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Numerical analysis of $In_xGa_{1-x}N$/SnS and $Al_xGa_{1-x}N$/SnS heterojunction solar cells

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ABSTRACT

In this work the photovoltaic properties of $In_xGa_{1-x}N$/SnS and $Al_xGa_{1-x}N$/SnS heterojunction solar cells are studied by numerical analysis. The photovoltaic performances of $In_xGa_{1-x}N$/SnS solar cells are enhanced with the decreasing In content and the GaN/SnS solar cell exhibits the highest efficiency. The efficiencies of GaN/SnS solar cell improve with the increased SnS thickness and the reduced GaN thickness. For the $Al_xGa_{1-x}N$/SnS solar cells, there is electron barrier in the $Al_xGa_{1-x}N$/SnS interface. The electron barrier becomes larger with increasing Al content and lead to the degraded efficiency of $Al_xGa_{1-x}N$/SnS solar cells. The simulation contributes to designing and fabricating SnS solar cells.

1. Introduction

Tin monosulphide (SnS) with orthorhombic structure as a novel "absorber" layer in the fabrication of thin film solar cells has attracted considerable attention in recent years [1–6]. SnS has several advantages for fabrication of photovoltaic devices. It has an optical band gap of 1.31 eV [1], which are suitable for the solar radiation and a high absorption coefficient ($\alpha > 10^4\ cm^{-1}$). Both Sn and S are abundant in nature and non-toxic. Semiconductor heterojunctions can be used as photovoltaic devices and can reach high efficiencies [7–9]. Reported experimental fabrication of SnS-based heterojunction cells includes the types CdS/SnS [1,10], Zn(O,S):N/SnO_2/SnS [2], SnS2/SnS [11], ZnS/SnS [12], SnS/c-Si [13], a-Si/SnS [14], ITO/SnS [15] and TiO_2/SnS [16]. However, the highest conversion efficiency of SnS heterojunction solar cells is still below 5% [2,3,17]. Xu et al. [18–20] have simulated CdS/SnS, ZnS/SnS, ZnO/SnS, a-Si/SnS and SnS/c-Si heterojunction structures and have reported the highest simulated conversion efficiency 19.9% using ZnS/SnS heterojunction.

$In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys are other promising material systems for optoelectronic devices [21]. The direct band gap of wurtzite $In_xGa_{1-x}N$ alloy system can extend continuously from InN (0.7 eV, in the near IR) to GaN (3.4 eV, in the mid-UV) by adjusting the values of In content, which match the solar spectrum very well. Therefore $In_xGa_{1-x}N$ alloy is a good candidate PV material for super-high-efficiency multi-junction solar cell [22]. And the band gap of wurtzite $Al_xGa_{1-x}N$ alloy system extends continuously from GaN (3.4 eV) to AlN (6.2 eV) by adjusting the values of Al content. $Al_xGa_{1-x}N$ alloy is often used as the barrier material for electronic and optoelectronic devices. $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys can be easily doped as n-type material [23], so they can be expediently used to form p–n junctions with p-type SnS thin films (SnS is intrinsically a p-type semiconductor and n-type doping is very difficult). In addition, with the excellent properties of radiation resistance, high temperature resistance, and superhigh hardness [24], $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys are very suitable as the window layers in the window/SnS heterojunction structures for space application. In this work we adopt new materials ($In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys) as the window layer and study the photovoltaic properties of $In_xGa_{1-x}N$/SnS and $Al_xGa_{1-x}N$/SnS heterojunction solar cells by numerical analysis. This work provides a guide to the design and fabrication SnS heterojunction solar cells.

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2. Modeling and simulations

2.1. Software and structure

AMPS-1D used in this study is a one-dimensional device physics code and is based on the basic equations of semiconductors and solar cells, which are listed as follows:

Poisson's equation:

$$\frac{d}{dx}\left[\varepsilon(x)\frac{d\Psi(x)}{dx}\right] = q^2 \times [p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (1)$$

where the local vacuum level Ψ (in unit of eV), absolute dielectric constant ε and the free electron n, free hole p, trapped electron n_t and trapped hole p_t, as well as the ionized donor-like doping N_D^+ and ionized acceptor-like doping $N_{\bar{A}}$ concentrations are all functions of the position coordinate x. q is the electron charge.

$$\text{The continuity equation for electrons}: \frac{1}{q}\left[\frac{dJ_n(x)}{dx}\right] = -G_L(x) + R(x) \quad (2)$$

$$\text{The continuity equation for holes}: \frac{1}{q}\left[\frac{dJ_p(x)}{dx}\right] = G_L(x) - R(x) \quad (3)$$

$J_n(x) = n\mu_n \frac{dE_f^n(x)}{dx}$ and $J_p(x) = p\mu_p \frac{dE_f^p(x)}{dx}$ are the electron and hole current densities, respectively. μ_n and μ_p are the mobilities of electron and hole, respectively. E_f^n and E_f^p are the electron and hole quasi-Fermi levels, respectively. $R(x)$ is the net recombination rate resulting from direct (band-to-band) recombination and indirect (Shock ley–Read–Hall) recombination traffic through gap states. $G_L(x)$ is the optical generation rate.

To be specific the solutions to Eqs. (1)–(3), must satisfy the following boundary conditions:

$$\begin{aligned} &\Psi(0) = \Psi_0 - qV, \Psi(L) = 0 \\ &J_p(0) = -qS_{p0}(p_0(0) - p(0)), J_p(L) = qS_{pL}(p(L) - p_0(L)) \\ &J_n(0) = qS_{n0}(n(0) - n_0(0)), J_n(L) = -qS_{nL}(n_0(L) - n(L)) \end{aligned} \quad (4)$$

The definition domain in AMPS is the region $0 \leqslant x \leqslant L$ (L is the length of solar cells). $\Psi(x)$ is the energy difference between the local vacuum level at point x and its value at the back contact. In thermodynamic equilibrium, its value is Ψ_0 at $x = 0$ and using the definition its value is zero at $x = L$. $\Psi(L)$ is always zero no matter what the light or voltage condition because of the choice of reference for Ψ. However, $\Psi(0)$ becomes $\Psi_0 - qV$ if a voltage bias, light bias, or both exist. $p_0(0)$ and $p_0(L)$ are the free hole concentrations at $x = 0$ and $x = L$, respectively, in thermodynamic equilibrium whereas $n_0(0)$ and $n_0(L)$ are the free electron concentrations at $x = 0$ and $x = L$, respectively, in thermodynamic equilibrium. The quantities $p(0)$ and $p(L)$ are the corresponding free hole concentrations, under operating conditions, at $x = 0$ and at $x = L$, respectively. The quantities $n(0)$ and $n(L)$ are the corresponding free electron concentrations, under operating conditions, at $x = 0$ and at $x = L$, respectively. The quantities S_{p0}, S_{pL}, S_{n0}, and S_{nL} are effective surface recombination velocities for holes at $x = 0$ and $x = L$, respectively, and for electrons at $x = 0$ and $x = L$, respectively.

Determining transport characteristics then becomes a task of solving the three coupled non-linear differential Eqs. (1)–(3), each of which has two associated boundary conditions. In AMPS, these three coupled equations are solved simultaneously to obtain a set of three unknown state variables at each point in the device: the local vacuum level, the electron and hole quasi-Fermi levels. From these three state variables, the free carrier concentrations $\left(n(x) = \frac{2}{\sqrt{\pi}} N_c F_{\frac{1}{2}}\left[-\frac{E_c(x) - E_F^n(x)}{kT}\right]\right.$ and $\left. p(x) = \frac{2}{\sqrt{\pi}} N_v F_{\frac{1}{2}}\left[-\frac{E_F^p(x) - E_v(x)}{kT}\right]\right)$, where N_c and N_v are the effective density of states in the conduction band and the valence band, respectively. k is the Boltzmann constant, T the temperature and $F_{\frac{1}{2}}(\xi)$ the Fermionic integral), fields $\left(E(x) = \frac{1}{q}\frac{d\Psi(x)}{dx}\right)$, currents, etc. can then be computed.

To solve these three coupled non-linear differential Eqs. (1)–(3), a finite difference scheme is utilized in AMPS. AMPS firstly breaks the structure of solar cell (the definition domain is $0 \leqslant x \leqslant L$) down into several slabs and major grid points, and then discretizes these differential equations into a set of algebraic equations. The Newton–Raphson method is used in AMPS to solve this set of algebraic equations.

Since most of the reported SnS thin films exhibit p-type electrical conductivity, the p-type SnS is used as the material of base. The structure as designed is shown in Fig. 1. The lifetime model is adopted in this work and the simulation is performed under AM1.5G illumination (100 mW cm^{-2}, 0.32–1.32 μm).

2.2. Parameters for simulations

The expressions of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys are listed in Table 1 and the values of SnS, $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ material parameters used in the simulations are shown in Table 2. Absorption coefficient $\alpha(\lambda)$ of SnS thin film used in this paper is the same as Ref. [34] and the minority electron lifetime is 0.8 μs [37]. For n-$In_xGa_{1-x}N$/p-SnS and n-$Al_xGa_{1-x}N$/p-SnS heterojunction solar cells, the minority electron lifetime strongly affects the overall efficiency since most of the light absorption occurs in the p-type layer. The electron and hole mobilities of SnS are 4.3 [37] and 130 cm^2 V^{-1} s^{-1} [1], respectively. The electron mobility, along with the minority electron lifetime, will determine the minority electron diffusion length which in turns affects the device efficiency. The surface recombination velocities are 2×10^4 cm s^{-1} [37].

Constant bowing parameters 1.43 and 0.69 are used for the band gaps of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$, respectively (see the expressions of band gaps in Table 1). The formulae of the relative permittivity and effective density of states in the conduction band and valence band are obtained from the linear interpolation of the corresponding parameters of InN and GaN. Absorption coefficient $\alpha(\lambda)$ of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ is the same as Ref. [38]. Hole lifetimes as high as 6.5, 5.4 ns and 20 ns have been observed in GaN, InN and AlN, respectively [39–41]. However, $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys are likely to have lower lifetimes due to compositional fluctuations, and therefore 1 ns minority hole lifetime was assumed [25]. The electron and hole mobilities were calculated

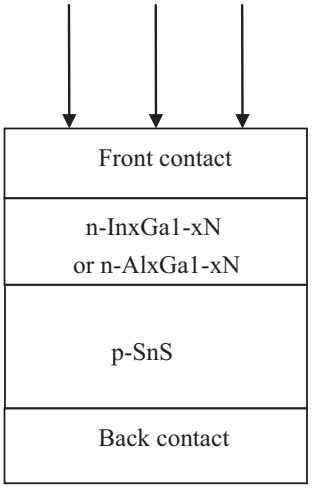

Fig. 1. Structure of InGaN/SnS and AlGaN/SnS heterojunction solar cells.