CRITICAL REMARK ON THE SOLAR CELL CONCEPT WITH A METAL INTERMEDIATE BAND

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Abstract

The solar cell concept with a metal intermediate band promises energy conversion efficiencies above the Shockley–Queisser limit. However, ideal absorption has to be taken into account for thermal generation including the metal intermediate band, and charge-selective contacts can only probe chemical potentials in the photovoltaic absorber. Solar cells with a metal intermediate band cannot exceed the Shockley–Queisser limit.

A solar cell has two basic functions: photo-generation and separation of photo-generated free charge carriers. Both functions are expressed in the diode equation including the diode saturation current density ($I_0$) and the short circuit current density ($I_{SC}$) as parameters:

$$ I = I_0 \cdot \exp \left( \frac{q \cdot U}{k_B T} \right) - 1 - I_{SC}. $$

The maximum possible energy conversion efficiency can be calculated under the assumptions that generation is equilibrated by radiative recombination (detailed balance) and that ideal absorption takes place (Shockley–Queisser limit [1]). Ideal absorption means that the quantum efficiency is equal to one for all photons with an energy equal or larger than the value of the band gap of the photovoltaic absorber ($E_g$). The open circuit voltage ($V_{OC}$) is limited to the $I_{SC}/I_0$ ratio. The energy conversion efficiency of a solar cell is defined as the product of $I_{SC}$, $V_{OC}$ and the fill factor divided by the power of incoming light. Losses by resistive heating are neglected in ideal solar cells.

Following Würfel [2], $I_0$ and $I_{SC}$ are given by the thermal and photo-generation rates ($G_0^{E_g}(h\nu)$ and $G_{sun}^{E_g}(h\nu)$, respectively) and can be calculated by integrating the photon flux of blackbody ($\Phi_0(h\nu)$) and solar ($\Phi_{sun}(h\nu)$) irradiation, respectively, from $E_g$ to infinite (or about 4 eV).

$$ I_0 = q \cdot G_0^{E_g}(h\nu) = q \cdot \int_{E_g}^{\infty} \Phi_0(h\nu) \cdot d(h\nu) $$

$$ I_{SC} = q \cdot G_{sun}^{E_g}(h\nu) = q \cdot \int_{E_g}^{\infty} \Phi_{sun}(h\nu) \cdot d(h\nu) $$

The detailed balance and the ideal absorption conditions must be taken into account for calculating $I_0$ and $I_{SC}$ of any ideal solar cell with maximum energy conversion efficiency.
A solar cell with a metal intermediate band [3] is based on a semiconductor with an additional band within the band gap of the photovoltaic absorber. The band gap of the semiconductor and the differences between the conduction band edge ($E_C$) of the photovoltaic absorber and the Fermi-energy of the metal intermediate band ($E_{F-MIB}$) and between $E_{F-MIB}$ and the valence band edge of the photovoltaic absorber ($E_V$) are denoted by $E_{g1}$, $E_{g2}$ and $E_{g3}$, respectively. The density of occupied and unoccupied states in the metal intermediate band is large so that photons with energies larger than $E_{g1}$, $E_{g2}$ and $E_{g3}$ are absorbed. Therefore, a solar cell with a metal intermediate band has a photovoltaic absorber with a band structure containing three band gaps.

The Fermi-energies of photo-generated electrons and holes are contacted separately, while the metal intermediate band disappears at the charge-selective contacts [3]. The charge-selective contact regions do not contribute to photo-generation. As remark, the potential difference at the external leads cannot be larger than the Fermi-level splitting in the photovoltaic absorber.

There is no internal driving force or circuit for charge separation within a homogeneous photovoltaic absorber, in contrast to multi-junction solar cells. Therefore, the metal intermediate band has only influence on the thermal and photo-generation rates.

Under the assumption of ideal absorption, the band gap of a solar cell with a metal intermediate band corresponds to the larger values of $E_{g2}$ or $E_{g3}$. Therefore, $I_{SC}$ or $I_0$ of a solar cell with a metal intermediate band cannot be larger or less, respectively, than $I_{SC}$ or $I_0$, respectively, of a solar cell with a band gap of $E_{g3}$ or $E_{g2}$. Consequently, solar cells with metal intermediate bands cannot exceed the Shockley–Queisser limit.

References