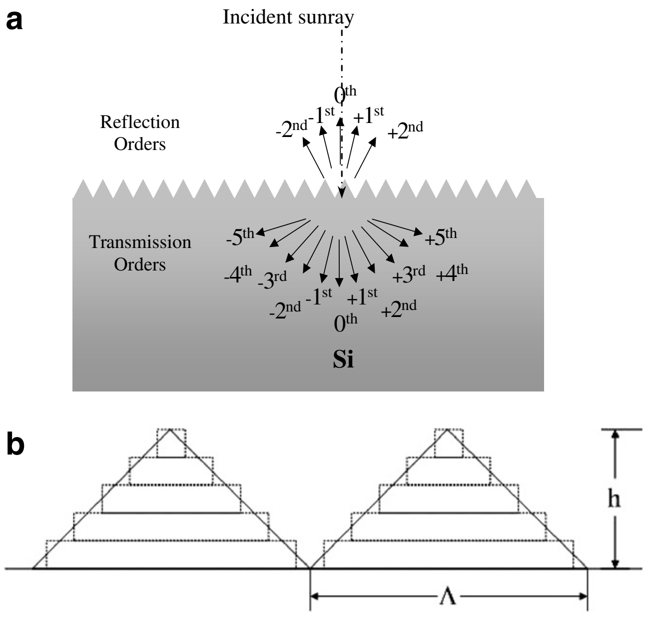

Fig. 1. Schematic diagram of: (a) reflection and transmission diffraction orders for incident sunray with pyramid structure and (b) pyramid structure for rigorous couple-wave simulation.

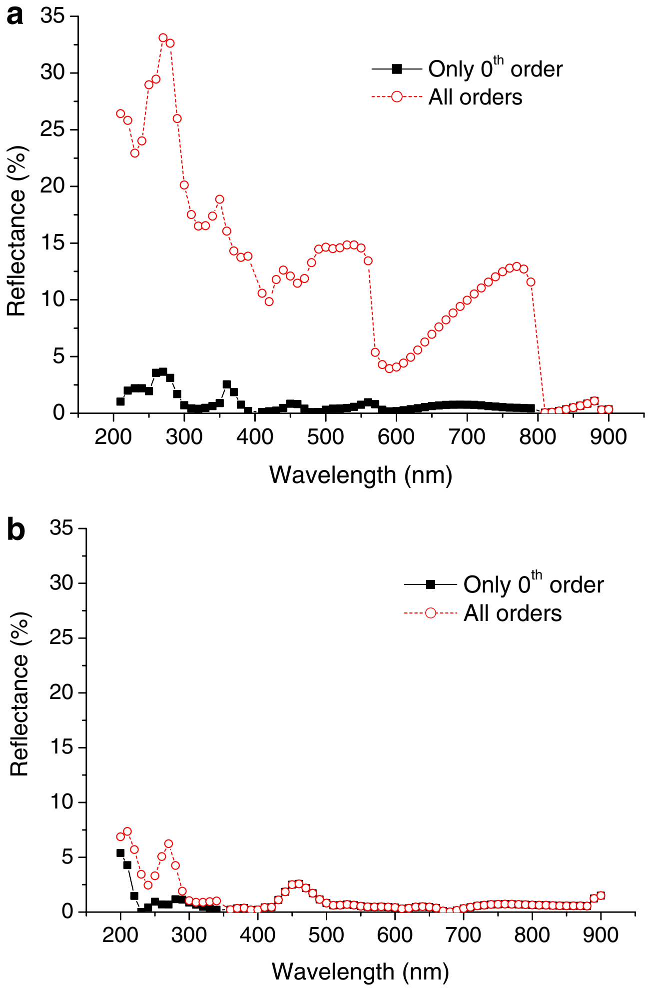

Fig. 2. Simulation reflectance spectra of pyramid silicon structures with period of: (a) 800 nm and (b) 350 nm obtained by rigorous couple-wave simulation.

reactive gases Cl_2, SF_6, and O_2. Finally, the cross-section profile was observed by the scanning electron microscopy (JEOL, JSM-6500F), and the optical properties were measured by optical spectrometer (Hitachi, U-4100).

3. Results and discussion

Fig. 2 shows the reflection spectra of pyramid structures consider with and without all diffraction orders for 800 nm and 350 nm periods. As shown in Fig. 2a, the reflectance is less than 3% from 200 to 900 nm for the consideration of only 0th-order reflection. As consideration of all diffraction orders, the reflectance is dramatically increased as the wavelength less than 800 nm for the pyramid structure with period of 800 nm and height of 450 nm. Similarly, Fig. 2b shows the reflectance is less than 3% from 350 to 900 nm as consideration of all diffraction orders for the pyramid structure with period of 350 nm. Results indicate that the reflectance is dramatically increased as the consideration of all diffraction orders. Therefore, patterning the subwavelength texturing structures for eliminating the diffraction order light is desired for solar cell applications. For the consideration of working wavelength region of silicon-based solar cells, the pyramid structure with period of 350 nm is suitable as the antireflective structure.

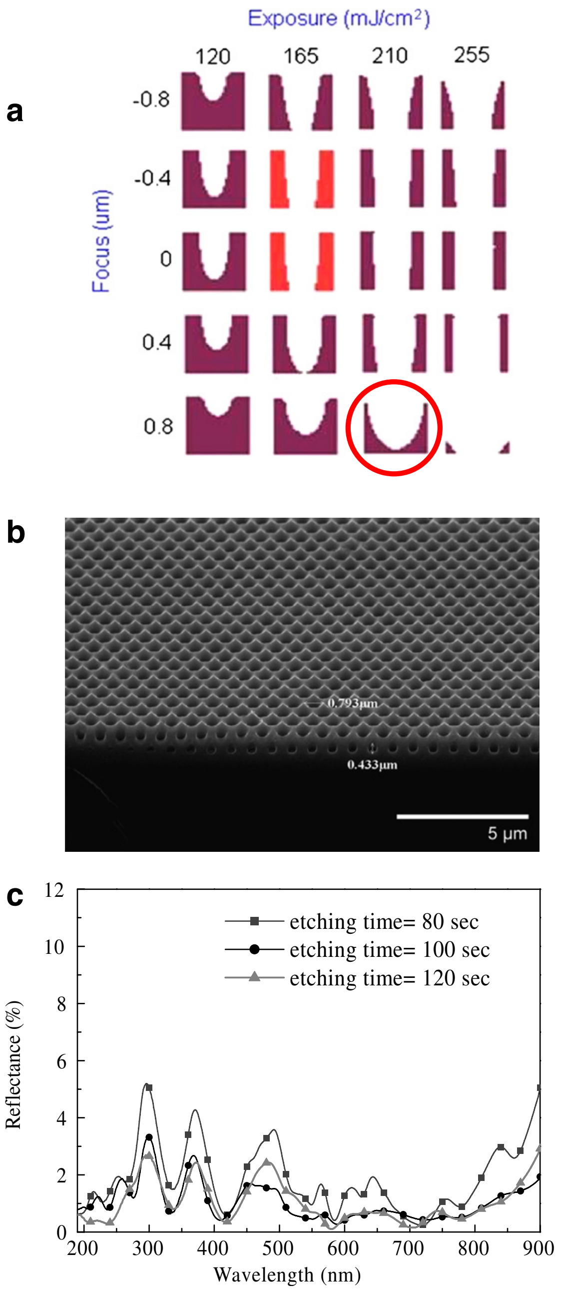

Fig. 3. (a) Resist profiles dependence of focus-dosage matrix, (b) the cross-section morphology with a large area of closed-packed pyramid structures in a silicon substrate and (c) reflectance spectra were obtained by varying the etching time in the RIE process.

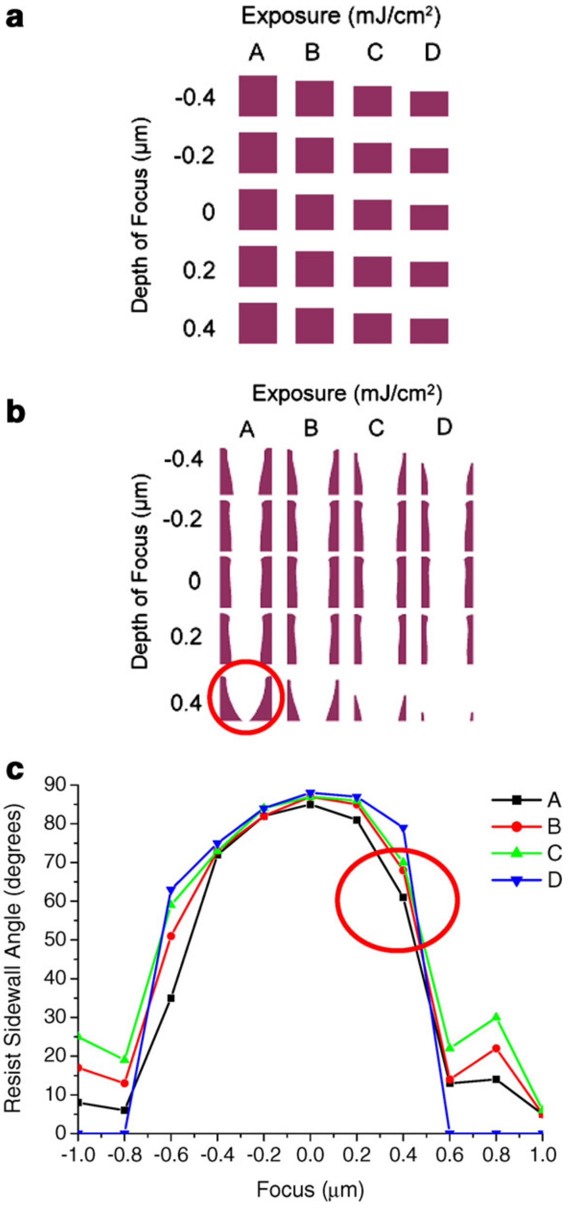

Fig. 4. Resist profiles with the 350 nm period dependence of focus-dosage matrix by: (a) I-line, (b) ArF laser and (c) resist side-wall angles depend on different defocus distance by an ArF exposure tool.

Fig. 3a shows the resist profile of a positive resist with thickness and period of 800 nm exposed by 365 nm (I-line, NA-0.65) on different defocus position with different exposure dosage. The optimized pyramid structures in resists that are simulated in dosage-focus matrix by the optical lithography simulator. The zero-defocus means the maximum intensity region is located on the surface of the resist. For zero-defocus in the resist, a vertical resist profile can be obtained by the exposure with suitable dosage. The +0.8 μm defocus means the maximum intensity is above the resist surface with 0.8 μm. The maximum intensity region is away from the surface of resist and the relative intensity decreased from the surface to the bottom of resists. Therefore, a gradient resist profile can be obtained with positive defocus-exposure. Suitable exposure dosage is also important for the fabrication of gradient resist profiles. According to the simulation results shown in Fig. 3a, we can obtained the optimized pyramid structures in resists by adjusting the exposure dosage and defocusing distance. These are the referable parameters to fabricate the pyramid structures in the resist.

Fig. 3b shows the SEM image of the pyramid structures were transferred to silicon substrates by the RIE processes with reactive gases Cl_2, SF_6, and O_2. We find the pyramid shape can be remained with the same 0.8 μm period after the dry etching process. Fig. 3b shows the cross-section morphology with a large area of closed-packed pyramid structures in the silicon substrate can be easily obtained. In this study, the texturing structures on silicon substrates are characterized by measuring the reflection spectra from deep ultraviolet (DUV) to near infrared ray regimes. Fig. 3c shows the reflection spectra of the texturing structures fabricated with different etching time but fixed defocusing distance (+0.8 μm) and exposure dosage. Results indicate that the reflectances are less than 5% for different etching time. We find the defocusing distance in an optical exposure tool is the key factor for the fabrication of optimal pyramid structures. If the resist is exposed at the suitable focusing position, we can get reasonable processing tolerance for the fabrication of pyramid structures by this defocusing method.

Furthermore, patterning the sub-wavelength texturing structures for eliminating the diffraction order light is desired. For the consideration of working wavelength region of silicon-based solar cells, the pyramid structure with period of 350 nm is suitable as the antireflective structure. Patterning sub-wavelength structures should use the shorter wavelength or resolution enhancement techniques (RET) such as modified illumination in an exposure system. Fig. 4a shows the structure with period of 350 nm

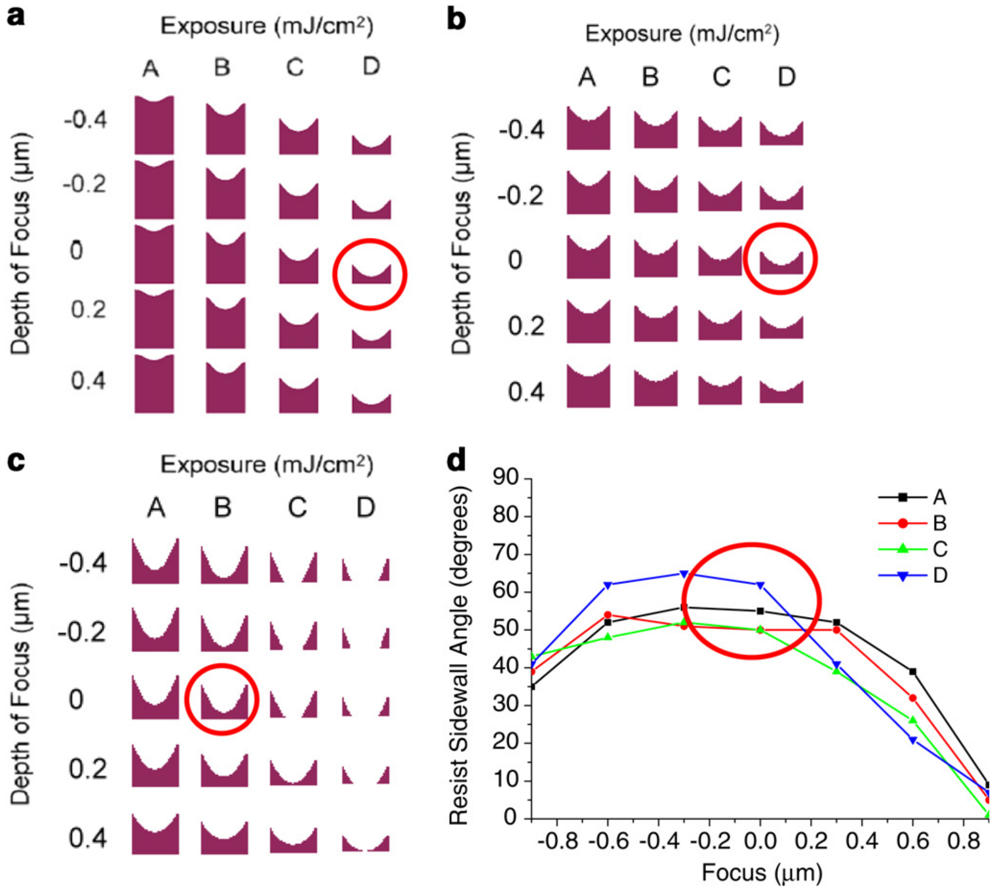

Fig. 5. Resist profiles with the 350 nm period exposed by: (a) I-line with high sigma value, (b) I-line with annular illumination system, (c) I-line with quadrupole modified illumination system and (d) resist side-wall angles depend on different defocus distance in (c).

simulated in dosage-focus matrix by I-line (365 nm) light source with common conditions (NA = 0.65, sigma = 0.6). Result indicates that the structure can not resolve by I-line with common conditions. Fig. 4b shows the pyramid structure with period of 350 nm exposed by 193 nm light source (ArF, NA = 0.65, sigma = 0.6). Result shows the pyramid structure with period of 350 nm can be easily obtained by +0.4 μm defocus exposure with suitable exposure dosage. As shown in Fig. 4c, the defocus distance for patterning pyramid structures can also be determined by resist side-wall angle. In general, the 50°–60° of side-wall angle is suitable to form a pyramid structure.

We would like to use a cheaper I-line exposure tool with modified illuminations to form pyramid structures with period of 350 nm. In general, the I-line resist is thicker and better etching resistance than the ArF resist. Therefore, the patterned I-line resist can be as a template to form a deep pyramid structure on an underlying silicon substrate. Fig. 5a shows the simulated dosage-focus matrix by using an I-line light source with high sigma value (sigma = 0.95, NA = 0.65) for patterning the 350 nm period structure. Result shows that only a few shallow pyramid structures with the period of 350 nm can be obtained. Similarly, Fig. 5b shows some shallow pyramid structures obtained by the I-line light source with annular illumination. Fig. 5c shows the simulated dosage-focus matrix by using an I-line with quadrupole illumination for patterning the pyramid structure. Results show the quadrupole illumination system with large process latitude can form deep sub-wavelength pyramid structures. By optimizing locations of the four source points for periodic structures in two-dimensions, quadrupole illumination is well suited for printing two-dimensional dense patterns [15]. Fig. 5d shows that resist side-wall angles depend on different defocus distance. For small depth of focus (DOF) in this exposure setup, no defocus exposure is required for patterning the sub-wavelength pyramid structure.

4. Conclusion

In this paper, we demonstrate a simple method, which is combining modified illumination and defocus techniques in optical lithography to fabricate sub-wavelength antireflective structures for solar cells. The optimum pyramid resist and silicon profiles can be obtained after exposure, development and common dry etching processes. The reflection and transmission properties are analyzed by the rigorous coupled-wave analysis in two-dimensional microstructure and find the reflectance is dramatically increased as consideration of all diffraction orders. Therefore, patterning the sub-wavelength texturing structures for eliminating the diffraction order light is important. Patterning sub-wavelength structures should use the short wavelength combining defocus exposure or using a suitable modified illumination exposure system. Results show the quadrupole illumination system with large process latitude is suitable for patterning sub-wavelength pyramid structures. This method is also suitable for the fabrication of antireflective structures on various kinds of solar cell materials.

Acknowledgement

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