Modelling III-Nitrides Optoelectronic devices with Quantum corrected drift-diffusion

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III-Nitrides



- III-Nitrides exhibit unique <u>optoelectronic</u>
 <u>properties</u>:
 - <u>Wide range of bandgaps</u>, allowing absorption or emission from UV to IR.
 - Direct band gap
 - Wide bandgap for <u>high temperature applications</u>
 - High efficiency of LEDs and Solar cells.
- However, the <u>high difference in lattice constant</u> makes heterostructures complex.
 - Only <u>few nm</u> of InGaN can be grown on GaN
 - <u>Multi-quantum well</u> structures needed to overcome this issue
 - Results in a <u>high density of defects</u> detrimental to the device performance



Experimental data



- Diode follow the <u>Shockley equation</u>
 - $I = I_S \cdot \left(\exp\left(\frac{qV}{\eta k_B T}\right) 1 \right)$
 - η is the ideality factor and should <u>not be higher</u> <u>than 2</u> according to the SRH theory
- But, Experimentally, ideality factors higher than 2
- Explained in literature as <u>trap-assisted tunneling</u>.
 - Need to add <u>quantum correction</u> to drift diffusion
- However, not enough to explain some of these high ideality factors
 - Donor-acceptor pair model needed



Quantum correction



- Quantum effects does not allow to use normal simulation tools.
- Quantum corrections need to be included in the <u>Drift Diffusion</u> method.
- Two methods implemented, based on finding an <u>effective</u> <u>quantum potential</u>
 - Density Gradient
 - Poisson-Schrodinger



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Donor-acceptor pair



- Due to the high density of defects interaction between traps cannot be neglected
- Two <u>coupled defect levels</u> must be considered.
- If the level are set as a <u>Donor-acceptor</u> <u>pair</u>, the coupling rate between the levels can saturate the recombination channel.
 - The recombination current will grow slower, <u>increasing the ideality factor</u>



Single QW LED



- Single QW LED structure.
- Dashed line show the <u>effective</u> <u>quantum band edges</u>.
- Where it is below E_c , E_v indicates the presence of <u>tail states</u>, where there can be tunneling.
 - Where Trap-assisted tunneling can take place



Single QW LED



- At low voltage, trap-assisted tunneling increase the ideality factor to around 6.
 - Due to Trap-assisted tunneling
- After 2 V, the recombination channel is saturated increasing further the ideality factor.
 - Due to <u>Donor-Acceptor pair</u> model



Thank you for the attention