Directions for Further Development of GaAs/CuInSe \textsubscript{2} Thin Film Tandem Cells

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Summary

Multijunction thin film solar cells utilizing GaAs and CuInSe \textsubscript{2} as semiconductor absorbers are rapidly developing, becoming a viable technology for space power systems with an unparalleled combination of high efficiency, low mass, and high radiation tolerance. The prospect for evolutionary improvement of this type of cell towards efficiency of \(\approx 30\%\) and specific power greater than 1 kW/kg while retaining the attribute of high radiation tolerance are good. Limitations of the present configuration and possible avenues for circumventing these problems are presented.

Introduction

In the nine years since the first demonstration of both thin film CuInSe \textsubscript{2} cells and the CLEFT process for fabricating thin film single crystals of GaAs, tremendous strides have been made in the maturation of both technologies. Each has been shown capable of fabricating large-area films [refs. 1 & 2] of high quality as attested to by the recent achievement of tandem efficiency greater than 20\% AM0. Bereft of excess high density semiconductor bulk, the practical lower mass limit for these cells is determined by their support structures, shifting the focus of mass reduction efforts to the module, panel, and array level designs. It is the conjunction of this inherently low mass with both high efficiency and high radiation tolerance, however, which enables the array designer to capitalize on this asset, since the array size may be smaller relative to other options and still guarantee adequate End-Of-Life (EOL) system power.

Although there there is little benefit at the systems level of further reducing the direct cell mass, improvements in EOL specific power may still be achievable by reducing mass contributions of associated components, increasing Beginning-Of-Life (BOL) efficiency, and increasing radiation tolerance. The remainder of this paper will comprise a discussion of means by which this may be achieved.

Bandgap Engineering of AlGaAs/CuInSe \textsubscript{2} Tandem Cells

CuInSe \textsubscript{2} is a ternary chalcopyrite semiconductor, which unlike the ternary alloy of AlAs and GaAs, Al\textsubscript{x}Ga\textsubscript{1-x}As, has a fixed bandgap (to first order). Its attributes that commend its use in space photovoltaics include one of the highest known absorption coefficients of any semiconductor [ref. 3], an optimum bandgap for the lower cell in two-junction tandems [ref. 4], and an exceptional tolerance to high-energy particulate radiation [ref. 5]. In a heterojunction with CdZnS it has shown excellent minority carrier collection, achieving internal quantum efficiencies nearing unity [ref. 6]. Its greatest liability is the low voltage of the cell compared to its bandgap. Conventional diffusion-current dominated ideal photodiodes with this bandgap would be predicted to exhibit open-circuit

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References:

1. Ref. 1
2. Ref. 2
3. Ref. 3
4. Ref. 4
5. Ref. 5
6. Ref. 6
voltages as high as $\approx 560$ mV [ref. 7] at comparable current levels to those of CuInSe$_2$/CdZnS in tandem with GaAs, compared to an observed $V_{oc} \approx 380$ mV. The reasons for this low voltage are an active area of research and debate in the literature, but it is most likely due to interface states acting as a recombination pathway for minority carriers [ref. 8 and 9], with deep level defects in the bulk possibly playing a role [ref. 10]. Improvements in CuInSe$_2$ cell voltage are most likely to result from refinement of the component materials and their fabrication processes. Certainly any success in improving the voltage performance of CuInSe$_2$ cells will contribute to the overall performance of the tandem. In practice this plays a crucial role, however, in selection of the optimum bandgap for the Al$_x$Ga$_{1-x}$As upper cell.

Hybrid Tandem Cells

The present state-of-the-art thin film solar cells are hybrid or mechanically stacked, each component cell fabricated independently before being incorporated into the tandem. There are numerous advantages to this approach, foremost being flexibility. A range of bandgaps for upper and lower cell are possible, permitting their design to be tailored to the requirements of the mission and properties of the available materials. Other advantages include series/parallel bus interconnect flexibility and less sensitivity to temperature effects on orbit. The principal disadvantage of hybrid tandems is the increased complexity of fabrication and interconnection concomitant with its increased flexibility.

Previously published calculations [Table 1 in ref. 11] for Al$_x$Ga$_{1-x}$As shallow homojunction cells in four-terminal tandem configuration with CuInSe$_2$ cells showed minor ($\leq 0.7\%$) losses in BOL efficiency for increasing $x \leq 0.3$ though it still remained over 22% in all cases. This was due in part to assumptions regarding minority carrier lifetimes in Al$_x$Ga$_{1-x}$As subsequently shown to be overly pessimistic [ref. 12]. This was also a consequence, however, of the upper cell with increased bandgap losing current to the lower cell operating at less than ideal voltage. These considerations indicate that the aluminum content ($x$-value) that maximizes BOL efficiency for Al$_x$Ga$_{1-x}$As/CuInSe$_2$ tandems is less than the theoretical optimum of $x \approx 0.3$ calculated for ideal cells in reference 4. Radiation degradation effects, however, provide a countervailing influence on the optimum choice of aluminum content in the upper Al$_x$Ga$_{1-x}$As cell for four-terminal tandem operation. Since both CuInSe$_2$ and Al$_x$Ga$_{1-x}$As cells are more radiation resistant than GaAs cells [refs. 5, 13, and 14], and available data suggest that the radiation effects in Al$_x$Ga$_{1-x}$As are less severe for higher aluminum content [refs. 15 and 12] in the range $x \leq 0.37$, EOL efficiency maximization for many missions will increase the optimum value of $x$ over the optimum for BOL efficiency.

Another available path for improved efficiency in the hybrid tandem configuration is the use of a monolithic Al$_x$Ga$_{1-x}$As/GaAs tandem cell mechanically stacked on a CuInSe$_2$ cell. The choice of bandgaps is near optimum in this case for $x \approx 0.4$ [ref. 4], and practical efficiencies near 30% should be achievable.

Monolithic Thin Film Tandem Cells

Certain components to the successful fabrication of high efficiency monolithic tandems appear important. Current matching (at some optimum point in the mission lifetime) is necessary. The calculations reported in reference 11 predict BOL current matching at an upper cell absorber layer composition near Al$_{0.2}$Ga$_{0.8}$As, a modest aluminum content for which high quality films should be
readily achievable. Fabrication of an Intercell Ohmic Contact (IOC) is one of the persistently vexing difficulties in the fabrication of monolithic tandem cells. One solution used successfully in references 16 and 17 has been fabrication of a tunnel junction between upper and lower cells, but steps must be taken to avoid interdiffusion at the highly-doped, abrupt interface which can result in a resistive, highly compensated transition region which destroys the tunnel junction.

The lattice mismatch between CuInSe₂ and GaAs is less than 2% and the chalcopyrite symmetry of CuInSe₂ is a ternary equivalent of two GaAs zincblende crystal unit cells distorted slightly along the connecting c-axis. Heteroepitaxial single-crystal cell structures in material systems with comparable or greater amounts of lattice mismatch have been widely pursued, utilizing the techniques of advanced epitaxial growth technology such as graded composition lattice-matching transition layers and superlattice dislocation propagation filters. Given the nearly perfect carrier collection efficiency in polycrystalline CuInSe₂ cells, it appears that the minority-carrier electron transport in the material is tolerant of the native defects in the material. This may relax the requirement for crystalline perfection compared to III-V based materials. Study of the epitaxial growth of CuInSe₂ on GaAs has been reported in reference 18 and references therein.

I propose a novel solution [ref. 19] to these problems which capitalizes on the unique abilities of the CLEFT process and properties of the constituent materials. Figure 1 shows a cross-sectional schematic of the proposed structure. Fabrication is begun by the overgrowth of a GaAs CLEFT buffer on a GaAs wafer. Next, the AlₓGa₁₋ₓAs cell is fabricated in an 'inverted' configuration with the emitter nearest the buffer. Since this is the first device structure deposited, it can be deposited at high temperature to improve the quality of the AlₓGa₁₋ₓAs without degrading the tunnel junction. The proposed tunnel junction is formed between a p⁺-AlₓGa₁₋ₓAs and subsequently deposited n⁺-ZnSe layer. This ZnSe layer is compositionally and dopant graded to form an n-Cds₂Se contact to the final semiconductor p-CuInSe₂ absorber layer. Back contacts are deposited, the film is cleaved from the bulk GaAs wafer, front contacts formed and the excess buffer layer removed before AR coating completes the device.

The technology for fabrication of the tunnel junction has only recently been demonstrated, although to the author's knowledge it has not yet been done. High-quality single-crystal ZnSe and GaAs lattice-matched ZnSe₀.₅Se₀.₉₉ can be deposited on GaAs or AlₓGa₁₋ₓAs by numerous processes including MBE [ref. 20] and MOCVD [ref. 21]. Recently, effective doping of ZnSe, long an elusive goal of research, has been demonstrated [ref. 22]. In fact, degenerate doping of ZnSe to levels of 2.8 x 10¹⁶cm⁻³ with Hall mobilities of 140cm²/V-s and resultant resistivity of 10⁻³Ω-cm have been reported at a temperature of 318°C [ref. 23], quite adequate for tunnel junction fabrication without significant interdiffusion. Though a reliable direct measurement of the ZnSe/GaAs conduction band offset is unavailable, application of the theory of Tersoff in reference 24 predicts a valence band offset of 0.04 volts, essentially zero within the accuracy of the theory, though this calculation is only thought to be accurate to within ±0.15 volts. Certainly recent evidence suggests that the density of interfacial surface states between ZnSe and GaAs can be very low [ref. 25].

Perhaps the greatest challenge in fabricating the monolithic AlₓGa₁₋ₓAs/CuInSe₂ tandem is the formation of a high-quality heterojunction between the CdZnSSe interconnect region and the subsequently deposited CuInSe₂ absorber. The results reported in reference 18 for deposition of epitaxial single crystal CuInSe₂ on GaAs suggest that careful control of composition can produce p-type films without a Cu-rich second phase which appears to minimize Cu out-diffusion. This is important since Cu forms a deep level trap in the ZnSe, ZnS, and CdS binary constituents of the interconnect alloy. It would appear from this previous work that the key to successful fabrication of this device is the development of a lower temperature process for the fabrication of high quality CuInSe₂ than
the elemental codeposition process presently employed. Given the widespread technological effort to
develop lower temperature processes for the deposition of other important semiconductor materials,
usually for the same reason of minimizing interdiffusion in multilayered structures, I believe the
solution of this problem to be feasible.

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Figure 1.- Schematic of monolithic AlGaAs/CuInSe$_2$ cell.