Modeling of epitaxially grown heterostructures with the nextnano software

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Testing and evaluating an epitaxial design via modeling before the actual growth takes place can save considerable amount of effort, time and money, especially when growing those compound semiconductors where material parameters are well known and thus modeling can be predictive. The commercial nextnano software [1, 2] is a semiconductor nanodevice simulation tool that has been developed for predicting and understanding a wide range of electronic and optical properties of quantum structures. The underlying idea is to provide a robust and generic framework for modeling device applications in the field of nanosized semiconductor heterostructures (quantum wells, wires and dots). The simulator deals with realistic geometries and any combination of materials in one, two, and three spatial dimensions. It focuses on an accurate and reliable treatment of quantum mechanical effects and provides a self-consistent solution of the Schrödinger, Poisson, and current equations. The electronic structure is represented within the single-band or multiband k·p envelope function approximation, including strain, piezo and pyroelectric fields and arbitrary crystallographic growth directions. The user interface simplifies running repetitive tasks such as parameter sweeps. The material database includes binaries, ternaries and quaternaries of group IV, III-V and II-VI materials in both zinc blende and wurtzite crystal structure.
In this contribution, we give a brief overview of the nextnano software and present typical examples that demonstrate the wide range of possible applications such as LEDs, Laser Diodes, HEMTs and Nanowires. For modeling transport and gain in Quantum Cascade Lasers, an advanced quantum transport model based on the nonequilibrium Green's function method is used.

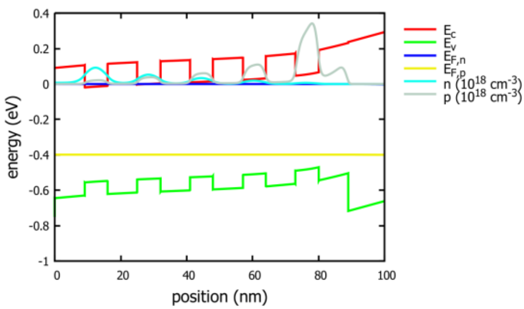

Figure 1: *Calculated conduction and valence band edge profiles, Fermi levels, and electron and hole densities of the active region of a laser diode.*

Finally, the question shall be raised whether a growth recipe of process control parameters such as temperature or shutter time, together with the growth monitoring of in-situ characterization of layer thicknesses can be used to automatically generate input files for modeling software. Such an integration would enhance the effectiveness of improving heterostructure design, reproducibility, benchmarking of different epitaxy machines, and the accurate determination of material parameters.

[1] http://www.nextnano.com
[2] S. Birner et al., nextnano: General Purpose 3-D Simulations, IEEE Transactions on Electron Devices **54**, 2137 (2007), DOI: 10.1109/TED.2007.902871