Solar Energy Materials & Solar Cells 93 (2009) 797–802

Contents lists available at ScienceDirect

Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

Impact ionization and Auger recombination at high carrier temperature

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ARTICLE INFO

Article history:
Received 11 January 2008
Accepted 27 September 2008
Available online 29 November 2008

Keywords:
Hot carrier solar cells
Hot carriers
Impact ionization
Auger recombination

ABSTRACT

We have calculated impact ionization (II) and Auger recombination (AR) lifetimes in hot carrier solar cells (HC-SCs) in operation, and found that these lifetimes are much longer than the average retention times of photo-generated carriers in the cells at an appropriate range of applied voltage, under practical conditions of 500–1000 times-concentrated solar irradiation and carrier thermalization times of several hundred picoseconds. This means that the particle conservation (PC) model, in which II and AR are completely excluded, can be applied to predict the conversion efficiency. In contrast, the PC model does not stand under the ideal condition of the maximally concentrated irradiation and no thermalization of carriers, as previously pointed out.

1. Introduction

Hot carrier solar cells (HC-SCs) are one of the attractive candidates of the third-generation solar cells [1]. The main concept to achieve very high conversion efficiency is to extract photo-generated carriers before thermalization, i.e., energy dissipation caused by carrier–phonon interaction. There are two contrasting models proposed to calculate conversion efficiency of HC-SCs: the particle conservation (PC) model [2] and the impact-Auger (IA) model [3]. In the PC model, impact ionization (II) and Auger recombination (AR), which are generally significant at a large carrier density and a high carrier temperature, are completely excluded. In contrast, the IA model is based on an assumption that significant II and AR result in a common quasi-Fermi level for electrons in the conduction band and holes in the valence band.

Although both the models predict around 85% of conversion efficiency under the ideal condition of no thermalization and the maximally concentrated solar irradiation [1–3], we have found that the maximal conversion efficiency calculated using the PC model is considerably lower than the values of the ideal case, under practical conditions of 500–1000 times-concentrated irradiation and thermalization times of several hundred picoseconds [4], and the value calculated using the IA model is even lower.

In this study, we investigate the influence of II and AR by calculating the II and AR lifetimes in HC-SCs in operation, and elucidate the coverage where the PC model can be applied.

Recently, significant II has been observed in semiconductor quantum dots using time-resolved laser spectroscopy techniques [5,6]. The experimental conditions of these observations are, however, considerably different from the focus of the present study. The II observations were carried out using pulsed lasers with very large peak power, under conditions corresponding to the open-circuit because photo-generated carries were not extracted to outside. To evaluate solar cells, steady states at appropriate voltage to achieve high output power (the so-called P_{max} condition) should be considered, rather than transient states at the open-circuit voltage.

2. Modeling and formulation

2.1. Conversion efficiency

An HC-SC consists of an absorber, where carriers are generated by photo-excitation, and energy-selective contacts (ESCs) on both sides of the absorber, through which mono-energetic electrons and holes are extracted to metal electrodes, as schematically illustrated in Fig. 1. In this study, the ESCs are supposed to be ideal, i.e., with infinite conductance and infinitesimal energy-selection width.

In the PC model, both particle number and energy are assumed to be conserved. The extracted carrier flux, J, is determined from the difference between the spectral photon flux absorbed, I_A, and

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doi:10.1016/j.solmat.2008.09.053

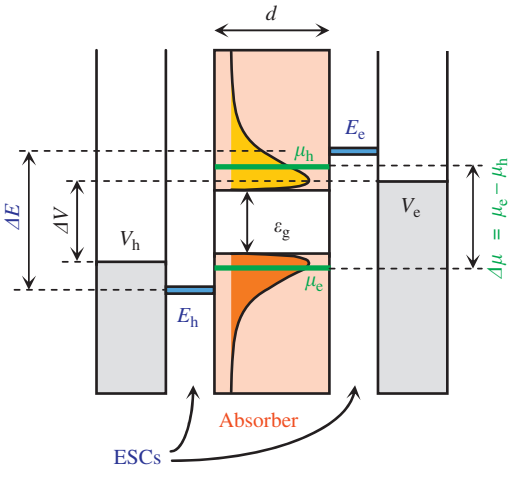

Fig. 1. Schematic configuration and energy diagram of a hot carrier solar cell. ε_g: bandgap of the absorber, d: thickness of the absorber, μ_e and μ_h: quasi-Fermi levels in the absorber, E_e and E_h: energy levels of the ESCs, V_e, V_h: Fermi levels in the metal electrodes. The suffixes e and h represent electrons and for holes, respectively.

that emitted from the absorber, I_E, i.e.,

$$J = \int_{\varepsilon_g}^{\infty} d\varepsilon (I_A - I_E), \tag{1}$$

where ε_g is the bandgap of the absorber.

The solar spectrum is approximated by the black-body radiation at a temperature of $T_S = 5760\,K$:

$$I_A = \frac{2\Omega_A}{h^3c^2}\frac{\varepsilon^2}{\exp[\varepsilon/k_BT_S]-1}, \tag{2}$$

where Ω_A is the solid angle under which the sun is seen, ranging from 6.8×10^{-5} for non-concentration to π for the maximal concentration, h the Plank constant, k_B the Boltzmann constant and c the velocity of light in vacuum. The influence of the radiation from the ambient has been confirmed to be negligible.

I_E depends on the quasi-Fermi levels, μ_e, μ_h and temperatures of photo-excited electrons in the conduction band and holes in the valence band, as well as on ε:

$$I_E = \frac{2\Omega_E}{h^3c^2}\frac{\varepsilon^2}{\exp[(\varepsilon-\Delta\mu/k_BT_c)]-1}, \tag{3}$$

$$\Delta\mu \equiv \mu_e - \mu_h, \tag{4}$$

where temperatures of the electrons and holes are assumed to be the same: T_c, for simplification. Ω_E equals π, since a flat geometry is premised.

The carrier energy extracted from the absorber through the ESCs, ΔE, equals the difference between the energy level of the ESC for electrons, E_e, and that for holes, E_h: $\Delta E = E_e - E_h$. The energy flux equals J times ΔE, and is similarly related to the difference between the spectral photon energy fluxes absorbed and emitted. When an electron–hole pair is generated, the incremental carrier energy equals the absorbed photon energy, ε. The energy is, however, decreased to be $\tilde{\varepsilon}$ due to thermalization when the carriers are extracted after the average retention time, τ_{re}. Therefore, the following relations are derived from the energy conservation:

$$J\Delta E = \int_{\varepsilon_g}^{\infty} d\varepsilon(\tilde{\varepsilon}I_A - \varepsilon I_E), \tag{5}$$

$$\tilde{\varepsilon} = \varepsilon F + (1-F)(\varepsilon_g + 3k_BT_{RT}), \tag{6}$$

$$F = \exp[-\tau_{re}/\tau_{th}], \tag{7}$$

where the thermalization times of the electrons and holes are assumed to be the same, τ_{th}; T_{RT} denotes the room temperature; τ_{th} is supposed to be independent of n_c and T_c for simplification, although they are actually dependent [7–10].

The carrier energy extracted from the metal electrodes to external loads, ΔV, should be smaller than ΔE, because of the difference between T_c and T_{RT}. ΔV is thermodynamically derived as follows (since the ESCs are assumed to be ideal and hence the energy transfer through the ESCs is isoentropic) [11]:

$$\Delta V = \Delta E - (\Delta E - \Delta\mu)T_{RT}/T_c. \tag{8}$$

The energy flux extracted to outside, P, equals J times ΔV, and the conversion efficiency, η, is the ratio of P to the incident energy flux:

$$\eta = J\Delta V / \int_0^{\infty} d\varepsilon\varepsilon I_A. \tag{9}$$

In the IA model, it is assumed that significant IA and AR result in $\Delta\mu = 0$. Therefore, the particle number is not conserved. The energy conservation leads to a simple expression of P:

$$P = J\Delta V = (1 - T_{RT}/T_c)\int_{\varepsilon_g}^{\infty} d\varepsilon(\tilde{\varepsilon}I_A - \varepsilon I_E). \tag{10}$$

The photo-generated carrier density, n_c, is determined from μ_e and T_c as follows:

$$n_c = 8\sqrt{2}\pi m_e^{3/2}/h^3 \int_{\varepsilon_g/2}^{\infty} d\varepsilon\sqrt{\varepsilon - (\varepsilon_g/2)}\frac{1}{\exp[(\varepsilon-\mu_e)/k_BT_c]+1}, \tag{11}$$

where m_e denotes the effective mass of the conduction electrons and n_c is related similarly to μ_h.

τ_{re} also determines n_c. When particle number is conserved, n_c is proportional to τ_{re} as follows:

$$n_c = J_A\tau_{re}/d, \tag{12}$$

where d is the thickness of the absorber. Large J_A, i.e., high concentration ratio leads to large n_c. This relation also provides rough estimation of n_c of the IA model, although it is not exact because of particle number non-conservation.

When ε_g, τ_{th}, d and ΔE characterizing the materials used in an HC-SC, and Ω_A proportional to the concentration ratio are given, n_c, τ_{re}, $\Delta\mu$ and T_c that satisfy Eqs. (5)–(8) and (11) and (12) are determined, depending on the applied voltage, v ($= \Delta V/q$, q the elemental charge). The current density, j ($= qJ$), is calculated as a function of v.

2.2. II and AR lifetimes

II and AR are significant in general when n_c is large and T_c is high. AR of III–V compound semiconductors is extensively studied, because it affects the performance of light-emitting devices using these materials. Among them, the bandgap of $In_{0.53}Ga_{0.47}As$ (0.73 eV) is close to the optimal value for HC-SCs. Therefore, II and AR lifetimes, τ_{II} and τ_{AR}, in operation of an HC-SC, in which a hypothetical material having a band structure identical to that of InGaAs is used as an absorber, were evaluated. Comparison of calculated τ_{AR} with experimental data supports the validity of the present calculation.

The band structure of InGaAs is schematically illustrated in Fig. 2. It has been already found that three kinds of II and AR processes, CCCH, CHHL and CHHS, shown in Fig. 2 are dominant in III–V compound semiconductors compared to other processes. The CCCH process involves three conduction electrons and a heavy hole. The transition probability of II-CCCH, R_{II}(CCCH), is