Solar Energy Materials & Solar Cells 94 (2010) 1704–1710

Contents lists available at ScienceDirect

Solar Energy Materials & Solar Cells

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

Evaluation of thermal radiation dependent performance of GaSb thermophotovoltaic cell based on an analytical absorption coefficient model

Y. Wang [a,*], N.F. Chen [b,*], X.W. Zhang [a], T.M. Huang [a], Z.G. Yin [a], Y.S. Wang [a], H. Zhang [a]

[a] Key Laboratory of Semiconductor Materials Science, Institute of Semiconductor, Chinese Academy of Sciences, Beijing 100083, China
[b] School of Renewable Energy Engineering, North China Electric Power University, Beijing 102206, China

ARTICLE INFO

Article history:
Received 10 September 2009
Accepted 10 May 2010

Keywords:
Thermophotovoltaic
Gallium antimonide
Absorption coefficient

ABSTRACT

Applying the model dielectric function method, we have expressed the absorption coefficient of GaSb analytically at room temperature relating to the contribution of various critical points of its electronic band structure. The calculated absorption spectrum shows good agreement with the reported experimental data obtained by spectral ellipsometry on nominally undoped sample. Based on this analytical absorption spectrum, we have qualitatively evaluated the response of active absorbing layer structure and its photoelectric conversion properties of GaSb thermophotovoltaic device on the perturbation of external thermal radiation induced by the varying radiator temperature or emissivity. Our calculation has demonstrated that desirable thickness to achieve the maximum conversion efficiency should be decreased with the increment of radiator temperature and the performance degradation brought by any structure deviation from its optimal one would be stronger meanwhile. For the popular radiator temperature, no more than 1500 K in a real solar thermophotovoltaic system, and typical doping profile in GaSb cell, a reasonable absorbing layer structure parameter should be controlled within 100–300 nm for the emitter while 3000–5000 nm for the base.

1. Introduction

In recent years, there is a renewed interest in solar thermophotovoltaic (STPV) [1] because of considerable progress received in the fabrication of high-quality, low-bandgap semiconductor converters, e.g., gallium antimonide (GaSb) as well as its ternary or quaternary alloys [2–5]. When compared with conventional photovoltaic (PV) application, an intermediate emitter, generally made by refractory materials such as tungsten [6] or ceramic oxides [7], is particularly introduced in thermophotovoltaic (TPV) scheme to heat itself by absorbing the concentrated solar illumination, then low-bandgap converters are used to convert the reemitted thermal irradiation of heated emitter into electric energy. Due to close space distance between emitter and converters, high density electric output and the generation of heat simultaneously are promised. Moreover, by modulating the thermal irradiation through some artificial engineering [8], a competitive thermal-to-electric conversion efficiency (η) is also attainable because of the enhanced spectral match between the incident spectrum and response of TPV cell, showing the potential application in both terrestrial and space [1,9].

However, for the real outdoor STPV application, operating temperature of intermediate emitter in a real STPV prototype is very difficult to keep invariant because the incident intensity of solar illumination is different from time to time, leading to the marked variation of thermal irradiation and further resulting in the potential perturbation on the generation of electricity and output stability. It is therefore very necessary to reveal this perturbation on device performance comprehensively. Disappointingly, even for the dominant GaSb device, relatively little work has been done to perform the design and structure optimization of GaSb cell because of the insufficient knowledge of device related parameters [10,11]. For example, both Stollwerck et al. [10] and Martín and Algora [11] have made an attempt to quantify the optical absorption in device simulation, but no analytical expression was given explicitly there. Therefore, the underlying goal of this work is to establish an analytical model for the absorption spectrum of GaSb in the range 0.5–6 eV, and further to enhance the qualitative understanding of performance perturbation of GaSb TPV cell illuminated by a varying incident radiation for the aforementioned reason.

This paper is organized as follows. In Section 2 we briefly describe the combined theoretical method to analytically express the absorption coefficient of GaSb, and the detailed procedure to simulate the performance of GaSb cell is presented in Section 3. The calculated result and comprehensive discussion is given in Section 4, and in Section 5 we conclude with a summary.

* Corresponding author. Tel.: +86 10 82304458; fax: +86 10 82304588.
E-mail addresses: ywang@semi.ac.cn (Y. Wang), nfchen@ncepu.edu.cn (N.F. Chen).

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doi:10.1016/j.solmat.2010.05.032

2. Analytical model for GaSb absorption coefficient

With an attempt to perform the structure optimization of GaSb cell, an accurate knowledge of optical absorption $\alpha(E)$ related to the radiation energy E of incident photon is thus strongly desirable. However, in spite of its significance in STPV application, relatively little investigation has been reported to determine $\alpha(E)$of GaSb. Experimentally, using spectral ellipsometry (SE) measurements, both Ferrini et al. [12] and Aspnes and Studna [13] have measured the room temperature complex dielectric function $\varepsilon(E)[=\varepsilon_1(E)+i\varepsilon_2(E)]$ of GaSb on nominally undoped sample, and the derived $\alpha(E)$ has been given as we depicted schematically in Fig. 1 with different symbols, circle for the former while star for the latter. Disappointedly, a desirable analytical form of $\alpha(E)$, important and convenient for the device simulation, was not given explicitly there. In the theoretical aspect, in the framework of the simple band-to-band single particle transition, Adachi [14] proposed a model dielectric function (MDF) method to calculate the optical absorption of zinc-blende-type semiconductor analytically in terms of its electronic band structure. Although a satisfied fit between theoretical calculation and scattered experimental data was not obtained, the underlying principle of this proposal, decomposing the integrated absorption of material under consideration into the specific contribution of various type critical points (CP) in its Brillouin Zone (BZ), are involved into subsequent model calculations [15–19].

Specifically, in zinc-blende-type GaSb, spin–orbit interaction splits $\Gamma^v_{15}(\Gamma^c_{15})$valence (conduction) band into $\Gamma^v_7(\Gamma^c_7)$ (degenerate band) and $\Gamma^v_8(\Gamma^c_8)$ (spin-split off band) with an energy splitting $\Delta_0(\Delta'_0)$, also the L^v_3 valence band is split into $L^v_{4,5}$and L^v_6 by spin–orbit interaction with an energy splitting Δ_1 [20]. Thus, the important CPs in BZ can be labeled as direct gap $E_0[\Gamma^v_8\rightarrow\Gamma^c_6]$, spin split off component $E_0+\Delta_0[\Gamma^v_7\rightarrow\Gamma^c_6]$, spin–orbit split doublet $(E_1[L^v_{4,5}\rightarrow L^c_6]$, $E_1+\Delta_1[L^v_6\rightarrow L^c_6])$, indirect gap E^{ID}_g $(E_X[\Gamma^v_8\rightarrow X^c_6]$ or $E_L[\Gamma^v_8\rightarrow L^c_6])$ and higher-lying E_2 transition along $\langle 1\,1\,0\rangle$ or near X point. Based on these CPs and additional higher CP if necessary, several modified MDF methods [16–19] have been proposed to express $\alpha(E)$ of GaSb analytically, but the detailed comparison between experimental data and theoretical calculation, to our knowledge, is still absent from the literature.

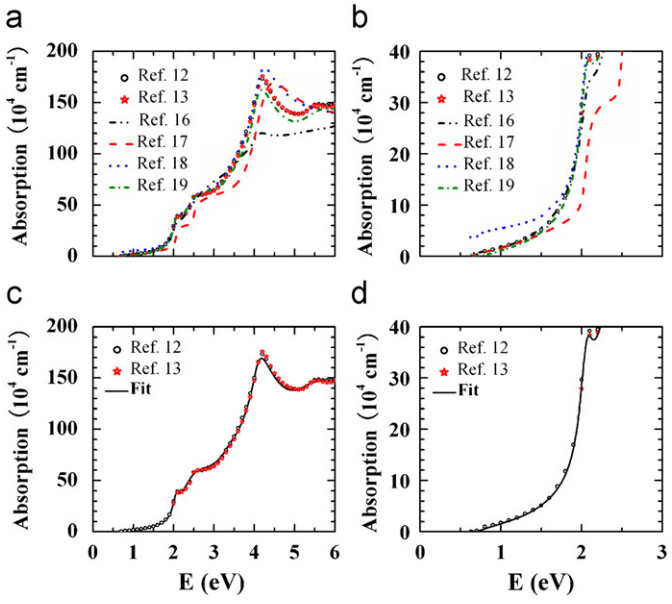

Fig. 1. Comparison of theoretical calculation and experimental measurements on GaSb absorption coefficient: (a) several reproduced theoretical curves calculated from the proposed physical models are compared with the experimental data measured by Ferrini et al. (open circle symbol) and Aspnes et al. (star symbol), and for clarity an expanded version in the range 0–3 eV is schematically shown in (b). Our calculated curves based on an improved model is shown and compared with experiments in (c), and in (d) the expanded picture near the fundamental energy is displayed.

In the top panel of Fig. 1, the reproduced theoretical curves calculated from the suggested parameters for each proposed model are shown for comparison, and for clarity, in Fig. 1(b), an expanded version near band edge is also shown. Evidently, both the calculation of Gonzalez-Cuevas et al. [17] (dashed line) and Djurišić et al. [16] (dash-dot-dot line) by developing the Adachi's modified MDF method [15], are failure to fit the experimental data well, indicating the theoretical insufficient of band-to-band single particle transition. However, it is noteworthy that additional incorporation of a frequency-dependent broadening [21–23] in Ref. [16] can give significant improvement in the range 0.5–2 eV while for E larger than 3 eV the increasing discrepancy are observed. In order to clarify the CPs in $\alpha(E)$ of GaSb, Muñoz et al. [18] have performed SE measurements again on nominally undoped sample and tabulated the model parameters by fitting their experimental data with the Holden's MDF [24,25] theory, where the contribution associating with the discrete and continuous exciton effect is also included. Unfortunately, direct comparison of $\alpha(E)$ between their experiment and theoretical calculation was absent from their report. For the comparison, we have reproduced their theoretical curve (short dashed line in Fig. 1) in line with their preferential model and suggested parameters. It is easily seen that, with the exception of optical absorption near the band edge (see Fig. 1(b)) and beyond the E_2 points (4.1 eV), excellent fit can be attained. To overcome the overestimation of theoretical $\alpha(E)$ near band edge, Djurišić et al. [19] have received significant improvement (see dash-dot line in Fig. 1) by replacing the Lorentzian broadening with an adjusting broadening. However, there is an unexpected degradation of optical absorption in the range $2.54(E_1+\Delta_1)$–$4.1(E_2)$ eV.

Based on the above analysis, we have improved the physical model to express GaSb optical absorption analytically by inheriting good feature from the aforementioned models. In the down panel of Fig. 1, our calculated result is shown for the comparison. Obviously, the impressive fit between our calculation and reported experimental data cannot only be attained near the band edge, but also for the whole interested range. In the following, specific model we used are briefly summarized and the corresponding parameter are tabulated in Table 1.

In our calculation, the modified Holden's MDF model [19] is mainly employed and the involved CPs are E_0, $E_0+\Delta_0$, E_1, $E_1+\Delta_1$, E_2, $E'_0[\Gamma^v_8\rightarrow\Gamma^c_7]$, $E'_0+\Delta'_0[\Gamma^v_8\rightarrow\Gamma^c_8]$, and an unlabeled CP E_3 to improve the fit for the broadening peak located at $E=5.3$ eV or so. Moreover, any contribution from the indirect transition is not included in our simulation. Following the modified Holden's MDF

Table 1
Values of model parameters to calculate the absorption spectrum of GaSb.

Parameters	Value	Parameters	Value	Parameters	Value
E_0 (eV)	0.728	E_1 (eV)	2.189	E'_0 (eV)	3.400
A (eV^2)	0.096	C (eV^2)	6.696	$F(E'_0)$ (eV^2)	13.879
$\Gamma_0=\Gamma^{ex}_0$(eV)	0.084	Γ_1 (eV)	0.101	$\Gamma(E'_0)$ (eV)	0.782
α_0	0.039	α_1	0.001	$E'_0+\Delta'_0$ (eV)	3.790
R_0 (eV)	0.0016	R_1 (eV)	0.035	$F(E'_0+\Delta'_0)$(eV^2)	14.795
$E_0+\Delta_0$ (eV)	1.453	$E_1+\Delta_1$ (eV)	2.544	$\Gamma(E'_0+\Delta'_0)$(eV)	0.644
B (eV^2)	0.037	D (eV^2)	34.708	E_2 (eV)	4.050
$\Gamma_{s0}=\Gamma^{ex}_{s0}$ (eV)	0.180	Γ_{1s}(eV)	0.359	$F(E_2)$ (eV^2)	24.484
α_{s0}	0.039	α_{1s}	0.001	$\Gamma(E_2)$ (eV)	0.481
R_{s0} (eV)	0.0016	R_{1s}	0.035	E_3 (eV)	5.310
ε_∞	0.775	$F(E_3)$ (eV^2)	19.771	$\Gamma(E_3)$ (eV)	1.379