

High-Efficiency Solar Cell Concepts: Physics, Materials, and Devices

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ABSTRACT

Over the past three decades, significant progress has been made in the area of high-efficiency multijunction solar cells, with the effort primarily directed at current-matched solar cells in tandem. The key materials issues here have been obtaining semiconductors with the required bandgaps for sequential absorption of light in the solar spectrum and that are lattice matched to readily available substrates. The GaInP/GaAs/Ge cell is a striking example of success achieved in this area. Recently, several new approaches for high-efficiency solar cell design have emerged, that involve novel methods for tailoring alloy bandgaps, as well as alternate technologies for hetero-epitaxy of III-V's on Si. The advantages and difficulties expected to be encountered with each approach will be discussed, addressing both the materials issues and device physics whilst contrasting them with other fourth-generation solar cell concepts.

1. Objectives

The phenomenon of giant bandgap “bowing” that has recently been observed in several III-V dilute nitride alloys offers the exciting promise of increasing the flexibility in choice of semiconductor bandgaps available with specified lattice constants. However, the poor solubility of nitrogen and the degradation of electrical transport properties that these materials exhibit seriously limit their usefulness. Novel ideas for overcoming these limitations are discussed below.

2. Technical Approach

The solubility of an acceptor (donor) impurity can be significantly increased using the method of simultaneous co-doping with a donor (acceptor). Using this approach, it has been possible to increase the doping concentrations of As donors and Ga acceptors in Si by almost 3 orders of magnitude [1]. This motivates the use of a similar strategy for overcoming the limitations of isoelectronic doping encountered with N in GaAs and in GaP. Bismuth is the heaviest element of the III-V semiconductor family. Like N, the size and core electronic structure of Bi are significantly different from those of P and As. It is therefore reasonable to expect that Bi could also behave as an isoelectronic impurity in some III-V semiconductors and show unusual alloy properties. Bi indeed forms pseudo-donor bound states in GaP located above the valence-band maximum [2]. Although it has been predicted theoretically that the isolated Bi impurity does not form a bound state in GaAs, it yet remains to be investigated experimentally [3,4]. Even if isolated Bi does not form a bound state (like N in GaAs),

the perturbation produced by the Bi localized potential and the surrounding lattice relaxation could significantly perturb the electronic band structure of GaAs and induce a variety of effects qualitatively resembling those observed for GaAs:N. Being complementary in size and potential, Bi and N could compensate for the strong local perturbation each introduces, which is detrimental to carrier mobility, while preserving other desirable effects such as the strong bowing of the bandgap. Also, simultaneous N and Bi doping allows one to reduce the bandgap energy at a fixed lattice constant. Thus, Bi and N co-doping is of interest for exploring the possibility of enhancing the solubility of the individual isoelectronic dopants, significantly lowering the bandgap of GaP and sharpening the absorption edge as compared to the soft edge that is obtained by doping with N alone.

3. Results and Accomplishments

GaAsBi layers between 0.2 and 0.3 μm thick were grown using molecular-beam epitaxy. Details on the growth conditions can be found in Ref. [5]. The Bi concentration was determined from Rutherford back scattering [5]. X-ray diffraction asymmetrical maps revealed that most of the samples were almost completely strained to match the GaAs in-plane lattice constant. Modulated electroreflectance was used to measure the energy of the optical transitions in the vicinity of the fundamental bandgap of GaAsBi. The linearized dependence of the bandgap transition energy with respect to the bandgap of GaAs is $-88 \text{ meV}/\% \text{ Bi}$, which is close to half that for GaAsN; but relative to the strain induced by the isoelectronic dopant, these values are comparable. Isoelectronically co-doping N and Bi in GaAs should result in significantly larger bandgap reductions whilst allowing for counterbalancing the lattice-mismatch strain. In the case of GaP, the direct-bandgap characteristics of the heavily isoelectronically co-doped material, combined with the ability to grow GaP:N:Bi epitaxially on Si substrates, would introduce exciting possibilities for use of this material in fabricating photonic devices such as solar cells, light-emitting diodes, and lasers. These features are of value for designing semiconductor alloys for use in multijunction solar cells. One example of this is the quadruple-junction GaInP/GaAs/GaAsN:Bi/Ge solar cell. In this case, it is hoped that simultaneous codoping of GaAs with both N and Bi should lead to a larger band gap lowering with a smaller amount of Nitrogen whilst concomitantly permitting the lattice mismatch strain to be eliminated. It is expected that such cells should be theoretically capable of achieving efficiencies exceeding 40%. Another example is the GaPN:Bi/Si solar cell in Fig. 1. Here, isoelectronic co-doping makes it possible to grow a

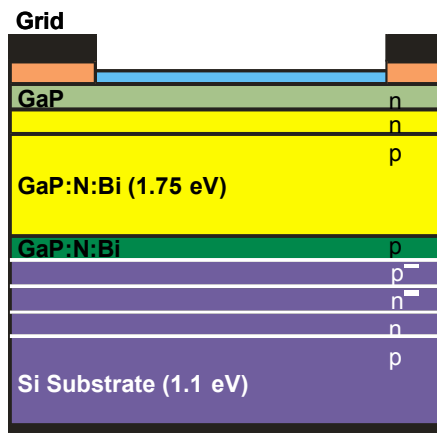


Fig. 1. GaPNBi/Si solar cell.

lattice-matched III-V semiconductor alloy with an optimal bandgap and strong absorption coefficient on inexpensive silicon substrates. The monolithic structure can be tailored close to the ideal requirements for a two-junction cell.

An alternative approach to get around the difficulty of synthesizing monolithic tandem cells with silicon serving as a substrate and bottom cell is to use the compliant-superstrate technique developed by Motorola [6-8]. A roughly 140-Å-thick epitaxial film of strontium titanate (SrTiO_3), henceforth referred to as STO, is grown on a (001) Si substrate using molecular-beam epitaxy. The film grows with the [110] edge of the perovskite-oxide aligned along the [100] cubic edge of Si whereby the 1.7% size-mismatch between the substrate and the film is accommodated elastically. Because its thickness is below the critical-thickness limit, the STO film is of high quality. A roughly 8-Å-thick layer of SiO_2 is observed to inadvertently exist between the STO/Si interface. GaAs has a cubic lattice that is 4% larger than that of Si. Because SiO_2 has a noncrystalline structure typical of a glass, it yields to any external strain at the growth temperature for GaAs. When a thick GaAs epitaxial layer is grown on the 140-Å thin STO layer, the STO layer elastically adjusts to the 2.3% larger GaAs lattice, with the SiO_2 layer accommodating itself to the mismatch between the STO and the SiO_2 layer. This enables epitaxial growth of high-quality GaAs on Si substrates. An advantage of the Si/ SiO_2 /STO superstrate is that it allows for the growth of III-V semiconductor alloys on a superstrate with a flexible lattice constant that can be easily adjusted anywhere between that of Si and that of GaAs. It allows for solar cell configurations to be optimized by designing the subcells from alloys with bandgaps that are closer to the ideal for two- and three-junction tandem solar cell structures [9]. An example of this is the GaInP/GaAsP/Si solar cell illustrated in Fig. 2 [10].

4. Conclusions

Si is far more abundantly available and its substrates are cheaper and more environmentally benign than GaAs substrates. Si also has greater mechanical strength and

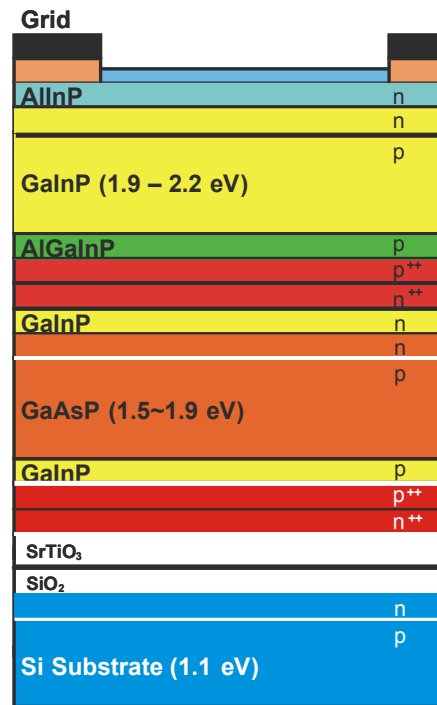


Fig. 2. GaInP/GaAsP/Si solar cell

thermal conductivity than GaAs. The isoelectronic co-doping approach or the compliant-substrate approach for Si-based high-efficiency photovoltaics are far more realistic in terms of near-term success than other fourth-generation concepts.

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REFERENCES

- [1] S. P. Withrow, O. W. Holland, S. J. Pennycook, J. Pankove, and A. Mascarenhas, *Mat. Res. Soc. Symp. Proc.* **157**, 143 (1990).
- [2] F. Trumbore, M. Gershenson, and D. Thomas, *Appl. Phys. Lett.* **9**, 4 (1966).
- [3] H. Hjalmarson, *Phys. Rev. Lett.* **44**, 810 (1980).
- [4] J. Shen, S. Ren, and J. Dow, *Phys. Rev. B* **42**, 9119 (1990).
- [5] S. Tixier, M. Adamcyk, T. Tiedje, S. Francoeur, A. Mascarenhas, P. Wei, and F. Schiettekatte, *Appl. Phys. Lett.* **82**, 2245 (2003).
- [6] J. Ramdani, R. Droopad et al., *Appl. Surface Science* **159-160**, 127 (2000).
- [7] Z. Tu, J. Ramdani, et al, *J. Vac. Sci. Technol.* **B 18**(4), 2139 (2000).
- [8] R. Droopad, Zhyi Yu, J. Ramdani, et al. *J. Crystal Growth* **227-228**, 936(2001).
- [9] NREL IR # 01-52, Patent pending
- [10] NREL IR # 02-11, Patent pending

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