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Mechanically Stacked Triple-junction GaInP / GaAs / Si Solar Cell Simulation

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Mechanically stacked triple-junction GaInP / GaAs / Si solar cell is simulated by Silvaco TCAD computer software and compared to more conventional GaInP / GaAs / Ge mechanically stacked configuration. External quantum efficiency, I-V characteristics and basic I-V parameters are obtained to demonstrate the advantages of using the silicon active substrate as the bottom sub-cell instead of the germanium substrate based bottom sub-cell.

Keywords: Solar cell, Triple-junction, Mechanically stacked, GaInP / GaAs / Si, Silvaco TCAD.

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1. INTRODUCTION

Multi-junction solar cells are regarded as photovoltaic devices which provide the most efficient way to convert solar energy to electric power. Currently these devices are widely used in space and terrestrial solar power facilities. Modern multi-junction monolithic GaInP / GaAs / Ge solar cells demonstrate total conversion efficiency over 30 % under 1-sun illumination and over 40 % under concentrated solar light [1].

Multi-junction (cascade or tandem) solar cells exploit so named spectrum separation principle [2]. It is well known that single-junction solar cells can convert to electric power solar radiation with photon energy equal and above the semiconductor material band-gap. However, if the photon energy sufficiently exceeds the band-gap, excessive energy is lost to the lattice for heating instead of charge carrier generation. To achieve more conversion efficiency rate, several junctions of semiconductor materials with different band-gaps are stacked on top of one another decreasing the band-gap value from the top junction to the bottom one. This makes it possible to split solar energy spectrum into several sub-bands and to treat separately each sub-band with an appropriate semiconductor material. Each upper junction absorbs photons with energy higher than band-gap value but within only relatively narrow energy sub-band and allows all photons with lower energy to pass through it to the lower junction which can absorb photons with energy from next sub-band. The total spectral response and conversion efficiency of a multi-junction solar cell can be obtained as a sum of those characteristics of all individual junctions (sub-cells). There is no formal limitation to the number of sub-cells, but in practice increasing the number of junctions over four or five has no significant effect. The most used multi-junction solar cells consist of three junctions however, investigations towards involving more junctions to the solar cell design are in the progress [3].

There are two different approaches to construct multi-junction solar cells, namely mechanically stacking sub-cells on top of one another or monolithically growing junctions on one substrate. Mechanically stacked sub-cells are electrically connected each another with conductors forming two-, three-, or multi-terminal circuit with various connection ways. In monolithic multi-junction solar cells, different sub-cells are connected in series through tunnel diodes forming two-terminal construction. Both approaches have advantages as well as drawbacks. From the technological point of view, the straightforward process of growing a monolithic construction on one substrate is much simpler, less time and cost consuming then separate producing each sub-cell and assembling them in a mechanically stacked structure. That fact determines the domination of monolithic multi-junction solar cells over their mechanically stacked counterparts in modern solar energy facilities. However, monolithic cell growing technology requires lattice matching for semiconductor materials involved in a multi-junction solar cell and allows to obtain only two-terminal series connected construction where sub-cells should be current matched for effective energy conversion. At the same time, mechanically stacked solar cells are highly flexible and free from many limitations inherent to monolithic devices. First of all, they do not require lattice matching and can use various ways of multi-terminal electric connection allowing us to alleviate the demand for current matching which decreases the sensitivity of multi-junction cells to spectrum variations. Therefore, applying mechanically stacked multi-junction solar cells, one can make essentially simpler the choice of appropriate semiconductor materials and sub-cell parameters to get more effective energy conversion. It is obvious that technological drawbacks of mechanically stacked solar cell manufacturing process can be overcome in the nearest future and should not create obstacles for the further investigation of these potentially very effective devices.

The most widely applied multi-junction solar cell design is a triple-junction solar cell build by monolithic technology with GaInP as the top, GaAs – the middle, and Ge – the bottom sub-cells. These materials are almost lattice matched and therefore can be successfully grown on one substrate without defect creation. However, the band-gaps of the semiconductors under consideration are not optimal enough to ensure the second important requirement for multi-junction solar cells – current matching. Indeed, the band-gaps of

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GaInP, GaAs and Ge are 1.9 eV, 1.42 eV, and 0.66 eV, respectively. There are too big difference between band-gap values of GaAs and Ge, comparing to that of GaInP and GaAs. This fact means that the bottom sub-cell has to absorb photons with energy which sufficiently exceeds its band-gap value. Excessive energy photon absorption leads to entire solar cell overheating and current overproducing by the bottom sub-cell comparing to currents generated by the two upper sub-cells. The optimal band-gap value for the bottom sub-cell should be near 1 eV. However, lattice matched to GaInP and GaAs semiconductor materials with 1 eV band-gap and adequate photovoltaic properties have not been obtained. Widely used in solar energetic silicon has the necessary band-gap value near 1 eV but it is lattice mismatched with GaInP and GaAs. The 4 % difference in the lattice constant value between Si and GaAs leads to appearing high density of dislocations in the semiconductor grown on Si which results in deteriorating GaAs photovoltaic properties and reducing overall multi-junction cell performance. Aside this problem, Si is very suitable especially as an active substrate semiconductor material for multi-junction solar cells. Comparing to germanium, silicon has many advantages, such as high availability, low cost, good thermal conductivity, great wafer mechanical strength and large wafer diameter. Benefits of silicon as a prospective material for multi-junction solar cells stipulate numerous efforts of researchers to use it instead of germanium or incorporate it as an additional sub-cell between GaAs and Ge.

There are a few ways to overcome the main obstacle to applying silicon in multi-junction solar cells – lattice mismatching between Si and traditionally used in these devices semiconductor materials. The most common approach for reducing dislocation density is involving additional graded buffer layers between lattice mismatched sub-cells [4]. This can be fulfilled by growing stepwise or continuously graded buffer layer of Ge_xSi_{1-x} on Si substrate starting with a minimal Ge fraction and ending with a pure Ge. The main drawback of this approach is that the buffer layer should be at least 10 μm thick to obtain sufficient dislocation density reducing. A thick buffer layer between GaAs and Si leads to the thermo-mechanical fragility of the multi-junction structure. Second problem is associated with the poor transparency of the buffer layer within wavelength range where the silicon bottom sub-cell can effectively absorb and convert solar energy. This prevents using Si as an active sub-cell for energy conversion, though its advantages as a good substrate material are still maintained.

Recently, another very promising approach has been demonstrated – direct wafer bonding of Si and GaAs sub-cells. Generally, wafer bonding may be considered as a technological process where two thoroughly prepared wafers are brought into contact to each other forming connection due to van der Waals forces [5]. Using additional annealing, the connection can be strengthened by creating strong covalent bonds between the wafer interfaces. "Sticking" materials by wafer bonding makes it possible to connect semiconductors with any degree of lattice mismatch. In case of bonding lattice mismatched materials, defects caused by mismatching are located on the interface only and cannot propagate into semiconductor material spoiling its photovoltaic properties. A wafer-bonded GaInP / GaAs / Si triple-junction solar cell has been produced by Fraunhofer ISE researchers [6] revealing its high efficiency. GaInP / GaAs dual-junction solar cells were grown lattice-matched on a GaAs substrate by metal organic vapour phase epitaxy (MOVPE) and finally bonded to the preliminary prepared silicon bottom cell.

And, at last, the third approach is available – mechanically stacked sub-cells [7] instead of grown on one substrate monolithic multi-junction solar cell construction. Actually, mechanically stacked multi-junction cells are rather close to wafer-bonded cells because they require no lattice matching. However, wafer-bonded stack of sub-cells can only maintain the series-connected two-terminal configuration like conventional monolithically stacked multi-junction solar cells and therefore they are subject to the current-matching limitation. As mentioned before, mechanically stacked solar cells not only ensure the free choice of sub-cell materials including lattice-mismatched semiconductors such as GaAs and Si but also grant the great flexibility in sub-cell electrical connection methods.

In this paper a mechanically stacked GaInP / GaAs / Si solar cell is simulated by Silvaco TCAD [8] computer package and compared to more traditional GaInP / GaAs / Ge solar cell configuration. I-V characteristics and quantum efficiency are obtained for the individual sub-cells and the total triple-junction structure. This allows us to investigate how changing material of the bottom sub-cell from germanium to silicon influences on multi-junction cell photovoltaic characteristics.

2. SOLAR CELL STRUCTURES AND SIMULATION TOOLS

Two mechanically stacked solar cell structures shown in Fig. 1 are considered for the analysis and comparison. Both structures have identical top and middle sub-cells formed from thin films of GaInP and GaAs. Each of the sub-cells consists of uniformly doped emitter and base layers. Similarly to the monolithic design, window and back-surface field layers are applied on the top and the bottom of each sub-cell to create the barrier field for minority carriers and to reduce their surface recombination. However, for mechanically stacked sub-cells, these layers do not alleviate the problem of lattice mismatching as it would be for monolithic design, and they had been kept for the purposes of comparing. The bottom sub-cells are different for the two structures under study. Conventional Ge bottom sub-cell with GaAs window layer is used for the first structure and Si bottom sub-cell with amorphous a-Si window layer is applied for the second one. Thicknesses of the bottom sub-cells are the same in both cases. To minimize unavoidable optic losses inherent to mechanically stacked solar cells, transparent adhesive layers are located between sub-cells to bond them together. A virtual one-layer anti-reflecting coating (not shown in the figure) is applied for each sub-cell to reduce reflective losses. Aluminum contacts are attached to each sub-cell aligned throughout the multi-junction stack.

Individual contacts for each sub-cell create the multi-terminal configuration of electric connection which makes it possible to calculate spectral response and photovoltaic characteristics of separate sub-cells and estimate their contribution to overall multi-junction solar cell performance. Moreover, connecting the sub-cells in series, we can obtain two-terminal configuration for the simulation of the total mechanically stacked as well as wafer-bonded multi-junction solar cells.

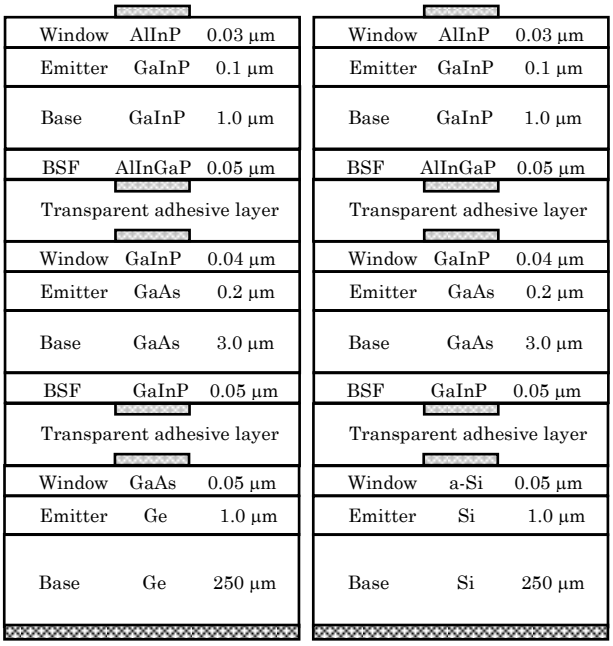

Fig. 1 – Schematic cross-section of mechanically stacked triple-junction solar cells: GaInP / GaAs / Ge solar cell (a), GaInP / GaAs / Si solar cell (b)

There are a number of works where similar multi-junction solar cell structures with silicon based bottom sub-cell are investigated. All works available to the authors are devoted to experimental researches focused mainly on technological aspects of multi-junction solar cell design. It should be noted that experimental researches provide the most reliable way to have a deep insight into physics of processes or devices under consideration. However, for experimental researches, it is hardly possible to analyze the influence of the large variety of structure parameters on device characteristics and to discover an optimal set of parameters for the best device performance. That is why, methods and tools of computer modeling gain growing importance in the design of semiconductor devices. There are a few computer softwares widely applied for the simulation of solar cells. One of them is Silvaco TCAD software package. Recently, this software has been applied to the simulation of the conventional GaInP / GaAs / Ge triple-junction monolithic solar cell [9]. In the present work, Silvaco TCAD is used to analyze mechanically stacked multi-junction solar cell configurations.

Silvaco TCAD is the sophisticated tool which capable to simulate any type of semiconductor devices in both two and three dimensional domains. Silvaco TCAD consists of two main components – process simulator ATHENA and device simulator ATLAS. ATHENA provides the physically-based simulation of technological processes used in semiconductor industry like ion implantation, diffusion, annealing, deposition, etching, etc. ATLAS makes it possible to predict the electrical behavior of semiconductor devices at specified bias conditions using different physical models – transportation, carrier statistic, mobility, recombination, etc.

In this paper we apply ATLAS software to determine solar cell electrical characteristics under the framework of the drift-diffusion transport model. This model consists of a set of fundamental equations including Poisson's equation, the continuity equations and the transport equations, which link together the electrostatic potential and the carrier concentrations inside a simulation domain.

Poisson's equation relates the electrostatic potential to the space charge density:

$$div(\varepsilon\nabla\psi) = -\rho\,, \tag{1}$$

where ε – the local permittivity, ψ – the electrostatic potential, ρ – the local charge density described in terms of the carrier and impurity concentrations.

The continuity equations for electrons and holes are defined as follows:

$$\begin{aligned} \frac{\partial n}{\partial t} &= \frac{1}{q} div\vec{J}_n + G_n - R_n \\ \frac{\partial p}{\partial t} &= -\frac{1}{q} div\vec{J}_p + G_p - R_p \end{aligned}, \tag{2}$$

where n and p – the electron and hole concentrations, q – the electron charge magnitude, $\vec{J}_n$ and $\vec{J}_p$ – the electron and hole current densities, G_n and G_p – the generation rates for electrons and holes, R_n and R_p – the electron and hole recombination rates.

The transport equations are the secondary equations which specify a physical charge transport model. The simplest drift-diffusion transport model determines the current densities in the continuity equations as:

$$\begin{aligned} \vec{J}_n &= qn\mu_n\vec{E}_n + qD_n\nabla n \\ \vec{J}_p &= qp\mu_p\vec{E}_p - qD_p\nabla p \end{aligned}. \tag{3}$$

where μ_n and μ_p – the electron and hole mobilities. $\vec{E}_n$ and $\vec{E}_p$ – the effective electric fields defined by the following expressions:

$$\begin{aligned} \vec{E}_n &= -\nabla\left(\psi + \frac{kT_L}{q}\ln n_{ie}\right) \\ \vec{E}_p &= -\nabla\left(\psi - \frac{kT_L}{q}\ln n_{ie}\right) \end{aligned}, \tag{4}$$

where T_L – the lattice temperature, n_{ie} – the effective intrinsic carrier concentration. D_n and D_p in equations (3) are the diffusion coefficients for electrons and holes, which can be expressed in terms of the mobilities using the Einstein relations:

$$D_n = \frac{kT_L}{q}\mu_n$$
$$D_p = \frac{kT_L}{q}\mu_p \quad . \qquad (5)$$

Carrier recombination is described by Shockley-Read-Hall model used concentration dependent minority carrier life-times and by Auger recombination model. Concentration dependent empirical mobility model, optical generation and recombination model and band-gap narrowing are also taken into account.

The set of the coupled non-linear partial differential equations (1)-(3) are discretized on the irregular mesh of nodes within considered device using the finite-difference method. Then, an obtained discrete system of algebraic equations is solved by Gummel and Newton non-linear iteration techniques.

3. RESULTS AND DISCUSSION

To simulate the solar cells shown in Fig. 1, command files with ATLAS statements have been composed to accurately describe the structure of mechanically stacked multi-junction solar cells under study. The command files define a finite-difference mesh, geometry parameters of regions loaded with homogeneous materials, doping levels for semiconductor materials, properties of all used materials including their optical data, models chosen for simulation etc. The simulation has been performed for normally directed solar light illumination with 1-sun intensity under AM0 conditions.

Simulation results are highly dependent on optical properties of the semiconductor materials involved in the solar cells. Refractive indexes and extinction coefficients for plenty of different materials are available from SOPRA NK database. However, this database mainly contains optical data for single elements and binary compounds. Most of ternary compounds such as GaInP are unavailable in the database. In such a case, required refractive indexes and extinction coefficients can be derived from corresponding optical data of known binary compounds by interpolation [10]. For example, optical data for GaInP have been obtained from available in the database n and k coefficients for GaP and InP using MATLAB program which realizes an interpolation algorithm.

Frequency responses of both GaInP / GaAs / Ge and GaInP / GaAs / Si mechanically stacked triple-junction solar cells have been calculated and displayed in Fig. 2 and Fig. 3 as the dependence of the external quantum efficiency on the optical wavelength. External quantum efficiency provides the essential information on the photocurrent produced by the sub-cells under solar light illumination at a particular wavelength. The thicknesses of the base layers with Ge and Si as the active substrate materials are varied from 50 μm to 550 μm. The frequency responses produced by the two upper sub-cells remain the same if the bottom sub-cell is changed from Ge to Si. So, we focus on the frequency response of the bottom sub-cell in the stack.

For both structures under consideration, the quantum efficiency of the bottom sub-cell decreases with decreasing the substrate thickness due to shortening an optical path length less than diffusion length available. This is more significant for large wavelength values because the charge carriers generated near the rear side of the base layer, where a "red" portion of the solar spectrum are absorbed, have less probability to be collected. Due to the absence of BSF layers in both bottom sub-cells, surface recombination increases at the rear sides of the sub-cells and therefore it contributes to decreasing the quantum efficiency in the "red" zone.

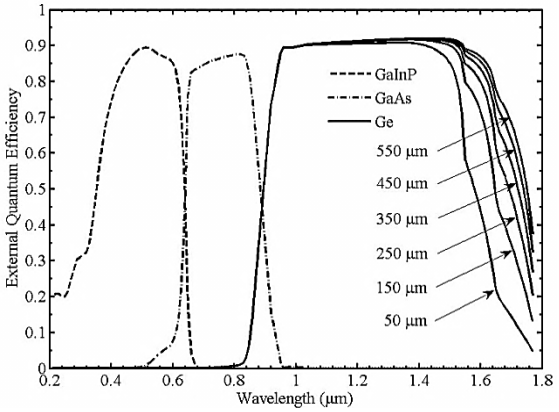

Fig. 2 – External quantum efficiency of GaInP / GaAs / Ge solar cell for various thicknesses of the bottom sub-cell base layer

Comparing external quantum efficiency behavior for Ge and Si substrate based sub-cells it can be observed that the Si sub-cell is more subjected to decreasing the quantum efficiency with substrate thinning. This difference in behavior appears due to larger absorption for Ge than Si, especially for the long wave range.

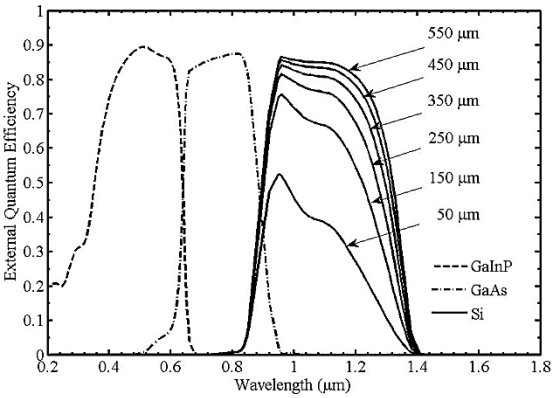

Fig. 3 – External quantum efficiency of GaInP / GaAs / Si solar cell for various thicknesses of the bottom sub-cell base layer

I-V characteristics of GaInP / GaAs / Ge and GaInP / GaAs / Si mechanically stacked triple-junction solar cells are shown in Fig. 4. The characteristics are demonstrated for each individual sub-cell in the stack as well as for the complete mechanically stacked structures under series connection of the sub-cells. The connection of the sub-cells in series limits the total current output of the mechanically stacked solar cell to the minimum current produced by the sub-cells. At the same time, the voltages of the individual sub-cells are added together to gain the total mechanically stacked solar cell voltage. Basic I-V parameters calculated from corresponding I-V characteristics are collected in the Table 1.

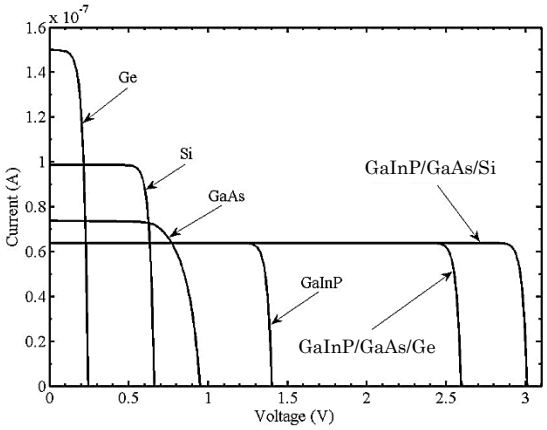

Fig. 4 – I-V characteristics of GaInP / GaAs / Ge and GaInP / GaAs / Si mechanically stacked solar cells

It can be seen that the upper GaInP sub-cell has the highest efficiency among the other sub-cells of both structures because its voltage is the highest although its current is the lowest. In the mechanically stacked solar cells, GaInP is the current-limiting sub-cell material at least for given layer thicknesses where the shadowing effect is not strong enough to greatly decrease the currents produced by the lower sub-cells.

Table 1 – I-V parameters for the mechanically stacked solar cells and their individual sub-cells

Parameters / Solar cells	J_{sc} [mA/cm^2]	V_{oc} [V]	η [%]
GaInP sub-cell	12.76	1.4	14.74
GaAs sub-cell	14.75	0.95	9.91
Ge sub-cell	29.92	0.24	4.95
Si sub-cell	19.73	0.66	10.9
GaInP / GaAs / Ge	12.76	2.59	29.6
GaInP / GaAs / Si	12.76	3.01	35.55

Conversely, both Ge and Si bottom sub-cells produce the highest current of the other sub-cells. But they have the relatively low efficiency because their voltage is too low. High current values produced by these sub-cells individually do not influence on the multi-junction solar cell performance because the total current is limited by the upper sub-cells. Comparing Ge and Si bottom sub-cells, one can note that Ge sub-cell voltage is much smaller than this one of Si. Open circuit voltage of Si sub-cell is nearly three times as much than that of Ge sub-cell. Accordingly, the efficiency of Si sub-cell is twice as much than that of Ge sub-cell resulting in the total efficiency of GaInP / GaAs / Si mechanically stacked solar cell equals 35.5 % versus 29.6 % for GaInP / GaAs / Ge solar cell. So, the choice of Si as the bottom sub-cell semiconductor material with larger band-gap than that of Ge and consequently with higher open-circuit voltage results in near 20 % increase of overall solar cell efficiency. Si sub-cell produces one-third less current than that of Ge leaving nevertheless the main current overproducer in the stack. To come near current matching for the actual parameters of the solar cells, the upper sub-cells have to be thickened to increase their energy conversion and to shade the bottom sub-cell. But in case of Si bottom sub-cell, current matching can be approached with thinner upper sub-cells saving costly semiconductor materials.

4. CONCLUSION

The substitution of germanium by silicon as an active substrate material in multi-junction solar cells is very attractive due to silicon availability, low cost, and mechanical strength. One of the possible ways to incorporate Si in a multi-junction solar cell together with common GaInP and GaAs semiconductors is to apply mechanically stacked sub-cell design or sub-cell wafer-bonding. In this paper GaInP / GaAs / Si mechanically stacked triple-junction solar cell has been analyzed and compared to its GaInP / GaAs / Ge counterpart using Silvaco TCAD computer software. Spectral responses have been studied for different thicknesses of Si as well as Ge base layers and I-V characteristics have been obtained to determine basic I-V parameters such as short-circuit current, open-circuit voltage and efficiency. It has been demonstrated that changing the bottom sub-cell material from conventional Ge to Si allows us to raise solar cell efficiency from 29.6 % to 35.5 % under 1-sun illumination.

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