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GaAsP/Si tandem solar cells: Realistic prediction of efficiency gain by applying strain-balanced multiple quantum wells

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ABSTRACT

The combination of tunable direct bandgap III-V absorbers with active Si substrates promises high-efficiency tandem solar cells. To yield the ideal III-V bandgaps between 1.6 and 1.8 eV which is considered to achieve current matching with the Si bottom-cell, however, either a big lattice-mismatch or dilute nitrides had to be considered so far. Here, we propose a new structure for a two-terminal III-V-on-Si solar cell which bases on strain-balanced III-V multi-quantum wells (MQWs) embedded in a metamorphic GaAsP top-cell matrix. Strain-balanced MQWs extend the absorption edge to a longer wavelength and enable a reduction of the As content in the GaAsP metamorphic top-cell matrix. And accumulation of carriers in MQWs favors radiative recombination, which is beneficial for high efficiency while deep quantum wells lower the charge carrier collection efficiency. Here, we predict solar energy conversion efficiencies over 42.6% with an entire MQW as thin as 500 nm. The applied model takes into account the drawbacks of MQWs, such as limited light absorption and the bottleneck of charge carrier collection from the confinement.

1. Introduction

Integration of III-V semiconductors with Si substrates allows for significant cost reduction of photovoltaic [1] and water splitting devices [2,3] with very high conversion efficiency. In a tandem device, an active Si cell combined with a top absorber with a bandgap of 1.73 eV has the theoretical potential to achieve 45% conversion efficiency under one sun (in the idealized detailed balance limit) [4]. Classical III-V semiconductors, such as (In,Al,Ga)(As,P) [1,5,6], with such bandgaps in the desired range, are mostly realized at the lattice constant of Ge/GaAs or require dilution with nitrogen, such as Ga(As,P,N) [7–9], for lattice matched growth on Si. For the former, lattice mismatch is large which leads to high threading dislocation densities [6] or requires bonding approaches [1]. The latter strongly suffer from poor minority carrier diffusion lengths [7].

A realistic device concept for a high-efficiency two-terminal III-V-on-Si solar cell should consider III-V top absorbers with (i) direct bandgaps in the range of 1.6–1.8 eV, (ii) reduced lattice mismatch and advanced strain-balancing, (iii) high internal quantum efficiency, as well as (iv) reduced material consumption. The optimum top absorber bandgap of 1.73 eV [10] could, for example, be achieved with GaAsP alloys containing 75% of As [6,11]. However, 75% of As translates to a large lattice mismatch of 2.8% between the top cell and a GaP seed layer, which requires a thick graded buffer layer (4–5 μm) [11]. Incorporation of less As would decrease the lattice mismatch and by that the minimum buffer thickness; but it would also increase the absorption edge energy of the GaAsP top cell and by that reduce the device efficiency due to increased current mismatch to the Si subcell. To overcome this limitation, we propose a new structure: a GaAsP/Si two-junction solar cell with multi-quantum wells (MQWs) in the top cell, as shown in Fig. 1. As an example, $GaAs_{0.5}P_{0.5}$ is adopted as matrix of the top cell. The corresponding bandgap of 2.05 eV is not suitable for high efficiency solar energy conversion. However, by inserting MQW layers in the top cell, the absorption edge can be shifted to longer wavelengths [12–14] and thus the current mismatch with regard to the Si cell can be mitigated. $GaAs_{0.5}P_{0.5}$ can reduce the lattice mismatch to GaP to about 1.8% compared with 2.8% for $GaAs_{0.75}P_{0.25}$, and the thickness of the metamorphic buffer layer can be substantially decreased. In addition, MQWs facilitate the radiative recombination of carriers by concentrating carriers in narrow-gap wells [15], which in turn supresses non-radiative recombination and thus heat dissipation. In multi-junction cells, radiative recombination enhances luminescence coupling and

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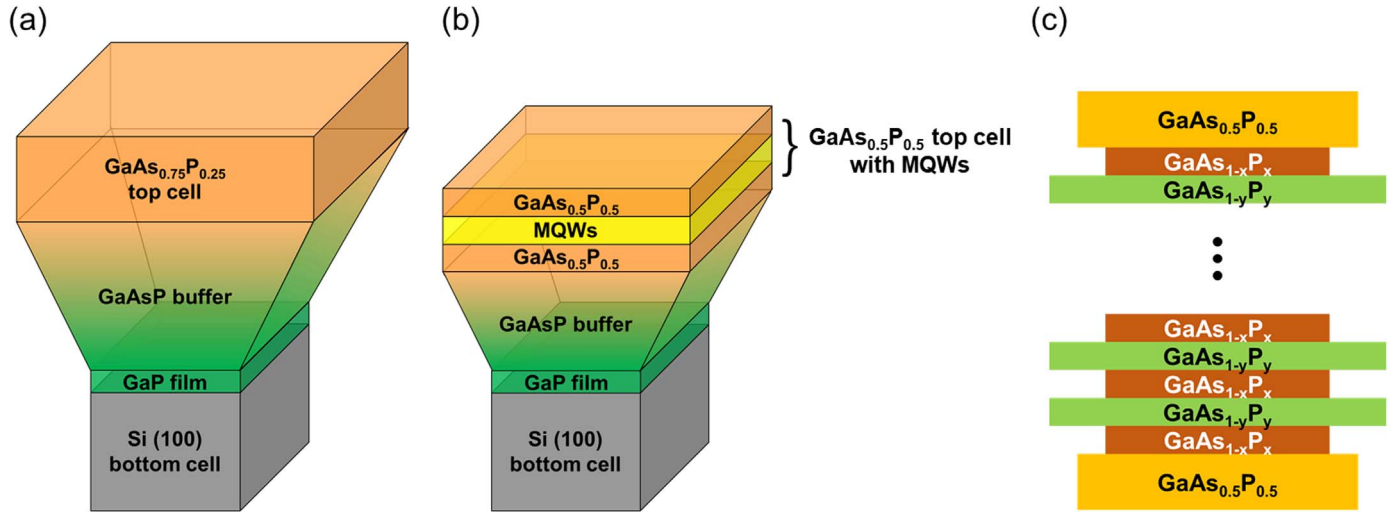

Fig. 1. Schematic of GaAsP/Si dual-junction solar cell with top cells containing (a) 75% of As and (b) 50% of As with multi-quantum wells (MQWs), respectively. (c) Structure of MQWs.

makes a cell more tolerant against current mismatch induced by spectrum fluctuations of the solar irradiation [16]. For on-Si cells, in which the crystal quality of III-V layers tends to be worse than the layers on native substrates, the efficiency of radiative recombination tends to be degraded significantly and the ability of MQWs to enhance radiative recombination will be quite vital for achieving high efficiencies with III-V on Si tandem solar cells.

In this paper, we present the new structure of GaAsP/Si two-junction solar cell with MQWs and estimate obtainable efficiency as a function of the structure of MQWs, such as the atomic content, thickness and stacking number. The model we apply is realistic in the sense that it takes the drawbacks of MQWs, such as limited light absorption and the bottleneck of carrier collection from the confinement states, into account.

2. Model for the efficiency prediction

2.1. Structure of the GaAsP top cell with MQWs

As mentioned in the previous section, $GaAs_{0.75}P_{0.25}$ top absorbers are required for conventional GaAsP/Si current-matched dual junction solar cells. The As content can be significantly reduced by applying MQWs embedded in the GaAsP layer. The amount of As incorporated into the host matrix is an important structural parameter for the overall efficiency. In this paper, we adopt $GaAs_{0.5}P_{0.5}$ as bulk host material of the top cell, which is arbitrarily chosen as a simple example. The efficiency predicted in this paper, therefore, is not the maximum efficiency as a result of global optimization, which needs to be pursued in future work.

For the MQWs, the content of wells and barriers are set to $GaAs_{1-x}P_x$ and $GaAs_{1-y}P_y$, respectively, and their thicknesses were set to L_W and L_B, respectively. Here, $x < 0.5 < y$ for strain balancing. The P content for the barrier, y, is determined to satisfy the strain-balancing condition, with the given P content in the well, x, and barrier thickness, L_B,

$$\frac{A_w L_w + A_B L_B}{L_w + L_B} = A_{bulk}, \tag{1}$$

where A_{bulk} is the lattice constant of the host $GaAs_{0.5}P_{0.5}$ layer. The thickness of a well, L_W, is fixed at 5 nm for simplicity although it is also an important structural parameter and its optimization is subject to future survey. The barrier thickness, L_B, is set as a variable because it significantly affects the efficiency of carrier collection and the total thickness of MQWs. A_W and A_B represent the lattice constants of well and barrier, respectively, which are obtained according to x and y on the basis of Vegard's law between GaAs and GaP.

It must be emphasized that L_W has only a small impact on the light absorption in the entire MQW structure. Although it is counterintuitive, the absorption coefficient in a well with significant carrier confinement is almost independent of its thickness for a photon energy range adjacent to its absorption edge, which is the functional energy range of quantum wells for our purpose. This physical principle implies that the light absorption near the absorption edge energy is almost proportional to the *number* of quantum wells, but not to their total thickness. Several experiments and theory supported this important design principle [17–19]. If multiple confinement states are included in a well, similar light absorption which is dependent on the number of wells takes place for each light absorption between the excited states. From the perspective of cost reduction, the thinner the MQW structure is, the less material is consumed and the crystal growth process takes the shorter time. We thus focus on thinner quantum wells as long as strong quantum confinement never prevents the absorption edge energy of MQWs from reaching the desired value for current matching in tandem configuration.

2.2. Assumptions for evaluating light absorption and photocurrent in MQWs

The bandgaps of the well and barrier were calculated taking into account the impact of strain, such as elastic stiffness, shear modulus and deformation potential. The band-edge energies were calculated following the method and parameters by Van de Walle [20], and all the parameters are indicated in Table 1. The quantum confinement energies were calculated using an effective-mass approximation for a rectangular confinement potential field, with an effective mass obtained using linear interpolation between GaAs and GaP where m_0 is the mass of an electron in vacuum.

There are several additional assumptions in the simulation.

(1) No optical loss in the metamorphic buffer layer and the GaP seed layer so that there is no performance degradation due to these layers.
(2) 100% light absorption in Si and $GaAs_{0.5}P_{0.5}$ matrix for the photon energy larger than the bandgap.
(3) The absorption coefficient corresponding to the transition between the ground states of the electrons and holes in a well was set to $3.2 \times 10^8\ cm^{-1}$, a value taken from the experimental result for InGaAs quantum wells [21], corresponding to 1.6% light absorption per a 5-nm-thick well and approximately 80% absorption in 100-period MQWs.
(4) The absorption between the excited states was considered. The