The nextnano software for the simulation of semiconductor heterostructures

Stefan Birner

next**nano** GmbH, Südmährenstr. 21, 85586 Poing b. München, Germany

stefan.birner@nextnano.com

The quickly progressing technology of semiconductor quantum structures requires and depends on reliable predictive theoretical methods for systematically improving, designing and understanding the electronic and optical properties of such structures. Nanodevice modeling nowadays has become a convenient tool for both, educational purposes as well as to support experimentalists while analyzing measured data or to design new experiments. The challenge is to make available to this audience a tool that covers the most important improvements that have been made over the past decades, i.e. to go beyond the simple "single-band effective-mass" model that is still widely used successfully due to its simplicity. More sophisticated models take into account the nonparabolicity and anisotropy of the electron and hole masses, usually employed within an 8-band **k·p** model. Such a model allows the calculation of broken gap type-II (InAs/GaSb) or type-III (HgTe/CdTe) superlattices. Strain is an important degree of freedom to optimize the electronic and optical properties of heterostructures. During the past decade 2D and 3D quantum confinement has been studied intensively in nanowires and quantum dots. These heterostructures require 2D or 3D simulation environments which go beyond simple self-written codes for 1D quantum wells. Most of these structures require the application of a bias. Therefore, a model that calculates the current has to be implemented.

The next**nano** software [1] allows one to study the realistic electronic structure of arbitrarily shaped three-dimensional semiconductor nanostructures crystallizing in the diamond, zinc blende and wurtzite structure. First, the strain is calculated within a continuum elasticity approach. Then the multi-band Schrödinger, Poisson and current equations are solved self-consistently, taking into account doping and piezo- and pyroelectric charges. For quantum cascade lasers, quantum transport is calculated with a nonequilibrium Green's function (NEGF) approach. The software is not limited to certain types of devices and thus perfectly suited for both, currently existing devices and novel devices, like for instance building blocks of quantum computers.

[1] The next**nano** software can be obtained from http://www.nextnano.com.