RAISING THE EFFICIENCY CEILING WITH MULTIJUNCTION III-V CONCENTRATOR PHOTOVOLTAICS


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ABSTRACT: In this paper, we look at the question "how high can solar cell efficiency go?" from both theoretical and experimental perspectives. First-principle efficiency limits are analyzed for some of the main candidates for high-efficiency multijunction terrestrial concentrator cells. Many of these cell designs use lattice-mismatched, or metamorphic semiconductor materials in order to tune subcell band gaps to the solar spectrum. Minority-carrier recombination at dislocations is characterized in GaInAs inverted metamorphic solar cells, with band gap ranging from 1.4 to 0.84 eV, by light I-V, electron-beam-induced current (EBIC), and cathodoluminescence (CL). Metamorphic solar cells with a 3-junction GaInP/ GaInAs/ Ge structure were the first cells to reach over 40% efficiency, with an independently confirmed efficiency of 40.7% (AM1.5D, low-AOD, 240 suns, 25°C). The high efficiency of present III-V multijunction cells now in high-volume production, and still higher efficiencies of next-generation cells, is strongly leveraging for low-cost terrestrial concentrator PV systems.

Keywords: III-V Semiconductors, Concentrator Cells, High-Efficiency, Multijunction Solar Cell, Gallium Arsenide Based Cells, Lattice-Mismatched, Metamorphic

1 INTRODUCTION

Most concentrator photovoltaic systems are now being built using III-V multijunction cells, due to the unprecedented efficiency levels that this cell technology has reached. III-V multijunction cells with a 3-junction metamorphic GaInP/ GaInAs/ Ge structure were the first solar cells of any type to reach over 40% efficiency in 2006, with an independently confirmed efficiency of 40.7% (AM1.5D, low-AOD, 240 suns, 25°C) [1], and inverted metamorphic 3-junction cells have now reached 40.8% [2]. The rapid growth in cell efficiency in recent years [1-12], and its strongly leveraging effect to lower system cost, both motivate reexamination of the upper limits of cell efficiency. In this paper, we look at the question "how high can cell efficiency go?" from both theoretical and experimental perspectives.

2 EFFICIENCY LIMITS

In Fig. 1 below, first-principle efficiency limits are analyzed for some of the main approaches for achieving new heights in performance for terrestrial multijunction solar cells. Many of these architectures are basically ways to achieve more nearly optimal combinations of subcell band gaps in multijunction cells for conversion of the terrestrial solar spectrum, combinations that are not straightforward to reach in standard lattice-matched multijunction cell structures. These cell architectures include: cells using metamorphic (MM) subcell materials, designs with 4 or more subcells, wafer-bonded multijunction cells, and inverted metamorphic (IMM) terrestrial concentrator cells.

Figure 1. Fraction of available power in the solar spectrum used by subcells in a 3-junction cell, showing the impact of various fundamental efficiency losses. The effects of concentration and of more nearly optimal 3- and 6-junction band gap designs are shown toward the right.
The fundamental loss mechanisms of non-absorption of low-energy photons, thermalization of electrons and holes to their respective band edges, and the difference between band edge energies and quasi-Fermi levels, and their impact on the available power density in the solar spectrum, are plotted for several of the main candidate designs for next-generation terrestrial concentrator cell designs in Fig. 1. Beginning at the left hand side, the portions of power in the terrestrial solar spectrum used by each subcell in a 3-junction 1.9-eV GaInP/ 1.4-eV GaInAs/ 0.67-eV Ge is shown, based on the subcell band gaps. The power of each subcell is traced through the non-absorption, thermalization, and band edge to Fermi level offset losses mentioned above. Increasing the concentration level, to 500 suns in the figure, is an effective way to reduce the band edge to Fermi level loss.

At the right of Fig. 1, the increased power densities available with two more advantageous band gap combinations for partitioning the solar spectrum are shown: a 3-junction inverted metamorphic cell with a 1.9-eV GaInP/ 1.4-eV GaInAs/ 1.0-eV Ge structure, and an AlGaInP/ GaInP/ AlGaInAs/ GaInAs/ GaInNAs/ Ge 6-junction terrestrial concentrator cell.

Figure 2 plots these fundamental efficiency losses, as well as the losses due to series resistance and grid shadowing, and ideal fill factor and subcell current matching, as a function of the indium content in subcell 2 of an upright metamorphic 3-junction GaInP/ GaInAs/ Ge solar cell, plotting the relative importance of each mechanism as the indium content and lattice mismatch is increased, and the band gap of the top two junctions is correspondingly decreased.

![Figure 2](image_url)

**Figure 2.** Fundamental power losses in 3-junction upright metamorphic GaInP/GaInAs/Ge terrestrial concentrator cells at 500 suns (50.0 W/cm²), 25°C, and series resistance and grid shadowing losses, as a function of the indium content of the GaInAs middle subcell.

3 DISLOCATIONS IN METAMORPHIC SEMICONDUCTOR MATERIALS

Semiconductor compositions with the desired band gaps for solar photovoltaic energy conversion can be grown easily enough, but many of those compositions are not lattice-matched to any readily available epitaxial growth substrate. As a result, the crystal lattice of these lattice-mismatched materials can become riddled with dislocations, which mediate Shockley-Read-Hall (SRH) recombination in the cell and lower cell voltage. The formation of dislocations tends to become more severe the greater the amount of lattice mismatch to the substrate, and constitutes the main barrier to using lattice-mismatched compositions freely to reach the optimal band gaps for maximum terrestrial solar cell efficiency.

The formation of dislocations can be mitigated by the use of a metamorphic buffer layer, in which the lattice-constant is transitioned to a different value than that of the growth substrate. In the metamorphic buffer, a layer or series of layers with graded composition is grown, allowing the strain in those graded layers to relax by dislocation formation in the metamorphic buffer, so that relaxed semiconductor layers can be grown with a much reduced density of dislocations on the virtual substrate with a new lattice constant formed by the metamorphic buffer. These low-defect-density layers with relaxed crystal structure grown on top of the metamorphic buffer are also termed metamorphic, such as the metamorphic active subcell regions in a multijunction solar cell, since they benefit from the metamorphic buffer. In many multijunction cell architectures, such as inverted metamorphic multijunction solar cells, sunlight must pass through the metamorphic buffer to subcells beneath, so it is advantageous to use high-band-gap semiconductors such as AlGaInAs or GaInP to form a transparent metamorphic buffer region.

It is important to quantify the degree to which the metamorphic buffer can suppress dislocation density in metamorphic cells to better understand how metamorphic materials can be used in multijunction solar cells. Since there are a wide variety of multijunction cell designs in which metamorphic cells can be used, such as 4-, 5-, and 6-junction cells, wafer-bonded solar cells, and others, and the optimal band gaps vary widely for these different designs, it is valuable to know how the dislocation density varies as a function of composition and lattice mismatch to the substrate. Furthermore, since it is the electron-hole recombination mediated by the dislocations that influences solar cell performance, it is important to measure the recombination activity of dislocations in metamorphic materials. The recombination activity of a single dislocation is found to vary widely depending on degree of lattice mismatch, semiconductor composition, e.g., In content in GaInAs, as well as in GaInP contrasted to GaInAs, and dislocation type, e.g., dislocation clusters vs. dislocation dipoles. This variation in the recombination activity of dislocations has a profound effect on the efficiency of metamorphic solar cells, separate from the effects of dislocation density alone.

To investigate the properties of dislocations in a relevant metamorphic device structure, single-junction inverted metamorphic GaInAs solar cells were grown on a transparent AlGaInAs metamorphic buffer by metal-organic vapor-phase epitaxy (MOVPE), on 100-mm Ge substrates. A range of GaInAs inverted solar cell base compositions were grown, from ~2 to 44% indium, corresponding to band gaps from 1.39 to 0.84 eV, and lattice mismatch from ~0 to 3.1%. Solar cell parameters such as open-circuit voltage Voc and external quantum efficiency (EQE) were measured by illuminating the inverted cells through a grid on the back surface, to characterize the cells in a state close to their as grown condition, without the complicating factors introduced by
the usual process for bonding inverted epitaxial solar cells to a handle substrate, removing the growth substrate to expose the sunward surface, and completing device fabrication on the now right-side-up cell. Dislocation density was measured on the same solar cells for which I-V characteristics were measured, by cathodoluminescence (CL) and electron-beam-induced current (EBIC) at the National Renewable Energy Laboratory (NREL). In addition, the recombination activity of the dislocations was measured by CL, by comparing the lowest photon intensity corresponding to the dislocation to the background intensity in parts of the base away from dislocations. A schematic of the inverted solar cell test structure is shown in Fig. 3.

Figure 3. Schematic of the single-junction inverted metamorphic solar cell test structure used in the experiment, with illumination from the back surface of the inverted cell, for the case with a 0.97-eV GaInAs base.

Images formed by EBIC are shown in Fig. 4, for inverted solar cells with band gaps of 1.39, 1.10, 0.97, and 0.84 eV as measured by EQE, corresponding to indium compositions in the GaInAs base of approximately 2% (nearly lattice matched), 23%, 33%, and 44%, respectively. The expected increase in dislocation density with increasing lattice mismatch can be seen, as well as a change in the type of dislocation as the In content is increased. At the lowest indium concentration at 1.39 eV, dislocations are seen in pairs, or dipoles, presumably propagating from a single defect deeper in the epitaxial material. For the 1.1-eV sample, two different types of dislocations are seen, a darker type on the EBIC scan and a lighter type with less severe recombination activity. In the 0.97 and 0.84 eV samples with highest indium content, alignment of the dislocations in streaks, aligned to the crystal lattice can be seen, perhaps due to interactions with the cross-hatch patterns seen in the surface topography of these highly lattice-mismatched samples.

Figure 4. Electron-beam-induced current (EBIC) images of dislocations in inverted metamorphic solar cells with band gaps of (a) 1.39 eV; (b) 1.10 eV; (c) 0.97 eV; and (d) 0.84 eV, as described in the text.
Figure 5 plots the band gap measured by EQE, Voc from illuminated I-V measurements at approximately one sun, and the band gap-voltage offset \( \text{Woc} = (E_g/q) - \text{Voc} \) as a function of indium content and lattice mismatch for four different GaInAs inverted metamorphic solar cells. The band gap-voltage offset provides a measure of crystal quality and minority-carrier lifetime since it is a measure of how far the electron and hole quasi-Fermi levels are from their respective band edges [1], with smaller values of Woc indicating lower recombination. Woc shows some variation in the different inverted MM solar cell samples, but is roughly constant over a wide range of In compositions and lattice mismatches. Dislocation densities measured by EBIC are also plotted in Fig. 5, and show a nearly linear dependence on In composition and lattice mismatch with respect to the Ge substrate.

Figure 6 plots the cathodoluminescence photon intensity for 4 compositions of inverted metamorphic GaInAs solar cells.

Figure 7. Dislocation density measured by EBIC, overall photon intensity measured by cathodoluminescence (CL), and average carrier loss measured for dislocations as described in the text, for 4 GaInAs inverted metamorphic solar cell compositions.

The impact of this average recombination activity at dislocations in different GaInAs matrices can be roughly gauged by combining the dislocation density \( N_{\text{disloc}} \) measured by EBIC with the fractional carrier loss at dislocations \( f_{\text{disloc}} \) measured by CL, and assuming an approximate radius \( r_i \) over which a dislocation can influence recombination of carriers. Choosing an approximate radius of influence of \( \approx 1 \mu m \), corresponding to the dark area surrounding each dislocation, allows one to calculate a total fractional carrier loss across the sample \( f_{\text{total}} \):

\[
f_{\text{total}} = N_{\text{disloc}} \pi r_i^2 f_{\text{disloc}} \tag{2}
\]

which reflects the recombination activity of dislocations as well as the dislocation density. This relative measure of total fractional carrier loss has a roughly exponential dependence on In composition and lattice mismatch. A more accurate analysis would include a measurement of the effective radius of influence of the dislocations on recombination from the CL data at each In composition.
Figure 8. Dislocation density, average carrier loss providing a measure of recombination activity of each dislocation, and relative total carrier loss from dislocations taking into account number of dislocations, average recombination activity for a single dislocation, and assuming an approximate radius of influence of ~1 μm surrounding each dislocation.

4 IMPACT ON PRODUCTION CELLS

Spectrolab is developing new high-efficiency terrestrial concentrator cell pathways based on metamorphic and other high-efficiency cell architectures in several research and development programs. In the DOE Solar America Initiative program at Spectrolab, the goals are to implement the efficiency advances in prototype cells to reach average production concentrator cell efficiencies of 40% in 2010, and 43% by 2015, as shown in Fig. 9.

To reach still higher efficiencies, it is important to push up the theoretical efficiency ceiling through the use of the more nearly optimal band gap configurations of next-generation multijunction cell designs. In this way, even with roughly constant offsets between production and best-experimental efficiencies — as well as between best-experimental and theoretical — higher production efficiencies can be realized by using a cell design with higher theoretical efficiency limits. These next-generation terrestrial multijunction cell designs include: an upright metamorphic approach, as in the record 40.7% efficient cell design; 4-junction GaInP/AlGaInAs/GaInAs/Ge terrestrial concentrator cells; inverted metamorphic terrestrial concentrator cells with a GaInP/1.4-eV GaInAs/1.0-eV GaInAs 3-junction structure, shown in schematic in Fig. 10; and wafer-bonded 3- to 6-junction cells. As the gaps between production and best-experimental efficiencies become narrower, through refinement of multijunction solar cell growth and fabrication processes, going to wholly different multijunction cell designs with a higher theoretical efficiency ceiling becomes the only approach that can keep cell efficiencies advancing at the encouraging rate of about one absolute percent increase in efficiency per year seen in the 1999-2006 time frame.

Figure 9. Average production terrestrial concentrator solar cell efficiency goals in the DOE Solar America Initiative program at Spectrolab.

Naturally, one fruitful approach to reaching these very high production efficiencies is to continue to minimize the gap between average production efficiency and the best experimental cell performance, and the gap between these champion experimental cells and theoretical efficiency.

Figure 10. Schematic diagram of an inverted metamorphic terrestrial concentrator 3-junction GaInP/1.4-eV GaInAs/1.0-eV GaInAs solar cell, showing removal of the growth substrate from the sunward surface.

Figure 11 plots light I-V data at 170-230 suns (17-23 W/cm²) from one series of terrestrial concentrator cell device structure experiments, showing that high efficiencies are possible for a range of current and voltage design tradeoffs. Figure 12 plots the independently confirmed light I-V data from the record 40.7%-efficient metamorphic 3-junction concentrator cell reported earlier [1]. It is worth noting that this first solar cell to reach over the 40% efficiency milestone was based on metamorphic materials, in this case in an upright configuration with metamorphic 56%-In GaInP and 8%-In GaInAs subcells 1 and 2.
5 SUMMARY

The backdrop of physically allowable efficiencies based on fundamental efficiency limits provides a framework for the practical best-experimental efficiencies likely to be reached, as well as for the efficiency of mass-produced terrestrial concentrator cells. A careful accounting of these fundamental losses not only provides better prediction, but points the way for creative new multijunction configurations that minimize first-principle losses. Most of these new designs make use of semiconductors with unconventional compositions and lattice constants to achieve the optimum band gaps for conversion of the solar spectrum, with theoretical efficiencies >70%, and practical cell efficiencies of 45% or even 50%. With metamorphic materials figuring so prominently in new types of 3- to 6-junction solar cells with band gaps tuned to the solar spectrum, a deeper understanding of the processes of nucleation, propagation, and the variable recombination activity of dislocations in these metamorphic materials is essential.

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