Silicon Thin Film with Si Nanopillar Surface Decoration for Solar Cell Application

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1. Introduction

Silicon nanowires (SiNW) or silicon nanopillars (SiNP) recently receive considerable attention for photovoltaic application due to their strong light trapping capability [1, 2]. It has been experimentally demonstrated that the nano-structured solar cell has higher spectrum absorption than the thin film [1]. In this paper, the optical properties of Si film with SiNP decorated surface are systematically studied via simulation, and the optimal structure in term of SiNP periodicity (P), diameter (D), and height (H) is proposed for solar energy absorption.

2. Results and Discussion

Fig. 1 shows the schematics of the periodic SiNP array under study. The thickness of the underlying Si thin film is set as 800nm. Light is assumed to be normally incident on the sample. The energy range of the incident light varies from 1 to 4eV, corresponding to the wavelength from ~1240nm to ~310nm. The optical properties of the structure are simulated by using Finite Element Method (FEM), from which the field strength profile and the carrier generation profile can be obtained for subsequent electrical simulation.

Our simulation result using the FEM is firstly verified against the data reported by Hu and Chen [3], which was obtained by the transfer matrix method (TMM). As shown in Fig. 2(a) and 2(b), the optical absorption data simulated by FEM and TMM are well matched. The light absorption in the low energy region ($< \sim$ 2eV) is close to zero in this case, as the SiNP array is assumed to sit on the non-absorption structure [3]. In Fig.2(c), our simulated data also shows reasonable agreement with the experimental result presented by Sivakov [4]. The slight variation may be due to the setting of SiNP L/D between the simulation and experiment is different.

Next SiNP array with various D/P ratio (with constant P) on Si thin film (as described in Fig. 1) is studied. Fig. 3(a)-(c) depict the absorption, reflection and transmission spectra of three SiNP structures with different diameters (100, 250 and 300 nm) at constant H (1µm) and P (400 nm). Fig. 3(a) shows that the SiNPs impart an increase in the absorption compared to the single thin film over whole solar spectrum, especially a significant improvement is seen at high energy region (> ~2.2eV), confirming the strong light trapping capability of SiNP. As D/P ratio increases, SiNP array acts more as a solid thin film due to the increase in the pillar top face area, resulting in higher reflectance as seen in Fig. 3(b). The transmission increases with decreasing D/P ratio, especially in long wavelength region, as in Fig. 3(c). This is understood as when the D is smaller than the wavelength of the incident light, the light is likely to get diffracted (reaching the Si thin film) while traversing the array, resulting in higher transmission. The

ultimate efficiency (η) at the Air Mass 1.5 direct normaland circumsolar spectrum is calculated using the formula listed in Table I to express the light absorption capability. As in Fig. 4, it is clear that the D/P value is optimized at ~ 0.5-0.6, which is consistent with data reported in [1].

The H effect of SiNP on optical properties is evaluated Fig. 5 shows the absorption spectra of SiNP with H of 200, 1000, or 2000 nm and a fixed D =150nm and P =300nm (D/P = 0.5). The absorption increases significantly when the H is increased from 200 nm to 1000 nm, but tends to be saturated after 1000nm. The impact on ultimate efficiency is insignificant for H>1µm, as in Fig. 6. If considering the materials volume / process controllability for final solar cell device fabrication, it is proposed that H of 1 µm seems to be sufficient being efficient for solar energy absorption.

Finally, we study the absorption spectra of the SiNP structures with different P (100, 500 and 600 nm) at constant D/P ratio (0.5) and H of 1 µm (Fig. 7). For small P (i.e. 100nm), in low energy region, as the wavelength of the incident light is much longer than P of SiNP array, the light is likely to pass through the SiNP, reaching the underlying silicon layer and getting absorbed. Hence the SiNP with P of 100 nm act more like the thin film sample, and the two have similar absorption/reflection/transmision in low energy region [Fig.7(a-c)). For the same small P in high energy region, as the wavelength of the incident light is comparable/smaller to the P, the light scattering between SiNPs is significantly enhanced. The effective path length for light rays confined within the arrays is prolongated, leading to low reflection and hence high absorption [Fig.7(b)). This explains also that the absorption edge of the SiNP array shift to longer wavelength region as P is increased (Fig.7a). When P becomes larger (i.e. P =600nm in this work), the reflection spectra is higher, as the light is not only scattered between SiNPs but also the underlying silicon layer. As in Fig. 7(d), P value is optimized at \sim 500 nm, where the ultimate efficiency reaching a maximum ~27%. Further increase in P beyond 600 nm will decrease the light trapping ability due to the increased light reflection in energy region above ~ 2.5 eV, which stands for the high energy density region in the solar spectrum.

3. Conclusion

The optical characteristics for SiNP textured thin film structure are studied, and the D, P, and L for effective solar energy harvesting is optimized, which can serve as a guideline for photovoltaic device design/fabrication.

References [1]. L. Tsakalakos, et al., J. Nanophoton. 1, 013552 (2007); [2]. N. S. Lewis, et al., J. Appl. Phys. 97, 114302 (2005); [3]. L. Hu and G. Chen, Nano Lett. 7 (11), 3249 (2007). [4]. V.Sivakov, et al., Nano Lett. 9 (4), 1549 (2009).



Fig. 1. Schematic of (a) the cross-sectional view (b) top-view of the simulated SiNP structure



Ultimate efficiency $\eta = \frac{\int_{E_g}^{\infty} \frac{E_g \times I(E) \times \alpha(E)}{E} dE}{\int_{0}^{\infty} I(E) dE}$	
Eg	Material bandgap
I(E)	Solar energy density spectrum
$\alpha(E)$	Absorption spectrum
Ε	Photon energy



Fig. 2. The absorption spectra (a) by FEM calculation (b) by TMM from Hu and Chen [3]. (c) by FEM calculation, with experimental data from V.Sivakov[4].



Fig. 3 (a) The absorption (b) reflectance (c) transmission spectra as a function of SiNP diameter (P=400nm).



Fig. 7 (a) The absorption (b) reflection (c) transmission (d) ultimate efficiency as a function of SiNP periodicity.