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Device modeling of HTL/$BaSi_2$ heterojunction solar cells

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***Abstract* — We simulated the optical absorptance of $BaSi_2$-based heterojunction solar cells with transition metal oxides as hole transport layer (HTL) using GENPRO4 software and optimized the device structures. The complex refractive index of each layer was used as an input in the optical simulations. We adopted ITO (80 nm) / HTL / a-Si (3 nm) / n-$BaSi_2$ (500 nm) / TiN (250 nm) / glass substrates (200 μm) structures. First, the implied photocurrent density (J_{ph}) loss caused by parasitic absorption in 20-nm-thick p^+-$BaSi_2$ layer was calculated to be 7.9 mA cm^{-2}. The J_{ph} increased to 29.1 mA cm^{-2} by substituting p^+-$BaSi_2$ with 2-nm-thick MoO_3. To figure out the optimal HTL materials and the structures for $BaSi_2$ solar cells, we simulated the absorption spectra as function of materials such as NiO, Cu_2O, MoO_3, V_2O_5, and WO_3, which have already demonstrated the HTL functionality, and their thicknesses. The highest J_{ph} was obtained with MoO_3, V_2O_5, or WO_3, meaning that these oxides are optically suitable HTL materials. By increasing the n-$BaSi_2$ absorber layer thickness to 2 μm and importing 3D random pyramidal texture structure with the height of 4 μm, the J_{ph} reached a maximum of 33.1 mA cm^{-2}. This is the largest value of all $BaSi_2$ solar cells ever reported.**

I. INTRODUCTION

Safe, stable, and earth-abundant materials are of great importance to realize a decarbonized society fueled by photovoltaic (PV) technology. Under such circumstances, we have paid special attention to $BaSi_2$, a semiconducting silicide composed only of earth-abundant elements.[1] $BaSi_2$ has a suitable band gap for single-junction solar cell application (1.3 eV). In addition, both a high absorption coefficient of 3×10^4 cm^{-1} at 1.5 eV and a prominent minority carrier diffusion length of 10 μm are realized. Solar cell materials possessing such properties are quite limited. According to the theoretical calculation, the conversion efficiency (η) of $BaSi_2$ homojunction solar cells exceeds 25%.[2] Moreover, the operation of $BaSi_2$ homo-junction solar cells was recently demonstrated[3] after the achievement of η = 9.9% for p-$BaSi_2$/n-Si solar cells architecture.[4] However, the η of $BaSi_2$ homojunction solar cells has been limited to 0.28% due to the parasitic absorption in $BaSi_2$ carrier collection layer containing a lot of defects.[5] The absorption coefficient of $BaSi_2$ is so high that such absorption loss is inevitable as long as $BaSi_2$ is employed as the surface layer. Therefore, it is crucial to explore the substitutional materials for the carrier collecting layer to fulfill high-η $BaSi_2$ solar cells. Since undoped $BaSi_2$ films usually shows n-type conductivity, we focused on hole transport layers (HTLs) to form $BaSi_2$ heterojunction solar cells and suppress the parasitic absorption. Several kinds of HTL materials such as MoO_3 have been studied so far and the η over 23% have been achieved in crystalline silicon PV technology.[6] However, there has been limited reports on HTL/$BaSi_2$ solar cells. In this study, we thereby aim to model HTL/$BaSi_2$ heterojunction solar cells using several kinds of HTL materials from the theoretical viewpoint.

II. SIMULATION METHOD

In this work, we carried out the optical simulations using GENPRO4 developed at the Delft University of Technology.[7] The complex refractive index ($n + ik$) of each layer was used as an input. It is noted that the extinction coefficient k of $BaSi_2$ layer was fixed to zero at wavelength above 950 nm, corresponding to the fact that no photoresponsivity is obtained experimentally beyond such wavelength. The implied photocurrent density (J_{ph}) was calculated by integrating the simulated absorption spectra of n-$BaSi_2$ absorber layer over the AM1.5 spectrum range. We adopted an ITO (80 nm) / HTL / a-Si (3 nm) / n-$BaSi_2$ (500 nm) / TiN (250 nm) / Glass (200 μm) structure to simulate the optical properties of HTL/n-$BaSi_2$ heterojunction solar cells using several HTL materials and changing their thickness. We chose MoO_3, WO_3, V_2O_5, Cu_2O, and NiO as HTL materials, for which the HTL functionality has been demonstrated.[8] For comparison, an ITO (80 nm) / a-Si (3 nm) / p-$BaSi_2$ / n-$BaSi_2$ (500 nm) / TiN (250 nm) / Glass (200 μm) structure was also simulated. The a-Si capping layers were inserted at the top of the $BaSi_2$ layer to suppress the oxidation of $BaSi_2$ layer, which is experimentally implemented.[9] We adopted the TiN as a back contact layer.[10] According to the previous research, TiN layer blocked the diffusion of oxygen atoms from the glass substrate and suppressed the intermixing at the $BaSi_2$/TiN interface, leading to the growth of $BaSi_2$ films with high photoresponsivity on glass substrates. First, we simulated the solar cell device using flat surfaces; then, we introduced the typical 3D random pyramidal texture at the front surface of the glass substrates to clarify the effect of the anti-reflection and the light trapping by the 3D random pyramidal texture on the above structures. An atomic force microscopy image of a pyramid-type texture obtained by

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chemical-etching of a Si substrate was adopted for the simulations as shown in Fig. 1.

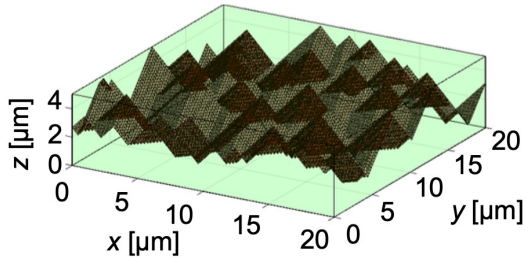

Fig. 1. 3D random pyramidal texture measured by atomic force microscopy.

III. Results and Discussion

It was experimentally revealed that at least 20 nm is necessary to form flat $BaSi_2$ films; otherwise, the $BaSi_2$ islands grow.[11] This island layer decreases the shunt resistance, resulting in the deterioration of solar cell performance. Therefore, we first calculate the parasitic absorption of 20-nm-thick p^+-$BaSi_2$ layer. Fig. 2 (a) shows the absorption spectra of pn-$BaSi_2$ solar cell on TiN/glass substrate. Owing to the high absorption coefficient of $BaSi_2$, the absorption in p^+-$BaSi_2$ with the thickness of 20 nm is markedly observed in the wavelength range of 300 – 900 nm. This parasitic absorption causes loss in the J_{ph} of 7.9 mA cm^{-2}, leading to the limitation of J_{ph} in n-$BaSi_2$ absorber layer to 20.3 mA cm^{-2}. We substituted the p^+-$BaSi_2$ with MoO_3 as an HTL layer to increase the absorption in n-$BaSi_2$ absorber layer. Only 1.7-nm-thick MoO_3 worked as an HTL layer and over 23% of η have been achieved for MoO_3/c-Si heterojunction solar cells.[6] The absorption in n-$BaSi_2$ distinctly increased and the J_{ph} reached 29.1 mA cm^{-2} (Fig. 2 (b)). The absorption of MoO_3 was negligible thanks to the large band gap of MoO_3. To figure out the suitable HTL materials for $BaSi_2$ in terms of the absorption, we simulated the absorption spectra of HTL/$BaSi_2$ solar cells with various kinds of HTL materials. Fig. 2 (c) reports the J_{ph} as a function of the HTL thickness. The highest J_{ph} of all structures was obtained when MoO_3, V_2O_5, and WO_3 were used as an HTL layer. The structure with Cu_2O showed the slightly small J_{ph} compared to the above three materials. NiO and p^+-$BaSi_2$ greatly decreased the J_{ph} in n-$BaSi_2$ absorber layer with increasing its thickness. Therefore, MoO_3, V_2O_5, and WO_3 are promising HLT materials for maximizing absorption in $BaSi_2$.

Fig. 3 shows the J_{ph} caused in the n-$BaSi_2$ absorber layer with pn-$BaSi_2$ and MoO_3/n-$BaSi_2$ structure as a function of n-$BaSi_2$ thickness $t_{n\text{-}BaSi2}$. The J_{ph} saturated when $t_{n\text{-}BaSi2}$ reached 2 μm for each structure. The maximum J_{ph} of 22.0 mA cm^{-2} was obtained for p^+-$BaSi_2$(20 nm)/n-$BaSi_2$ solar cells with flat

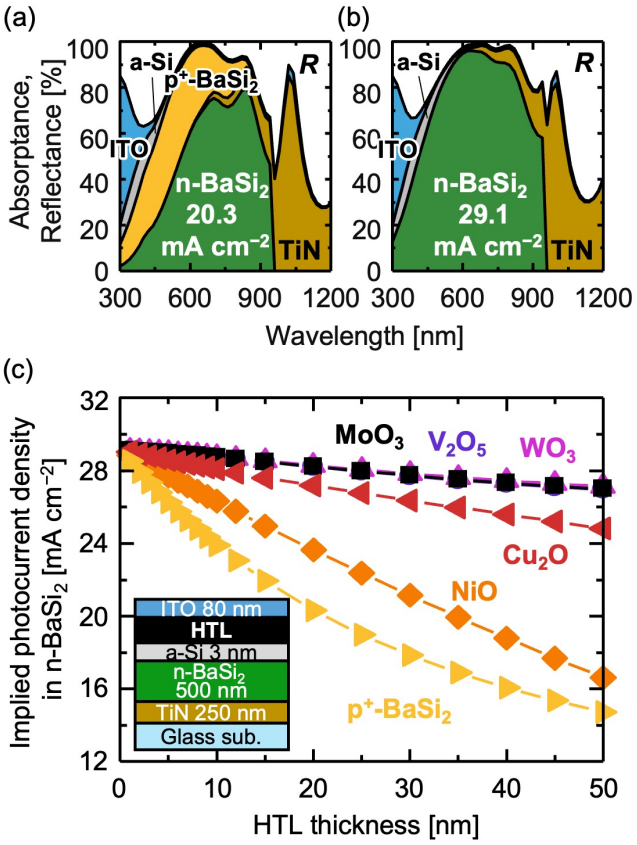

Fig. 2. Absorptance spectra of $BaSi_2$ solar cells with (a) 20-nm-thick p^+-$BaSi_2$ and (b) 2-nm-thick MoO_3. (c) HTL thickness dependence of J_{ph} in n-$BaSi_2$ absorber layer contacted with several kinds of HTL materials.

structure. The J_{ph} markedly increased by replacing p^+-$BaSi_2$ with 2-nm-thick MoO_3 and reached 31.1 mA cm^{-2}. Moreover, 3D random pyramidal texture further increased the J_{ph} up to 33.1 mA cm^{-2}. The absorptance spectra of MoO_3 (2 nm) / n-$BaSi_2$ (2 μm) solar cell on a textured glass substrate were depicted in Fig. 4. Compared to Fig. 2 (b), the absorption in the n-$BaSi_2$ absorber layer increased both in the short (<600 nm) and long (>700 nm) wavelength regions. Both light trapping effect thanks to the 3D random pyramidal texture and increment of the n-$BaSi_2$ thickness are contributed to this improvement. The J_{ph} of 33.1 mA cm^{-2} is slightly higher than that of Al-doped n^+-ZnO/p-$BaSi_2$ structures on textured glass substrates simulated in the previous study.

IV. Conclusion

We modeled the HTL/n-$BaSi_2$ solar cells using optical simulation GenPro4. The parasitic absorption of 20-nm-thick p^+-$BaSi_2$ layer caused the J_{ph} loss of 7.9 mA cm^{-2}. By replacing p^+-$BaSi_2$ with 2-nm-thick MoO_3, the J_{ph} increased up to 29.1 mA cm^{-2}. Among several kinds of HTL materials, MoO_3,

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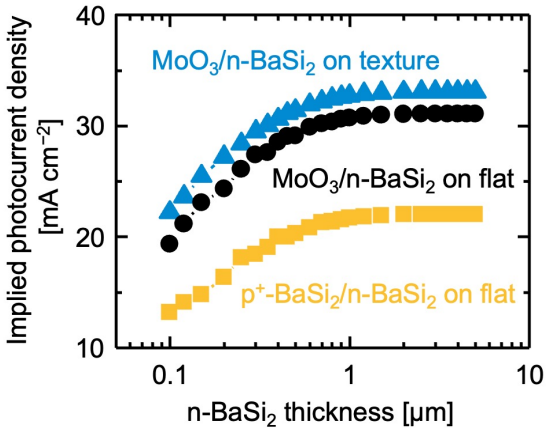

Fig. 3. n-$BaSi_2$ thickness dependence of the J_{ph} in n-$BaSi_2$ absorber layer contacted with 20-nm-thick p^+-$BaSi_2$ and 1-nm-thick MoO_3 on flat or 3D random pyramidal texture glass substates.

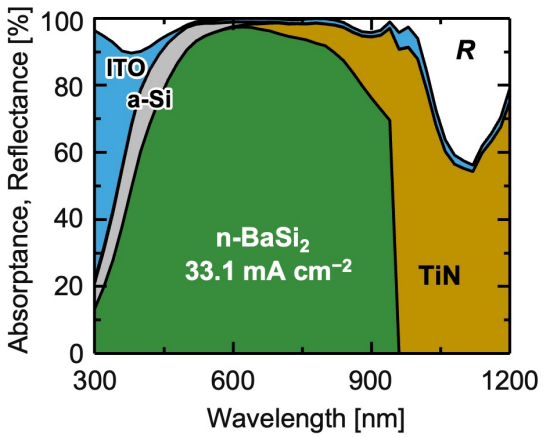

Fig. 4. Absorptance spectra of MoO_3(2 nm)/n-$BaSi_2$(2 μm) heterojunction solar cell on 3D random pyramidal texture structure.

V_2O_5, and WO_3 showed the lowest absorption, leading to the highest J_{ph}. Therefore, these oxides are promising HTL materials for $BaSi_2$ in terms of absorption. The J_{ph} increased with the thickness of n-$BaSi_2$ absorber layer and reached a maximum of 33.1 mA cm^{-2} by introducing 3D random pyramidal texture structure. This value is the highest of all $BaSi_2$ solar cells ever simulated.

Acknowledgements

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