Silicon quantum dots superlattice (Si-QDSL) solar cells are attracted as one of the novel concept solar cells [1]. Si-QDSL has the structure that the size-controlled silicon quantum dots (Si-QDs) are embedded in a wide bandgap material. Since the bandgap of the Si-QDSL can be tuned by controlling the size of Si-QDs [2], appropriate size control of Si-QDs would lead to realization of all silicon tandem solar cells. In our previous paper, the open-circuit voltage ($V_{oc}$) of 529 mV has been achieved in substrate-type Si-QDSL solar cells [3]. To improve the efficiency of the Si-QDSL solar cells, we considered that SiC mixed with Al$_2$O$_3$ would be promising for the barrier layer. Since Al$_2$O$_3$ is known as one of the excellent passivation materials for bulk Si, further improvement of $V_{oc}$ can be expected due to surface passivation of Si-QDs. The solar cell structure of ITO/p-type hydrogenated amorphous silicon (a-Si:H) or microcrystalline SiC ($\mu$-SiC:H)/Si-QDSL with a diameter of 5 nm/n-type a-Si:H/Al electrode was assumed as shown in Fig. 1. In order to investigate how the properties of the barrier layer affect the characteristics of the solar cell, quantum device simulation was carried out considering a virtual substance whose physical properties change with respect to the composition ratio of Al$_2$O$_3$ and SiC.

Figure 2 shows the effect of barrier height on the performance of Si-QDSL solar cells. Compared to SiC, Al$_2$O$_3$ has a low electron affinity and a large band gap. Therefore, higher Al$_2$O$_3$ composition ratio leads to higher barrier height and stronger quantum confinement effect, and it is inferred that the bandgap broadened. On the other hand, the short-circuit current ($J_{sc}$) decreased with increasing the barrier height. This is because the higher barrier height reduced the tunneling probability. However, since the influence of the $J_{sc}$ decrement is small, the open-circuit voltage ($V_{oc}$), and efficiency ($\eta$) almost correspond to the change in the band gap. When the p-type layer was changed from a-Si:H to $\mu$-SiC:H (the solid and broken lines in Fig. 2), there is a large difference in $J_{sc}$ and $\eta$. This may be attributed to the reduction of the absorption loss in p-type layer, since the $\mu$-SiC:H has wider bandgap than a-Si:H. In these results, it is important that the $J_{sc}$ was not decreased so much with increasing the barrier height. Although the defect density at the surface of Si-QDs was neglected in this simulation, it is predicted that higher composition of Al$_2$O$_3$ leads to higher $V_{oc}$ due to not only bandgap widening but also surface passivation. Therefore, Al$_2$O$_3$ is one of promising barrier materials to improve the efficiency of Si-QDSL solar cells.

References