Wurtzite InGaN/GaN Quantum Dots for Intermediate Band Solar Cells

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***Abstract* — Wurtzite InGaN quantum dots in GaN are investigated for intermediate band solar cells. A global limiting power conversion efficiency of 44% is predicted through detailed balance calculations with full freedom of allowed subgap transitions. We consider cylindrical quantum dots, predicting band structures using an 8-band k.p model, including deformation potential and piezoelectric fields from induced lattice strain. Taking the energy levels from the k.p model as absorption cutoffs in the detailed balance calculation, we determine the best device efficiency possible as a function of indium fraction and dot size. For small dots, of size ≈ 50 Å and indium fraction ≈ 0.7, efficiencies up to 42% are in principle attainable under 1-sun illumination.**

I. Introduction

The intermediate band solar cell (IBSC) has the potential to surpass the single junction solar cell efficiency limit of 31%, which is known as the Shockley-Queisser limit. Under a 1-sun 6000 K black-body (BB) illumination, the IBSC has a theoretical efficiency limit of 47% [1]. An intermediate band (IB) material has three bands: a valence band (VB), a conduction band (CB) and an IB energetically between the VB and the CB (see Figure 1). An IBSC operates with a voltage that is only limited by the large band gap while still being able to absorb photons that have smaller energy than the band gap by use of the IB enabling high efficiencies. We investigate the use of wurtzite InGaN QDs in GaN for IBSCs. The band gap of $In_yGa_{1-y}N$ varies from 0.78 to 3.51 eV, giving great flexibility in matching the solar spectrum. InGaN IBSC devices have already been made and the IB effect verified [2]. We give an optimal design for the growth of InGaN dots in GaN based on making optimal use of each absorbable photon.

First, detailed balance calculations (DBCs) are used to predict the limiting efficiencies of the QD system, indicating the ideal electronic transition energies. The QD electronic structure is calculated using an 8-band k.p model which include strain and piezoelectric field effects. The QD size and indium fraction are optimized based on the DBC target energies. Efficiencies of 42% under 1-sun black-body illumination could in principle be attained.

II. Detailed Balance Calculations

Detailed balance calculations allow the prediction of limitting efficiencies under the idealized assumptions of infinite carrier mobilities and all recombination being radiative [3]. We also assume each photon is only absorbed by the lowest energy transition possible, with transition energies E_{vc}, E_{oi}, E_{ic} defined in Figure 1. This assumption minimizes thermalization losses. We set the valence to conduction band transition E_{vc} to 3.51 eV, the band gap of bulk GaN. In this model, the quantum dot and host hole populations are thermally connected, which is represented by the two populations having a shared quasi-Fermi level. This assumption allows for the thermal escape of holes without the need for additional photon absorption. A maximal efficiency of 44% is found under a 1-sun 6000 K BB spectrum illumination as shown in Figure 2. However, E_{oi} and ΔE cannot be chosen independently in the InGaN QD system. We study the potential efficiencies of the InGaN QD system in the next section.

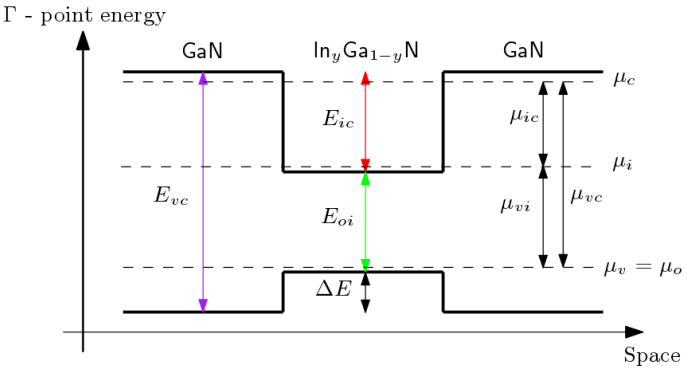

Fig. 1. E_{vc}, E_{oi} and E_{ic} are the allowed optical transition thresholds in the InGaN QD in bulk GaN system. The QD and host material hole populations have a shared quasi-Fermi level $\mu_v = \mu_o$, indicating that they are thermally connected. The operating voltage is given by the host material quasi-Fermi level splitting $\mu_{vc} = \mu_c - \mu_v$.

III. Electronic Structure Calculations

To know the possible optical transitions in a QD, we perform electronic structure calculations using an 8-band k.p model under an envelope function approximation [4, 5]. This model calculates single-electron energy levels in the vicinity of the Γ-point in k-space while imposing periodic boundary conditions [6]. We are interested in the properties of single dots and so have chosen unit cells large enough to ensure no dot-to-dot couplings. InGaN dots are typically lens shaped [7, 8], however we approximate them as cylinders for theoretical convenience, see Figure 3. Lattice-mismatch-driven strain

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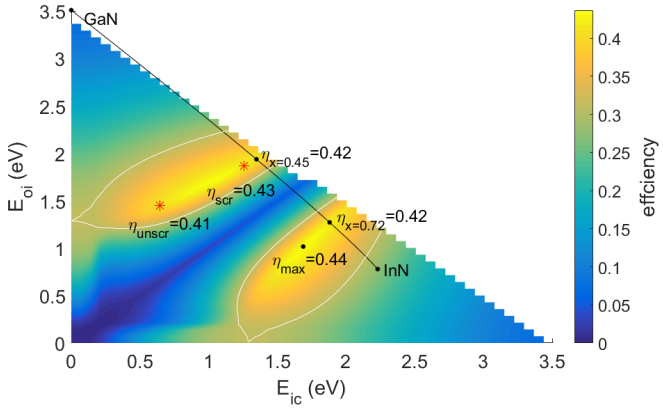

Fig. 2. Efficiency map of the InGaN QD in GaN system for varying subgap photon absorptions where E_{vc}=3.51 eV. E_{oi} and E_{ic} are the subgap transition, which are shown in Figure 1. The results are symmetric about the E_{oi}=E_{ic} line. The white contour indicates the Shockley-Queisser limit of 31%. The black line is the efficiency of bulk InGaN in bulk GaN. Black marker at 44% indicates the maximal efficiency of the QD system. Red markers indicate the realizable QD systems based on the electronic structure optimisation using the k.p model. η_{unscr} (η_{scr}) include (exclude) the piezoelectric fields.

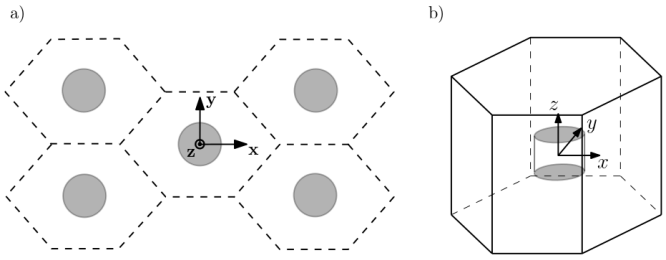

Fig. 3. (a) QD superlatice modeled by electronic structure calculations. Grey areas are indium-rich regions of the QD and white space the GaN host material. (b) Unit cell containing a single cylindrical quantum dot.

is calculated under a continuous medium approximation [9] and incorporated into the k.p model via deformation potentials [6].

Strain driven and spontaneous piezoelectric fields are calculated by solving Maxwell's equations assuming only dielectric screening [4, 9]. The piezoelectric fields can be quite intense in nitride materials [10, 11], leading to additional confinement and spatial separation of electron and hole states [7], which can lead to poor optical absorption due to small wavefunction overlap. To minimize this spatial separation, we have chosen to study dots having a radius of 25 Å and height of 50 Å. The piezoelectric fields can also be reduced through free-carrier screening [7] and thus also reduce the spatial state separation. We study the cases with zero and full piezoelectric fields, expecting that an experimental device would be in between.

The dot geometry fixed, we optimize over the indium fraction to achieve the highest efficiency possible with absorption threshold energies put into the DBCs (Figure 2). The unscreened case is found to have an optimal efficiency of $\eta_{unscr} = 41\%$ with an indium fraction of 0.72 and the fully screened case reaches $\eta_{scr} = 42\%$ with an indium fraction of 0.80. We note that both efficiencies are similar, but on opposite sides of the global maximum of 44%. Since a real device is expected to have some metallic screening, its limiting efficiency may lie somewhere in between, closer to the global efficiency maximum while maintaining a similar ideal indium fraction. Achieving QDs with such high indium is difficult, but we believe it would lead to the highest efficiencies.

IV. Conclusion

InGaN IBSCs have the potential to significantly surpass the Shockley-Queisser limit. Optimized InGaN quantum dots indicate the need for small quantum dots with high indium fraction. Partial screening of piezoelectric fields by free carriers would potentially increase performance.

Acknowledgments

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