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Efficiency Droop in Nanostructured III-N LEDs: Multiscale Numerical Analysis and Design Optimization<sup>1</sup> REZAUL NISHAT, VINAY CHI-MALGI, KRISHNA YALAVARTHI, SHAIKH AHMED, Department of Electrical and Computer Engineering, Southern Illinois University, Carbondale, IL — Recently, optical emitters using InGaN nanostructures have attracted much attention for applications in lasers, solid-state lighting, near-field photolithography, free-space quantum cryptography, consumer displays, as well as diagnostic medicine and imaging. Nanostructures can accommodate a broader range of lattice mismatch thereby allowing full-solar-spectrum emission characteristic, and provide larger active surface area and higher temperature stability. Nevertheless, performance of these III-N LEDs is determined by an intricate interplay of complex, nonlinear, highly stochastic and dynamically-coupled structural fields, charge, and thermal transport processes at different length and time scales. In this work, we study the effects of these coupled processes on the electronic and optical emission properties in nanostructured III-N LEDs. The multiscale computational framework employs the atomistic valence force-field molecular mechanics, the 10-band  $sp^3s^*$ -SO tight-binding models, and a coupling to a TCAD toolkit to determine the terminal properties of the device. Finally, a series of numerical experiments are performed (by varying different nanoscale parameters such as size, geometry, crystal cut, composition, surface and contacts, and electrostatics) that mainly aim to improve the efficiency droop and reliability of these LEDs.

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