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MULTISCALE-MULTIPHYSICS SIMULATION OF NANOSTRUCTURED DEVICES: THE TIBERCAD PROJECT

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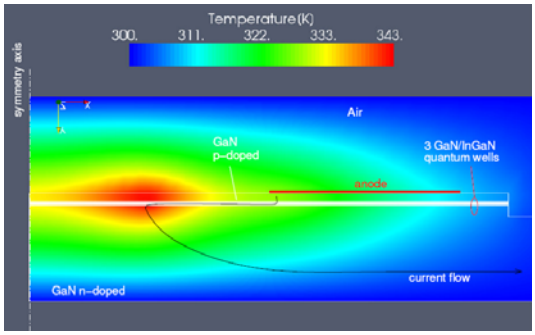
ABSTRACT

The TIBERCAD project [1] is aimed at the implementation of a device simulator which captures the most important physical concepts encountered in present and emerging electronic and optoelectronic devices. On the one hand the down-scaling of device dimensions requires the inclusion of more advanced quantum mechanical concepts which go beyond classical transport theories.
On the other hand, functionality of new emerging devices is based both on electrons/holes, and other quasi-particles such as excitons, polaritons, etc. Usually the active part of a device which needs a more elaborate and careful treatment is small compared to the overall simulation domain. The computational cost of the more accurate model however forbids its application to the whole domain, especially when using atomistic approaches. TIBERCAD implements the following physical models:
(a) A structural model that allows to calculate strain and shape deformation of lattice mismatched heterostructures based on linear elasticity theory of solids, assuming pseudomorphic interfaces between different materials [2]. External mechanical forces can be included in the simulation.
(b) Quantum-mechanical models to calculate eigenstates of confined particles based on the envelope function approximation including single-band and multiband $\mathbf{k}\cdot\mathbf{p}$ approach. We solve a stationary Schrödinger equation and obtain energy spectrum, particle density and probabilities of optical transitions [3].
(c) Semi-classical transport models that consider electrons, holes and excitons. Transport is treated in the drift-diffusion approximation. The electrochemical potentials are used as dependent variables such that the particle flux is equal to the gradient of a driving potential multiplied by a particle conductivity: $\mathbf{j} = -\sigma \cdot \nabla \phi$.
(d) Thermal transport considers the heating of the device due to Joule and Thompson effect and generation/recombination phenomena [4].
(e) Atomistic description of the most important regions of the device, based on empirical and semiempirical models, that includes structural, electronic and thermal properties [5].
The discretization of all PDE based models is done using an H^1-conforming finite element method [6]. The different physical models involved in the simulation of a

device can be solved on different space domains. The mesh of each model is derived from a common master mesh which facilitates data exchange for coupled multiphysics simulations. Adaptive h-refinement is used by some of the models. The nonlinear system resulting from the Galerkin-discretization of the drift-diffusion equations is solved using an approximate Newton method. The linear systems are solved by iterative methods [7].



As an example we present simulation results of a GaN pin-diode with three embedded $In_{0:05}Ga_{0:95}N$ QW, including an AlInN oxidization layer for current focusing. The heat transport simulation includes the air around the device, whereas the particle transport simulation is limited to the semiconductor. In Figure we show the temperature map at a bias voltage of 5.1 V, which corresponds to a current of approximately 88 mA. A temperature increase of about 43 K can be observed at the edge of the oxidization layer, where the carriers can cross the QW-stack and escape into the n-region.

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