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Device Simulation of Intermediate Band Solar Cells

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Abstract— **The intermediate band (IB) solar cells is one of the candidates to realize a higher conversion efficiency than the Shockley-Queisser limit of single-junction solar cells. By using device simulation of intermediate solar cells developed based on drift-diffusion method, we studied the fundamental properties of IB cell. Light concentration technique is very important to reduce the recombination via IB.**

Keywords-component; intermediate band solar cell; light concentration; device simulation

I. INTRODUCTION

Novel photovoltaic concepts to realize higher energy conversion efficiencies than the Shockley-Queisser's limit [1] are studied globally today. These types of solar cells are called as "third generation". The target of this generation is to utilize or reduce fundamental energy losses. The main fundamental loss mechanisms of solar cells are thermalization - energy relaxation process of carriers and transmission losses. If we use wide a bandgap semiconductor material for a single junction solar cell, the thermalization loss is reduced but the transmission loss is increased. On the other hand, use of a narrow bandgap material can reduce the transmission loss but increases thermalization loss. Thus, the optimal band gap material is decided. In the novel concepts, the key point is how to reduce or suppress these loss processes. For example, hot carrier and multi-exciton generation solar cells use a narrow band gap material with suppressing energy relaxation process of carriers in both conduction and valence bands by phonons and extracts carriers keeping a hot carrier temperature to the contacts and contribute to generate another electron-hole pairs within an energy relaxation process, respectively. In the case of multi-band or intermediate band (IB) solar cells [2], intermediate states are introduced in relatively wide band gap material to utilize lower energy photons than a host material band gap and increase total carrier generation rates in host material conduction and valence bands as shown in Fig. 1. The intermediate band solar cells are fabricated by using multi-stacked quantum dots [3, 4, 5], dilute alloy materials [6] and impurity bands [7]. The quantum dot solar cells show the concept of two-step photon absorption [5] and shows fundamental properties of the intermediate band solar cells. To improve conversion efficiency of the intermediate band solar cells, device simulations of the intermediate band solar cell can help to understand the inside physics and optimize the structure.

II. DEVICE SIMULATION OF INTERMEDIATE BAND SOLAR CELLS

We study properties of the intermediate band solar cells by using self-consistent device simulation of intermediate band solar cells in a steady state [8]. This simulation is based on the drift-diffusion method and includes carrier generation and recombination processes via the intermediate band. Electron densities in the intermediate band are decided by net transition rates via the intermediate band and affect to electrostatic potential. We assume the band as intermediate levels. Thus, the net transition rate is determined by a local balance equation,

$$G_{CI}(x) - U_{CI}(x) = G_{IV}(x) - U_{IV}(x) \qquad (1)$$

where G_{CI}, G_{IV}, U_{CI} and U_{IV} are optical generation and recombination rates between the conduction band - intermediate band, and the intermediate band and valence band, respectively. Thus, (1) describes transition rates should be balanced locally and decide the net carrier generation rate via the intermediate band. These terms in (1) have a dependence on an electron density in the conduction band, hole density in the valence band and electron density in the intermediate band. Therefore, we should solve the Poisson's equation, carrier continuity equations and the local balance equation self-consistently. We assume the carrier transport properties are well described by the drift-diffusion equation. In this calculation, we use GaAs material parameters except absorption coefficients and ideal Ohmic contacts for majority carriers and zero surface recombination velocities for minority carriers as boundary conditions. No surface recombination velocity expresses the presence of a well passivated surface or window layer.

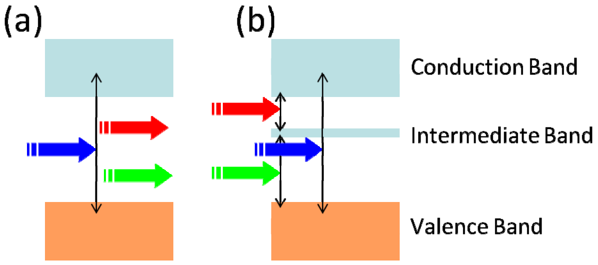

Figure 1. Schematic image of photon absorption process of the cases of single-junction solar cells (a) and intermediate band solar cells.

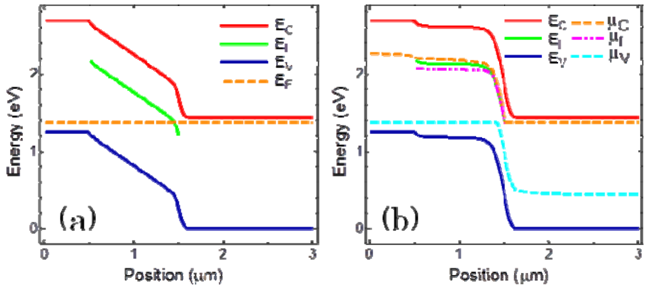

Figure 2. Calculated band diagrams in an equilibrium (a) and short-circuit condition (b), respectively. E_C and E_V are band edges of the condution and valence band. E_I is energetic position of the intermediate band. EF is the Fermi energy. μ_C, μ_I and μ_V are quasi-Fermi energies of the conduction, interemediate and valence band, respectively

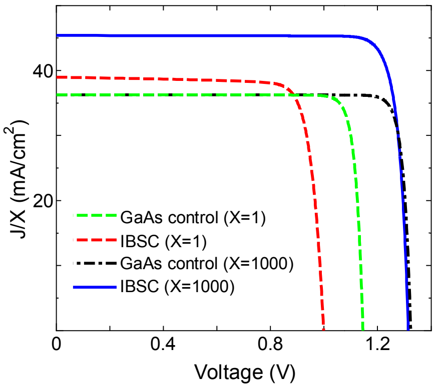

Figure 3. Curren-voltage characteristics of GaAs control cell and the intermediate band solar cell (IBSC). J and X are a current density and concentration ratio.

III. SIMULATION RESULTS

We used simplified absorption coefficients to focus on the fundamental properties of the intermediate band solar cells. The device structure consists of *p*-type top emitter layer, the intermediate band region and *n*-type bottom base layer. In the intermediate band region, the intermediate band is uniformly distributed and set 0.95eV from the band edge of the valence band. Calculated band diagrams in equilibrium and short-circuit conditions are presented in Fig. 2 (a) and (b), respectively. Electrons in the intermediate band affect the electrostatic potential profile. Under sun light illuminations, the electron density is calculated by (1) and strongly changes the band profile. Thus, the self-consistent calculation is important. In Fig. 3, current-voltage characteristics of the intermediate band solar cell and GaAs control cell which is the same structure except the intermediate band under 1 sun and 1000 suns are presented. Current densities are divided by light concentration ratio. Under 1 sun, short-circuit current of the intermediate band cell increase compared to the control cell but the open-circuit voltage and fill factor is degraded. This is the effect of the introduction of the intermediate band. The intermediate band works as carrier generation center but also recombination center. On the other hand, under 1000 suns illumination, the short-circuit current is largely increased while the current of the control cell is the same as under 1sun condition and degradations of the open-circuit voltage and fill factor are improved. In this case, the recombination via the intermediate band is suppressed by large carrier generation rates via the band. This effect is called as photo-filling effects [9].

IV. CONCLUSION

We studied fundamental properties of the intermediate band solar cells by using the self-consistent device simulation of intermediate band solar cells. The device simulation well describes inside properties of the photovoltaic and is a great tool to optimize the structure. The intermediate band works as both carrier generation and recombination centers. To minimize the negative effects of the introduction of the intermediate band, the light concentration is very important. In quantum dot based solar cells, the absorption coefficients related to the intermediate band are small [10]. In this case, light management technique can play an important role to achieve high conversion efficiencies.

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REFERENCES

[1] W. Shockley and H. J. Queisser, “Detailed balance limit of effciency of p-n junction solar cells,” J. Appl. Phys., vol 32, pp. 510-519, 1961.

[2] A. Luque and A. Marti, “Increasing the effciency of ideal solar cells by photon induced transition at intermeidate levels,” Phys. Rev. Lett., vol. 78, pp. 5014-5017, 1997.

[3] S. M. Hubbard, C. D. Cress, C. G. Bailey, R. P. Raffaelle, S. G. Bailey and D. M. Wilt, “Effect of strain compensation on quantum dot enhanced GaAs solar cells,” Appl. Phys. Lett., vol. 92, pp. 123512-123514, 2008.

[4] K. A. Sablon, J. W. Little, V. Mitin, A. Sergeev, N. Vagidov and K. Reinhardt, “Strong enhancement of solar cell efficiency due to quantum dots with built-in chrge,” Nanno Lett., vol. 11, pp. 2311-2317, 2011.

[5] Y. Okada, T. Morioka, K. Yoshida, R. Oshima, Y. Shoji, T. Inoue and T. Kita, “Increase in photoncurrent by optical transitions via intermediate quantum states in direct doped InAs/GaNAs strain-compensated quantum dot solar cell,” J. Appl. Phys., vol. 109, pp. 024301-024305, 2011.

[6] N. Lopez, L. A. Reichertz, K. M. Yu, K. Compman and W. Walukiewicz, “Engineering the electronic band structure for multiband solar cells,” Phys. Rev. Lett., vol. 106, pp. 028701-028704, 2011.

[7] Intermediate-band photovoltaic solar cell based on ZnTe:O,” Appl. Phys. Lett., vol. 95, pp. 011103-011105, 2009.

[8] K. Yoshida, Y. Okada and N. Sano, “Self-consistent simulation of intermediate band solar cells: Effect of occupation rates on device characteristics,” Appl. Phys. Lett., vol. 97, pp. 133503-133505, 2010.

[9] R. Strandberg and T. W. Reenaas, “Photofilling of intermediate bands,” J. Appl. Phys. vol. 105, pp. 124512-124519, 2009.

[10] S. Tomic, “Intermediate-band solar cells: influence of band formation on synamical processes in InAs/GaAs quantum dot arrays,” Phys. Rev. B, vol 85, pp. 195321-195335, 2010.