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Effect of Interface Properties on the Electrical Characteristics of InGaN-based Multijunction Solar Cell

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Summary

The InGaN ternary alloy has the potentiality to achieve high efficiency solar cells: tunable bandgap in the whole solar spectrum, high absorption coefficient, high stability and radiation tolerance. These very promising characteristics make InGaN potentially ideal for designing and developing next-generation high-efficiency thin films solar cells. However, challenging issues remain to address: (i) the difficulty to elaborate sufficiently thick monocrystalline InGaN layers with a high Indium content; (a) the high defects density and the spontaneous and piezoelectric polarizations; (iii) the p-doping which remains difficult to master. In this report, we use rigorous optimization approach based on state-of-the-art optimization algorithms to investigate the effect of defects and polarization (spontaneous and piezoelectric) on a double junction InGaN solar cell. A better understanding of the mechanisms involved in the heterostructure has a crucial impact on the design and elaboration of high efficiency InGaN thin films solar cells which require, in particular, a precise control of the Tunnel Junction elaboration which is still very challenging.

Double Junction InGaN Solar Cell: Effect of Spontaneous/Piezoelectric Polarization and Defects

DOUBLE JUNCTION INGAN SOLAR CELL STRUCTURE

SIMULATION PARAMETERS

→ Illumination : 1 Sun with AM 1.5G Solar Spectrum.

→ InGaN Bandgap, Affinity, Effective density of states, Permittivity, Absorption, SRH, Auger and direct recombination, Band discontinuity, Tunneling current, Polarization/Piezoelectric parameters, ...: taken from literature or extrapolated from GaN and InN experimental data.

Parameters	InN	GaN
Bandgap (eV)	0.7	3.42
Affinity (eV)	5.6	4.1
Carrier lifetime (ns)	1	1
Permittivity	15.3	8.9
N_c (cm ⁻³)	$9.1 \cdot 10^{17}$	$2.3 \cdot 10^{18}$
N_v (cm ⁻³)	$5.3 \cdot 10^{19}$	$4.6 \cdot 10^{17}$
Absorption	Extracted from experimental data [3]	
Mobility	Caughey-Thomas Model [4]	
Refractive Index	Adachi Model [5]	

[3] G. Brown, J. Ager III, W. Walukiewicz, J. Wu, *Finite element simulations of compositionally graded InGaN solar cells*, *Solar Energy Materials and Solar Cells* 94 (3) (2010) 478–483.

[4] F. Schwierz, *An electron mobility model for wurtzite GaN*, *Solid State Electronics* 49 (6) (2005) 889–895.

[5] A. B. Djurisic, E. H. Li, *Modeling the optical constants of hexagonal GaN, InN, and AlN*, *Journal of Applied Physics* 85 (5) (1999) 2848–2853.

DEFECTS AND POLARIZATION PARAMETERS

→ InGaN crystal structure: Wurtzite with Gallium or Nitrogen polarity. This polarity generates a spontaneous polarization creating an accumulation of charges at the InGaN surface.

→ Lattice mismatch induces strain and piezoelectric polarization. This polarization may either reduce or enhance the total polarization.

→ Without external polarization, the total polarization of the heterostructure is the sum of the spontaneous and piezoelectric polarizations:

$$P_{total} = P_{sp} + P_{pz} = P_{sp} + 2 \left(\frac{a_s - a_0}{a_0} \right) \left(e_{31} - \frac{c_{13}}{c_{33}} e_{33} \right)$$

$$P_{sp}^{In_xGa_{1-x}N} = x P_{sp}^{InN} + (1-x) P_{sp}^{GaN} - bx(1-x)$$

The spontaneous polarization bowing factor is taken equal to 0.038 C/m² [6].

[7]	InN	GaN
e_{31} (C/cm ²)	-0.41	-0.34
e_{33} (C/cm ²)	0.81	0.67
c_{13} (GPa)	94	100
c_{33} (GPa)	200	392
P_{sp} (C/cm ²)	-0.042	-0.034

The epitaxy of InGaN on lattice-mismatched substrates induces a high density of active defects at the heterointerface and in the bulk. Experimentally studied defects using DLTS, Photocurrent, Photoluminescence... e.g. [8]:

Indium Content (%)	Defects Energy vs E_c (eV)		Concentration (cm ⁻³)	
7	1.4	2.9	?	$1.4 \cdot 10^{16}$
10	1.5	2.8	10^{15}	$1.7 \cdot 10^{16}$
22	1.4	2.6	$7.5 \cdot 10^{15}$	$3.1 \cdot 10^{16}$
27	1.6	2.4	$4 \cdot 10^{15}$	$6 \cdot 10^{16}$

[6] F. Bernardini, V. Fiorentini, *Nonlinear behavior of spontaneous and piezoelectric polarization in III-V Nitride alloys*, *Physica Status Solidi (a)* 190 (1) (2002) 65–73.

[7] J. Piprek, *Semiconductor Optoelectronic Devices: Introduction to Physics and Simulation*, Academic Press, 2013.

[8] E. Gur, F. Akyol, S. Krishnamoorthy, S. Rajan, S. A. Ringel, *Deep level defects in N-rich and In-rich InGa_{1-x}N: In composition dependence*, *Superlattices and Microstructures* 99, 2016, 67-71.

SIMULATION METHODOLOGY

Cell optimized by a method using nonlinear optimization algorithms to calculate the set of parameters maximizing the efficiency [1]. This method and the resulting software we developed [2] permit to simultaneously optimize a large set of parameters (twelve parameters for the double junction solar cell) taking automatically into account their interdependence while drastically reducing the computing time when compared to the classical method where only one parameter is varying at a given time. The used backend simulator engine is Silvaco® Atlas.

[1] S. Ould Saad Hamady, A. Adaine, N. Fressegeas, *Numerical simulation of InGaN Schottky solar cell*, *Materials Science in Semiconductor Processing* 41 (2) (2016) 219–225.

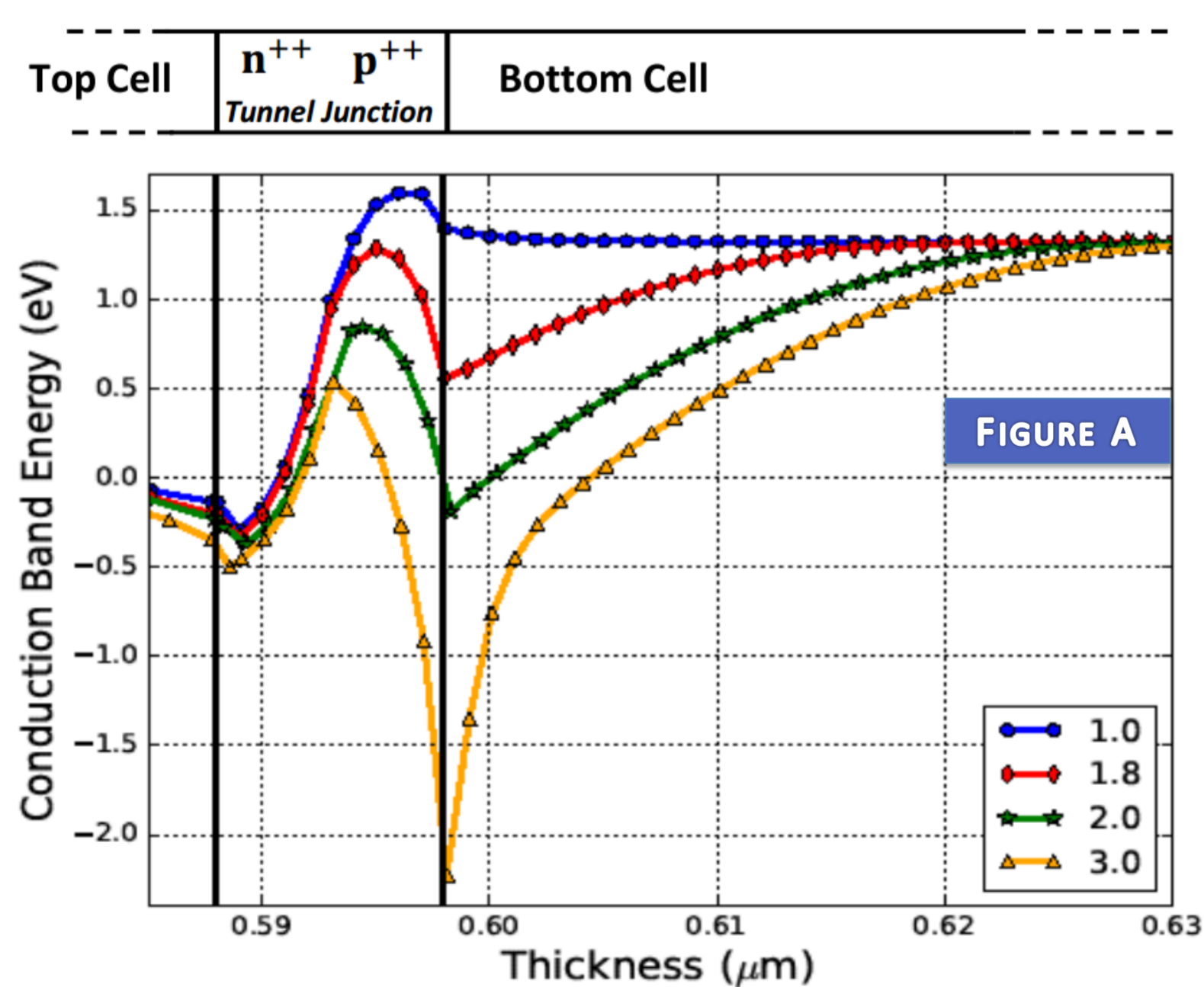
[2] SLALOM – Open-Source Solar Cell Multivariate Optimizer, to be released soon.

SPONTANEOUS/PIEZOELECTRIC POLARIZATION AND DEFECTS EFFECTS

Optimal InGaN double junction solar cell parameters giving efficiency of about 25%

InGaN Top Cell					InGaN Tunnel Junction					InGaN Bottom Cell					GaN	
Indium Content (%)	P-Doping (cm ⁻³)	N-Doping (cm ⁻³)	P-Thickness (μm)	N-Thickness (μm)	Indium Content (%)	P-Doping (cm ⁻³)	N-Doping (cm ⁻³)	P-Thickness (μm)	N-Thickness (μm)	Indium Content (%)	P-Doping (cm ⁻³)	N-Doping (cm ⁻³)	P-Thickness (μm)	N-Thickness (μm)	N-Doping (cm ⁻³)	N-Thickness (μm)
40	$8.04 \cdot 10^{18}$	$2.38 \cdot 10^{16}$	0.010	0.580	50	$5.00 \cdot 10^{19}$	$5.00 \cdot 10^{19}$	0.005	0.005	59	$2.51 \cdot 10^{18}$	$1.00 \cdot 10^{17}$	0.570	0.010	$1.00 \cdot 10^{19}$	0.160

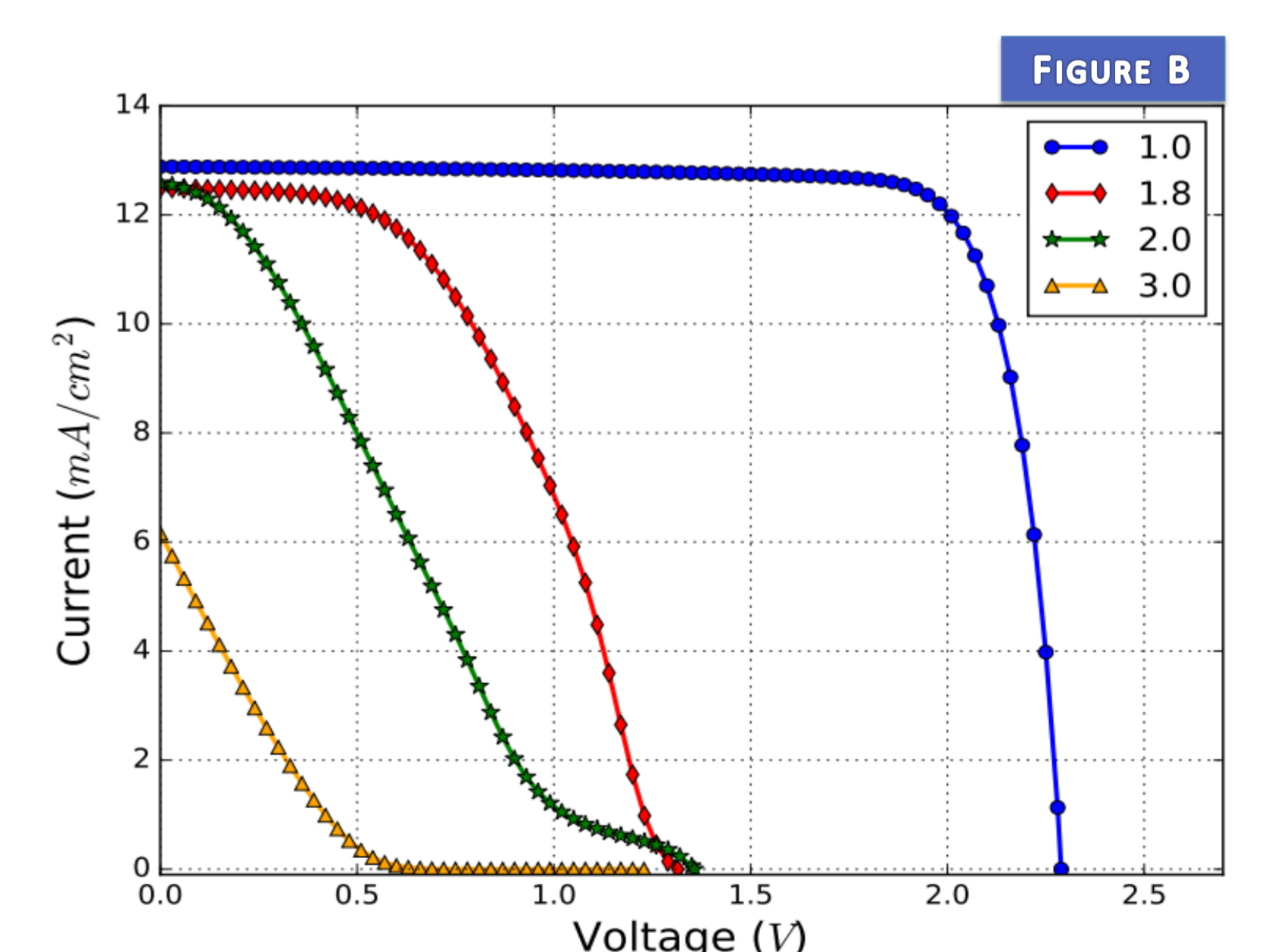
Efficiency = 25% less than what previous theoretical works predicted (35%) → comprehensive and empirical models (Absorption, Mobility, Recombination, Tunneling, Bandgap narrowing, etc.) → Effective result tightly linked to the actual device realization.



SPONTANEOUS/PIEZOELECTRIC POLARIZATION

Conduction band in the Tunnel Junction region (FIGURE A) and current-voltage characteristic (FIGURE B) variation with respect to the total (spontaneous + piezoelectric) polarization. The normalized polarization value of 1.0 corresponds to the nominal value in C/m² extrapolated from experimental data for GaN and InN. The polarization is increased up to 3 times its nominal value.

Polarization in the Tunnel Junction region → bands bend → charges accumulate at the interface and induce electric field in the direction opposite to that of the PN junction → “parasitic diode” in the double junction solar cell. This “parasitic diode” induces a decrease of the solar cell open-circuit voltage and, if the induced field is greater than that of the cell, a decrease of the short-circuit current.



DEFECTS AT TOP / TUNNEL JUNCTION / BOTTOM HETEROINTERFACES

Photogeneration and recombination rate distribution (FIGURE C) and effect of deep defects located in Top and Bottom Cells bulk (FIGURE D) and located at the Tunnel Junction heterointerfaces (FIGURE E) on the efficiency. The role of the Tunnel Junction is crucial in the multijunction InGaN solar cell by enhancing the current matching between the top and bottom cells and drastically reducing the voltage loss. It is very sensitive to the interface deep defects: the decrease of the efficiency begins at a defect concentration as low as 10¹² cm⁻³, while the effect of bulk deep defects becomes noticeable only at 10¹⁶ cm⁻³. The recombination rate around the Junction Tunnel (FIGURE C) illustrates this effect.

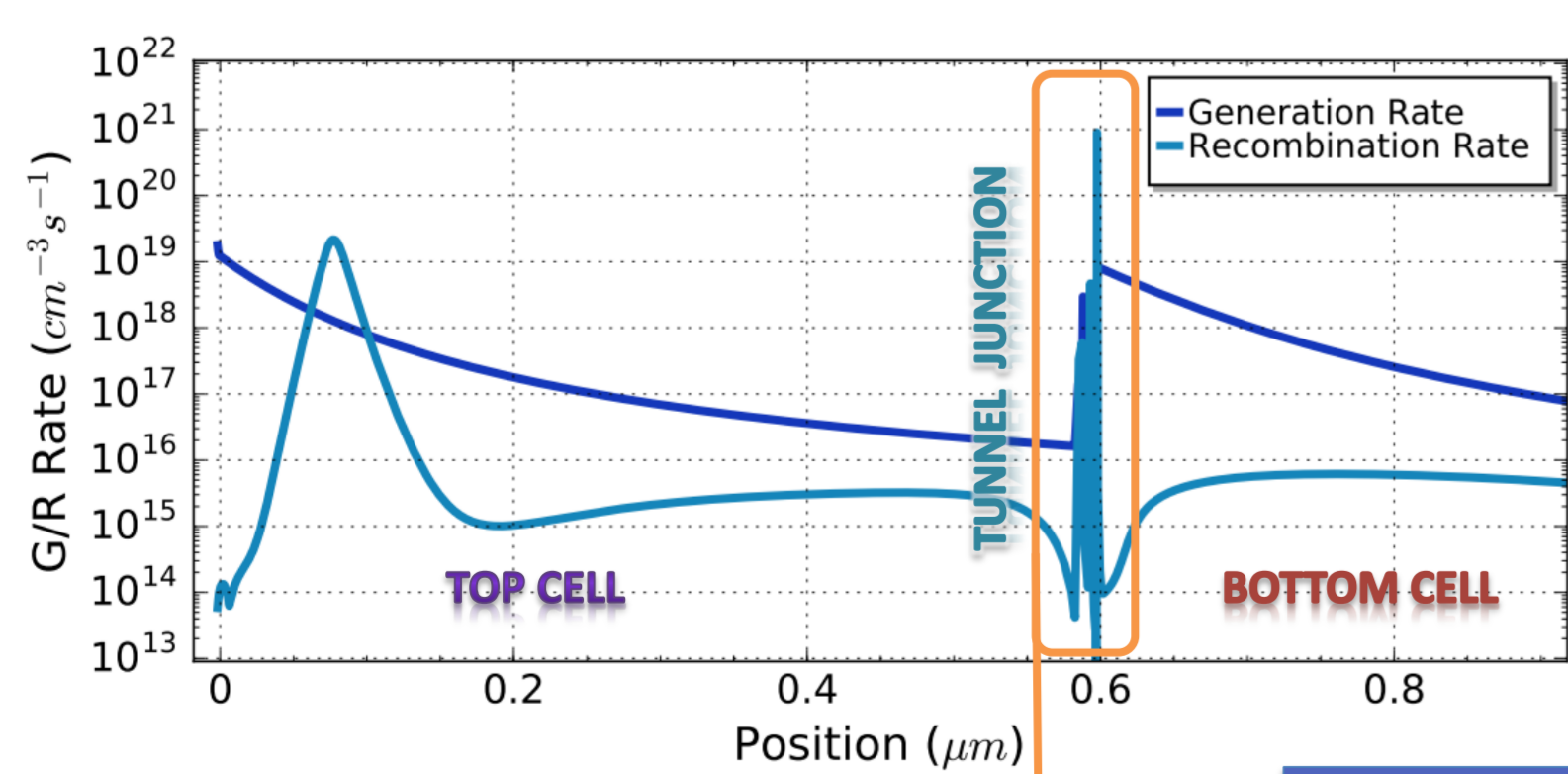
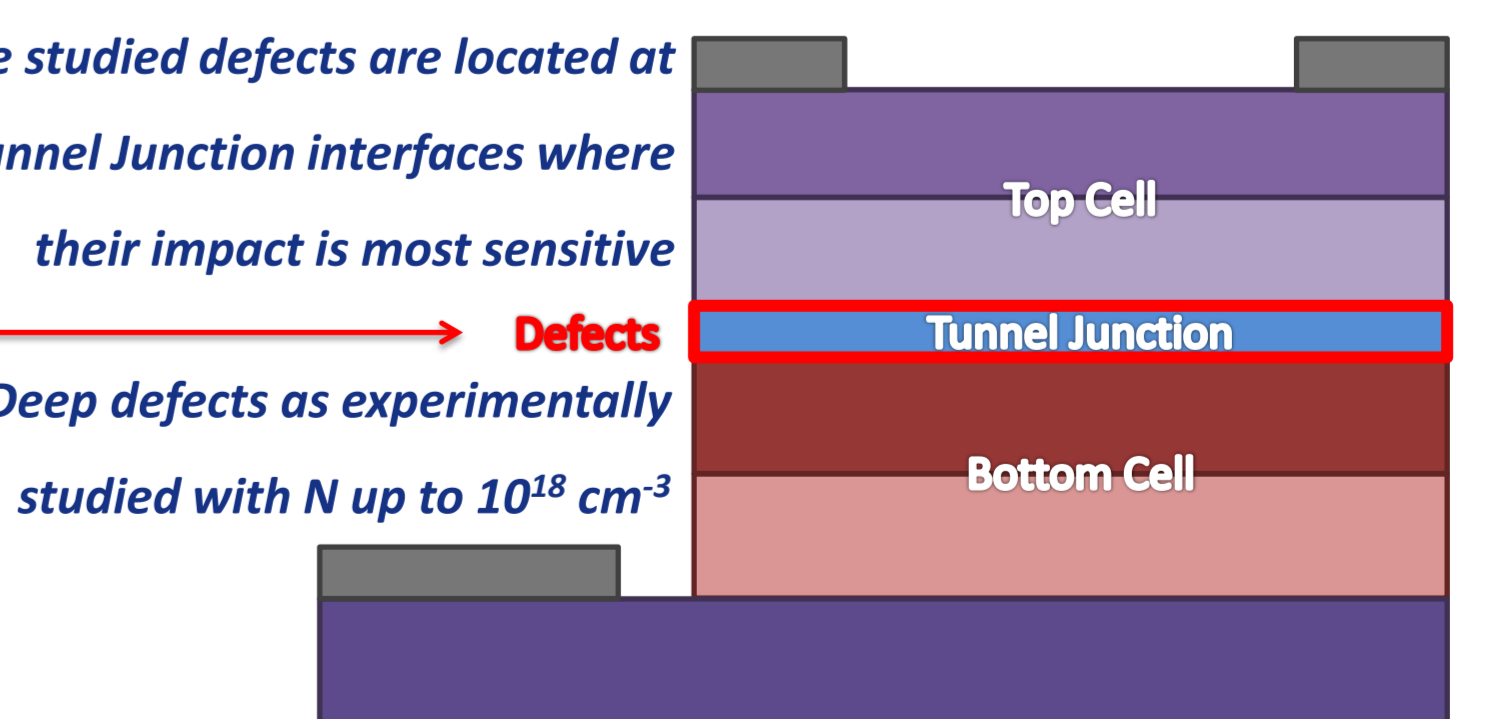
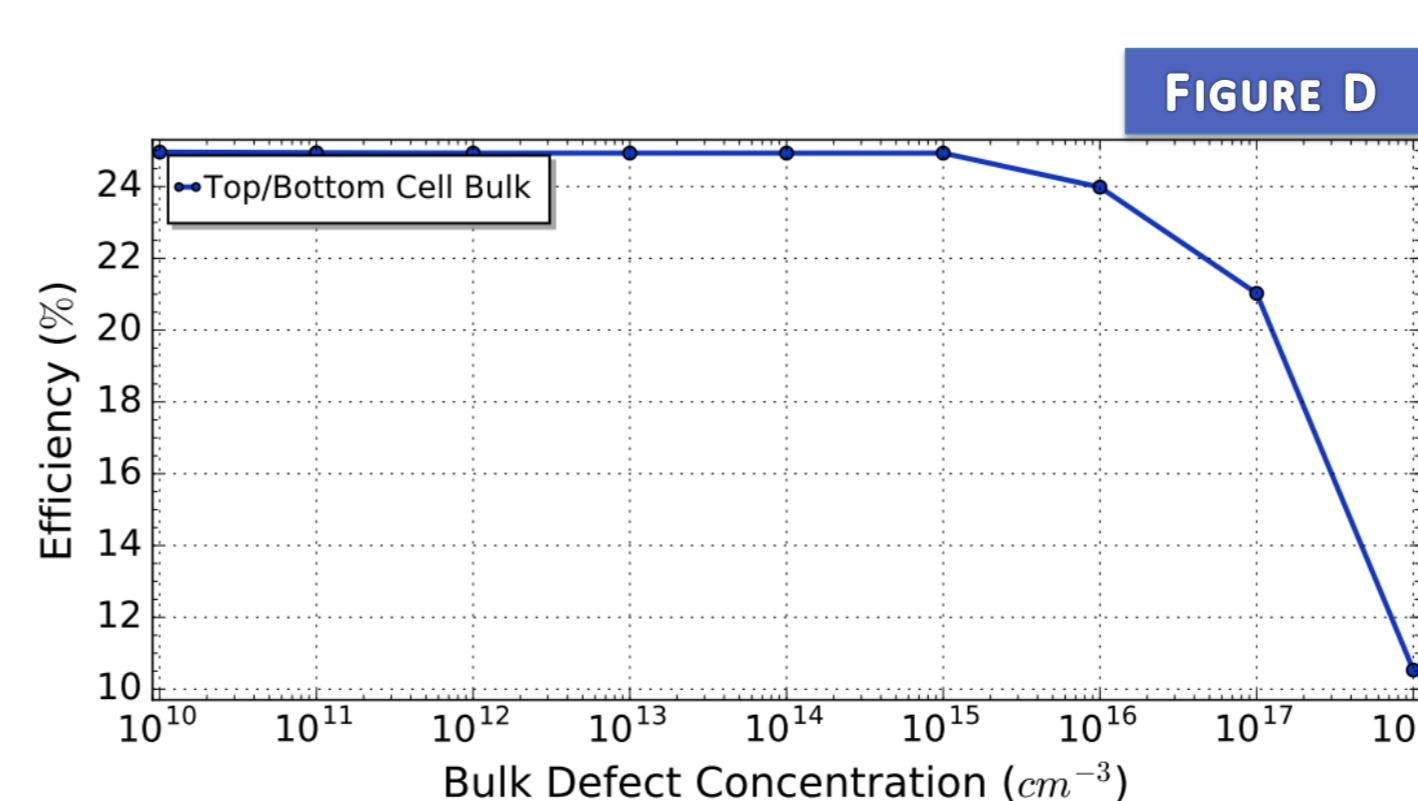


Figure C: Photogeneration and Recombination distribution in the InGaN double junction solar cell in full scale (top figure) and zoomed in the Tunnel Junction region (bottom figure).



The studied defects are located at the Tunnel Junction interfaces where their impact is most sensitive. Deep defects as experimentally studied with N up to 10¹⁸ cm⁻³.