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種別(和文)	論文要旨
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（博士課程）
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論 文 要 旨

THESIS SUMMARY

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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

In this thesis, the electrochemical passivation of porous silicon (PSi) for tandem solar cells is investigated with both experiment and simulation approaches.

Chapter 1 introduced the concept of all-silicon tandem solar cell, which has the potential to surpass the theoretical efficiency limit of a single-junction silicon solar cell. The structure also eliminates the lattice mismatch issue found in hetero-junction structures. The porous silicon (PSi) is selected as a candidate for a top cell of the tandem due to its adjustable band gap, which is reported to be in a range of 1.2 - 2.2 eV depending on its porous structure, and possibly originated from the quantum confinement effect. It can also enhance the light absorption due to its anti-reflective property. With these benefits, it provides the opportunity to use the PSi to improve the open circuit V_{OC}, short circuit current J_{SC}, as well as the efficiency η of the solar cell. However, as the surface area and defects greatly increase compared to crystalline silicon (c-Si) as a result of fabrication process, the surface recombination rate also increases. Therefore, a suitable passivation method for the nano-structured Si is necessary to minimize the surface recombination.

Chapter 2 described the statement of purpose of the thesis. The low-cost electrochemical passivation technique is proposed to achieve a uniform passivated layer on nanostructured surface like PSi. The PSi fabrication and the passivation process are varied in order to find the optimal fabrication condition that yields the best solar cell performance, which are compared with the conventional atomic layer deposition (ALD) method. Finally, in order to confirm the true electronic structure of PSi/c-Si system, various PSi models are created and calculated.

Chapter 3 explained the experimental PSi fabrication and the passivation conditions as well as the characterization details. The detail for the simulation part is also described, including the basis of calculation, the models creation, the analysis of the band structure.

Chapter 4 is divided into the experimental and the simulation part.

For the experimental part, the structure of PSi was fabricated to have a p-n junction depth at 200 - 250 nm where the PSi was introduced in the n layer of the p-n junction (Type III structure) with porosity of 25%. After passivation with the three methods, the carrier lifetime measurements results showed that the performance of each method was similar; all of the lifetimes are short (in a few microseconds range) compared to common Si solar cell (in millisecond range). However, while ALD and supercritical fluid methods passivated both sides of the PSi wafer, the

electrochemical method only applied to the front surface. Finally, the solar cell performance of electrochemical passivated and ALD-passivated samples was measured. With ALD passivation, all the solar cell parameters were poor, as well as its diode characteristics due to the formation of a resistive layer on the top surface. The reaction time of electrochemical passivation was varied to find the optimal passivation condition. The passivated PSi improved the quantum efficiency (QE) especially at the shorter wavelength, while the unpassivated PSi sample showed poor QE due to significant recombination. The solar cell efficiency result showed that the optimized passivation time is 30 seconds, at which the recombination is minimized, while the passivated oxide layer is not too thick and becomes more resistive. When compared to the c-Si solar cell and an unpassivated sample, it showed the improvement of J_{SC} and η of electrochemical passivated PSi solar cell, while all V_{OC} values are in the range of 0.51-0.54 V, i.e., not improved. Therefore, in order to verify the possibility to improve V_{OC} by using PSi, the simulation is used to clarify the electronic structure of the PSi/c-Si models.

In the simulation part, the band structures induced by porosity and passivation of Si were computed by the Density Functional Tight Binding (DFTB) method and compared. Four representative models of PSi were created: pillar, crater, internal sphere, and internal cube models. The results showed that the only component that determines the degree of expansion is not the pore, but the size of Si framework itself. The pillar diameter, the crater Si wall thickness, and the thickest Si skeleton part were varied including sizes which induce quantum confinement. The pillar height and crater depth have little to no effect on the band gap as long as the Si base is thicker than 1 nm. Moreover, only when two pillars are physically in contact and become crater model that the decrease of band gap is observed; the value converges to one of bulk Si (1.12 eV) as the pillars are more in contact to their neighboring pillars. On the other hand, when the crater diameters are large enough that the Si wall part is isolated, the band gap largely increases. Quantum confinement induced gap expansion was only observed when Si features approached 1 nm scale. To connect to the experiment to the simulation part, with the PSi wall thickness of more than 3.5 nm observed from TEM, the simulation result showed that the band gap expansion effect for this Si feature size is minimal (1.2-1.4 eV). Thus, the PSi framework must be fabricated with smaller sizes to utilize more quantum confinement effect.

In conclusion in chapter 5, this thesis investigated the possibility to use PSi as a top cell of the all-silicon tandem solar cell by both experiment and simulation approaches. With our original electrochemical passivation, the formation of the uniform and high coverage oxide layer could be achieved on PSi layer, resulting in the improvement of solar cell performance. The simulation on the electronic structure of PSi/c-Si models also provided an insight on the more suitable PSi structure that can further improve the performance of solar cell in the future fabrication.