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Carrier Transfer Simulation on Si/SiC interface in Quantum Dot Solar Cells

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1. Introduction

Solar cells (SCs) have been paid much attention for unlimited and pollution-free energy generation device. However, power-generating costs of SC are higher than commercial power sources. To decrease the costs, two methods are proposed: (1) Improvement of conversion efficiency, (2) Decrease of production cost.

In the former of them, the quantum dot solar cell (QDSC) using a quantum confinement effect is proposed. The theoretical value of the QDSC is more than 60% [1], and is much higher than other SCs. However, an actual efficiency of QDSC is at most about 20% [2]. It is suggested that the carrier trap at the QD/bulk interface defects decreases the conversion efficiency [3].

In this study, we calculated the electronic structure of QD/bulk interface by using the quantum chemical (QC) calculation to analyze the influence of interface defect on conversion efficiency. Moreover, we analyzed the carrier transfer at the QD/bulk interface by using electronic structures obtained from QC calculation.

2. Methods

Quantum chemical calculation

The QC calculation program, “Colors” based on original tight-binding approximation [4], was used for the electric structure analysis. This program can calculate a large scale model at high speed by constructing the Hamiltonian with the parameter determined from the first-principles calculation.

Carrier transfer simulation

The carrier transfer simulation based on Monte Carlo method was used to estimate the carrier transfer at the QD/bulk interface [5]. In this simulation, electron density of molecular orbital was divided into the three dimensional mesh (0.3 Å on a side) (Fig. 1). The carrier transfers according to the electronic density of each meshes obtained

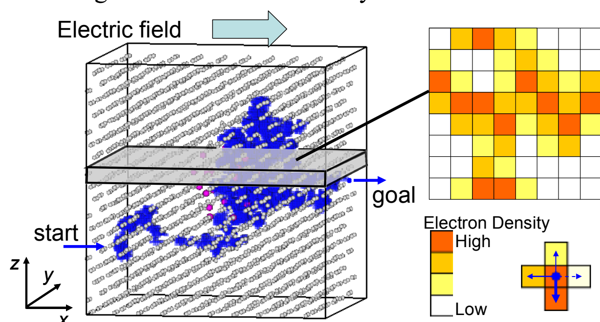

Fig. 1 The schematic figure of carrier transfer simulation

from QC calculation. In addition, we assumed that orbital transitions depend on the Boltzmann distribution and electron density.

Using this simulation, we calculated carrier trap rate (R_{trap}) as an index of the carrier transfer obstruction. To calculate R_{trap}, the number of steps until the carrier transfer from start side to goal side was analyzed. The rate of carrier passing over the model (R_{pass}) at the reference step S was calculated. In this paper, S was defined as a number of steps that R_{pass} becomes 0.9 in SiC bulk model. Then R_{trap} was obtained from equation (1) by using these results.

$$R_{trap} = R_{pass}(\text{SiC bulk}) / R_{pass}(S) \quad (1)$$

Calculation models

To consider the effect of the interface on the carrier transfer, we constructed a Si-QD/SiC model (Fig. 2). This model was created by implanting Si nano-crystal (1 nm in diameter) into the center of the SiC bulk (a = 30.72 nm, b = 32.21 nm, c = 30.14 nm). The relaxed structure by molecular dynamics was used for QC and carrier transfer simulations.

To compare the influence of the interface defects on carrier trap with that of the defect in bulk, we created a point defect model, which has a C atom defect at the center of SiC bulk (a = 30.72 nm, b = 32.21 nm, c = 30.14 nm). It was also relaxed and used for the simulations.

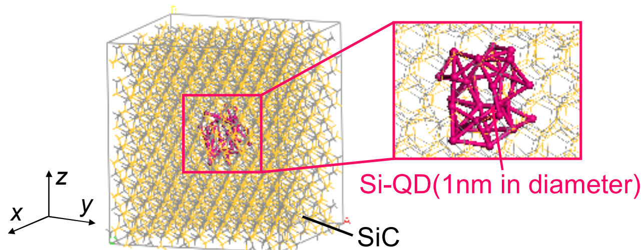

Fig. 2 Si-QD/SiC model

3. Results and Discussion

Electronic structure analysis

The electronic structure of QD/bulk interface was calculated by using QC calculation. Fig. 3 shows a partial density of states (PDOS) obtained from QC calculation. Fig. 3(a) shows the PDOS calculated for the whole model. In Fig. 3(a), the continuous energy levels between valence band top (V_b) and conduction band bottom (C_b) of SiC bulk was appeared. Fig. 3(b) shows the PDOS calculated only for Si-QD. Fig. 3(b) suggested that appeared energy levels contributed by Si-QD. Moreover, the orbital of the energy levels was localized at the Si-QD/SiC interface.

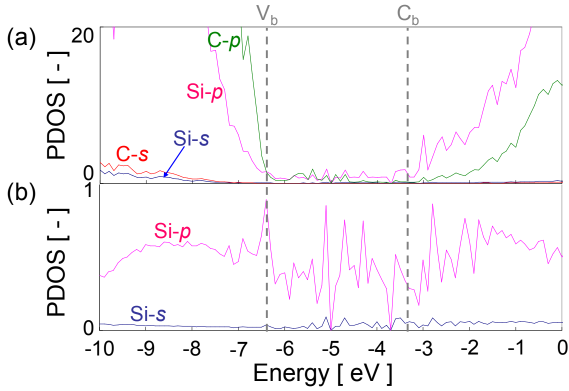

Fig. 3 PDOS of Si-QD/SiC model:
(a) Whole model, (b) Only Si-QD

The electronic structure of the point defect model was calculated. The energy levels in the forbidden band of SiC bulk were appeared. These levels appeared only in the center of the band gap and were not continuous. Moreover, these energy levels were also localized at the point defect.

Carrier transfer simulation

To analyze the carrier transfer at the Si-QD/SiC interface or point defect, we carried out the carrier transfer simulation. In this simulation, we observed that the carrier was trapped on the QD/bulk interface when the carrier transferred from the start side to goal side. Fig. 4 shows the distribution of the meshes that is high existence probability of electron after calculating for 100 electrons.

Fig. 4 shows that the meshes with high carrier existence probability concentrated at the QD/bulk interface. This result also suggested that the electron approached to Si-QD/SiC interface was trapped at the localized orbital.

Moreover, we simulated the carrier transfer in the point defect model. As the result, it was shown that the carrier was trapped around the point defect. The meshes with high carrier existence probability concentrated at the narrow area than QD/bulk interface.

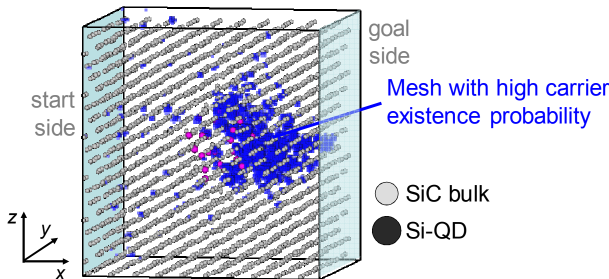

Fig. 4 Distribution of existence probability for Si-QD/SiC model

Estimation of carrier trap rate

To analyze the difference of the carrier trap rate (R_{trap}), we calculated R_{pass} for each of models. At first, we calculated the number of steps that R_{pass} in SiC bulk model by using the carrier transfer simulation, and this was a reference step. Then, R_{pass} at the reference step was calculated in each model.

Fig. 5 shows the results. In this study, the reference step was 1.13×10^5 steps. At this step, R_{pass} for the Si-QD/SiC

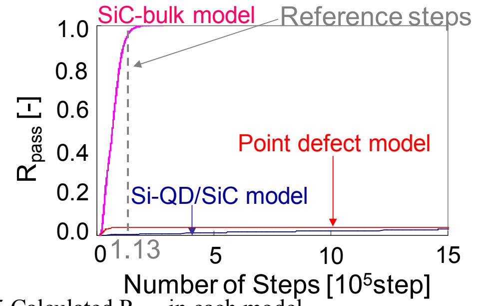

Fig. 5 Calculated R_{pass} in each model

model was 0.004 and R_{pass} for the point defect model was 0.040. At the reference step, R_{pass} for the point defect model was higher than R_{pass} for the Si-QD/SiC model. However, at the 15×10^5 steps, the value of R_{pass} were similar. This result shows that the carrier trapped at point defect could not escape. This is because of the defect levels are not continuous and the energy difference between Cb and defect levels were large.

Table 1 shows R_{trap} obtained from calculated R_{pass}. From Table 1, it was shown that R_{trap} of the Si-QD/SiC model was a ten times higher than the point defect model. This is because the volume of the defect levels localized at QD/bulk interface was larger than the defect levels localized at point defect. Therefore, the carrier could be trapped at the QD/bulk interface easily, and R_{trap} of the Si-QD/SiC model was larger than R_{trap} of the point defect model.

Table 1 Carrier trap rate

	Volume of defct levels [Å^3]	R_{pass} [-]	R_{trap} [-]
Si-QD/SiC model	1295	0.004	255
Point defect model	383.2	0.040	22.5

4. Conclusion

In this study, we analyzed the carrier transfer at the Si-QD/SiC interface and point defect. Consequently, it was suggested that the Si-QD/SiC interface traps the carrier easily and the point defect also contributes to the carrier trap. Therefore, it was suggested that the conversion efficiency could be improved by decreasing the defect at the interface.

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