

Heterostructure Design Studio



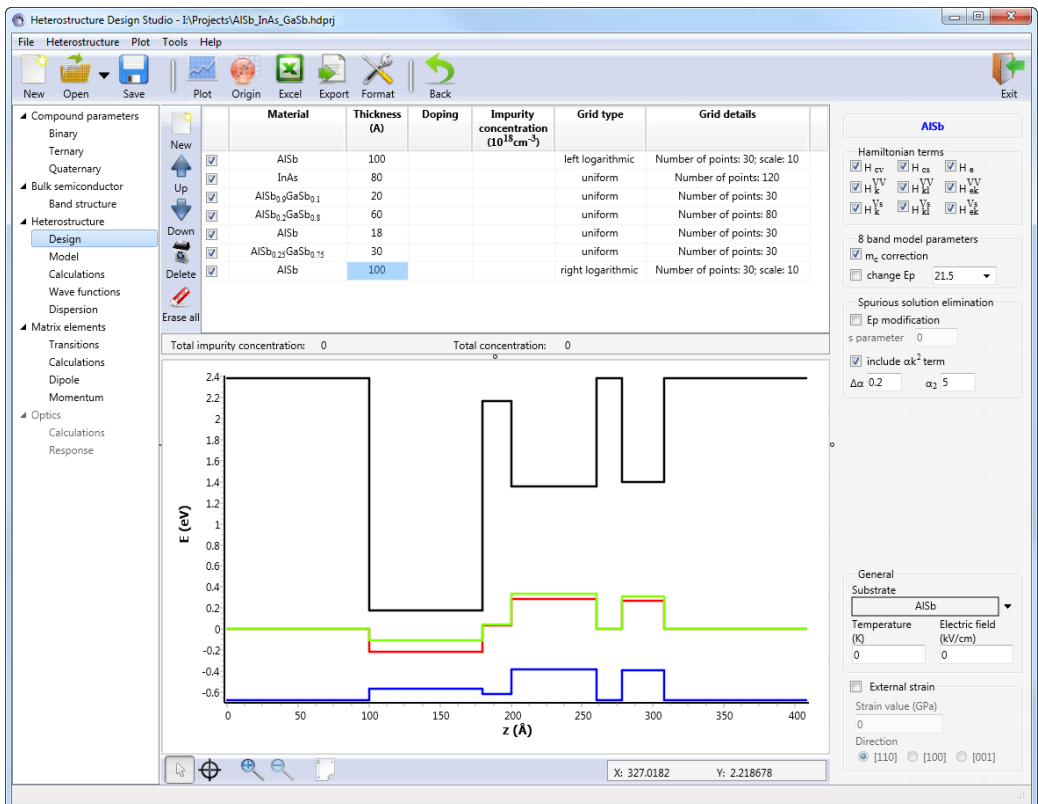
Nanostructure semiconductor
quantum simulation software for
scientists and engineers

Product description

Nowadays nanomaterials play an increasingly important role in modern technology. Artificially designed semiconductor heterostructures are basic material for electronic devices such as semiconductor lasers, photodetectors, field effect transistors etc. Computer Aided Design systems help in developing new devices predicting devices' properties that decreases costs of devices' design.

The **HETEROSTRUCTURE DESIGN STUDIO** is state-of-the-art quantum simulation CAD system developed for semiconductor heterostructure engineering. The **HETEROSTRUCTURE DESIGN STUDIO** performs calculations of energy levels' positions, corresponding wave functions and dispersion of confinement states in semiconductor heterostructures, dipole moments, momentum matrix elements, optical gain and optical absorption.

The **HETEROSTRUCTURE DESIGN STUDIO** was designed for scientists and engineers and was tested in NASA laboratories. Both scientists and engineers will find the **HETEROSTRUCTURE DESIGN STUDIO** to be an indispensable tool for heterostructure modeling, fast and convenient calculations of heterostructure properties, numerical theoretical study of novel structures.



Applications of Heterostructure Design Studio

Optoelectronic device engineering



Design of optoelectronics devices requires costly preparation of samples to get desired properties. The Heterostructure Design Studio allows predicting device properties by doing simulation. The calculations of wave functions, momentum matrix elements, optical gain etc with different input parameters of heterostructure provides the necessary information about device properties and its behavior under different external conditions that decreases the device design time and costs. Engineers involving in designing of semiconductor heterostructure devices will find the Heterostructure Design Studio an extremely helpful tool.

Theoretical studies of novel heterostructures in research labs and universities

The Heterostructure Design Studio provides scientists with precise and accurate calculations during all steps of heterostructure simulation. Knowledge of bandstructure calculated according to precise model and optical properties allows to work not only with novel structures but also to find hidden features properties in already known structures. Both scientists doing theoretical and experimental research will find the Heterostructure Design Studio an indispensable tool for their work.



Quantum mechanics training in semiconductor heterostructure studies at universities



Semiconductor heterostructures are subjects of study at quantum mechanics university courses. The base of courses is the theory of band structure and wave functions. Due to extremely complicated formulas, which include eigenvalue and eigenfunction problem of differential equations' system, it is impossible to get a result in analytical expressions. The Heterostructure Design Studio can be a working tool in solving exercises for the chapters in textbooks related to theory of heterostructures. Use of Heterostructure Design Studio provides students with both deep understanding of theory and practice in heterostructure calculations.

Key features and benefits

User friendly interface

- Easy to learn Windows based user interface
- Build-in heterostructure layers and grid editor
- Build-in material database with convenient access to parameters. Parameters used in calculations of well-known materials are placed in database
- Powerful graphical plotting tools

A₃B₅ semiconductors

The software allows working with all A₃B₅ semiconductors and their ternary and quaternary alloys with zinc-blend crystal structure as layer and substrate materials. Any new material can be added.

Multi-band k•p self-consistent calculations

Calculations are based on finite-difference self-consistent multi-band k•p method with symmetrized boundary conditions. Matrix part of calculations is done by using LAPACK library. The following models are included:

- Kane eight-band model
- Luttinger-Kohn valence six-band model
- Luttinger-Kohn valence six-band with conduction band model
- Luttinger-Kohn valence four-band model
- Luttinger-Kohn valence four-band with conduction band model
- Effective mass conduction band model

Main calculations parameters

- Temperature
- External DC electric field
- External uniaxial stress
- Quantum well and superlattice boundary conditions
- Self-consistent calculations mode
- Axial approximation
- Switch on/off the Hamiltonian terms

Spurious solution elimination

Spurious solutions' elimination mode for eight-band model

Optical transition calculations

Calculations of:

- momentum matrix elements,
- dipole moments.

Optical absorption and gain calculations

Calculations of optical absorption and gain in heterostructure medium

Bulk material band structure simulation

Calculations of bulk semiconductor band structure

Data export

Fast and convenient export of data to:

- Origin scientific software
- Microsoft Excel
- Text file
- Graphic file
- Clipboard

Parallel mode

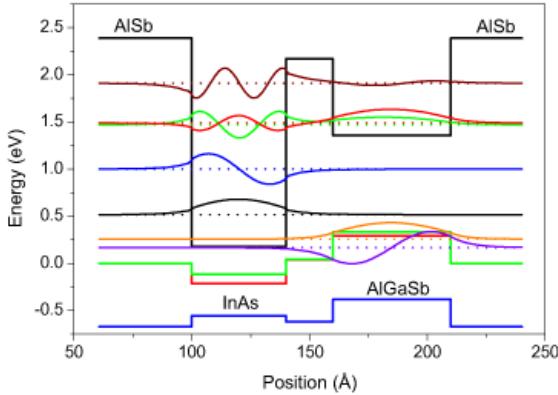
Use of several threads (processors) in calculations

System requirements

- IBM PC compatible computer
- 512 MB of RAM or higher
- 100 MB of available disk space
- Microsoft Windows 7 or later
- Connection to the Internet

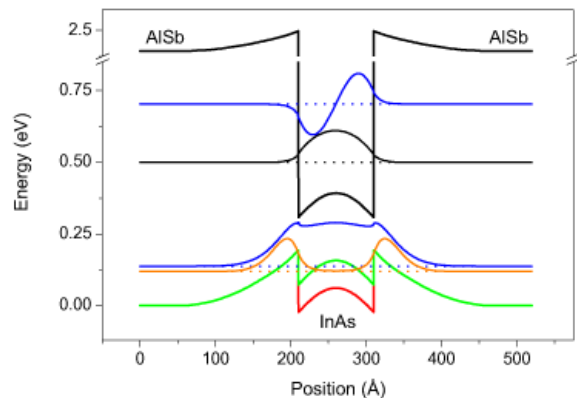
Simulation samples

Envelope wave functions

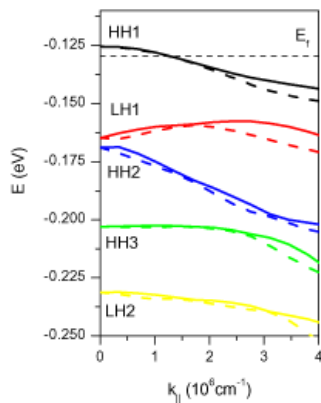


Valence and conduction band potentials with envelope wave functions of **AlSb/InAs/Al_{0.9}Ga_{0.1}Sb/Al_{0.2}Ga_{0.8}Sb/AlSb** double quantum well structure calculated from eight-band $k \cdot p$ theory.

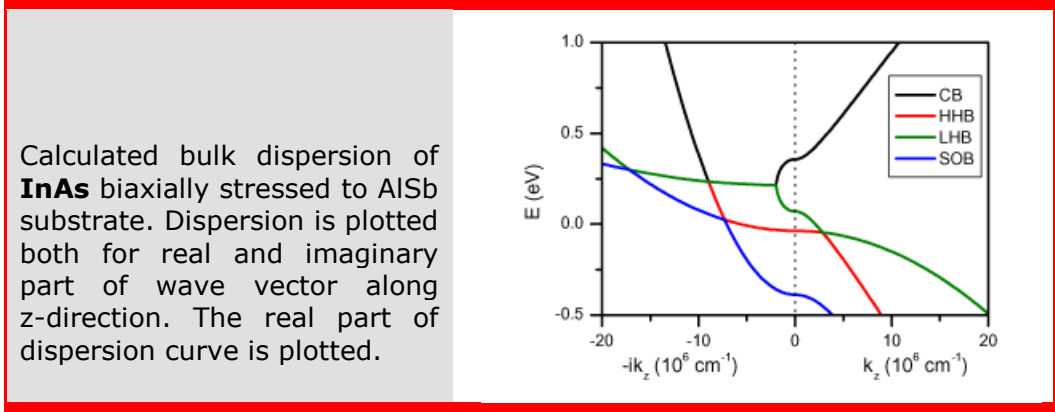
Self-consistent valence and conduction band potentials with envelope wave functions of **AlSb/InAs/AlSb** quantum well structure calculated from eight-band $k \cdot p$ theory. Heavily doping leads to type II \rightarrow type I transition due to the strong valence band bending.



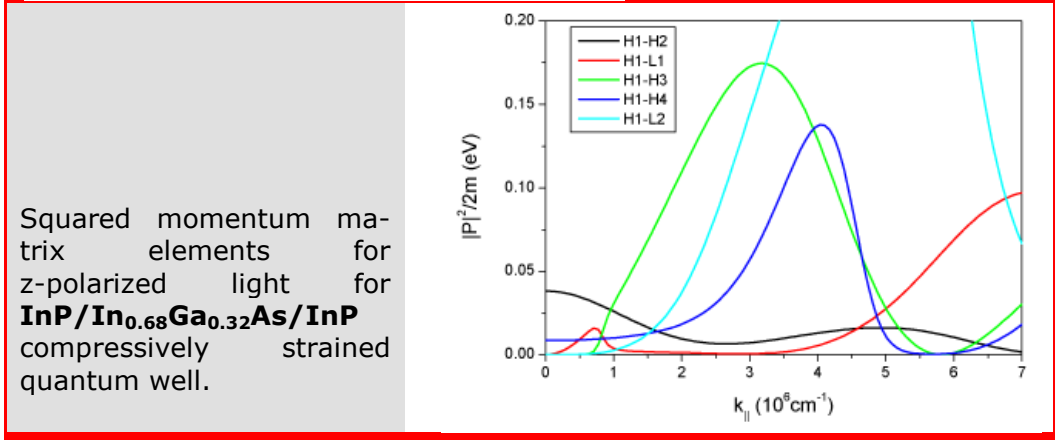
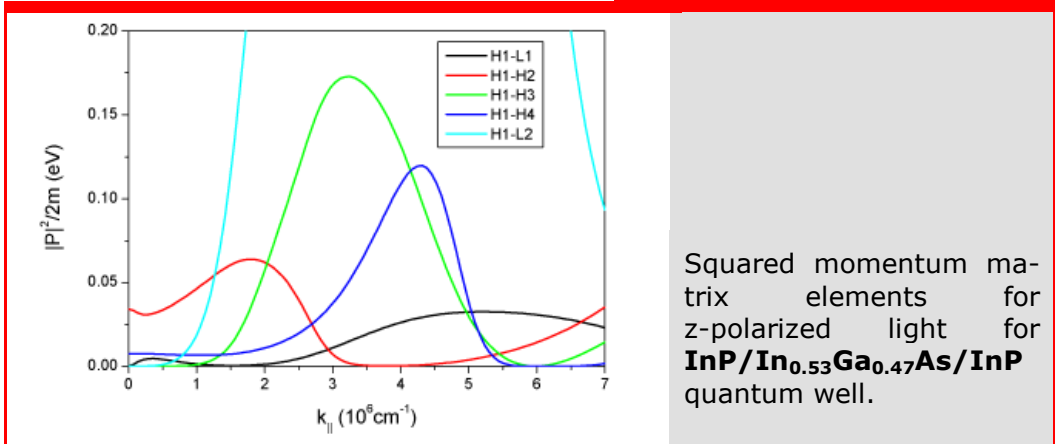
Dispersion



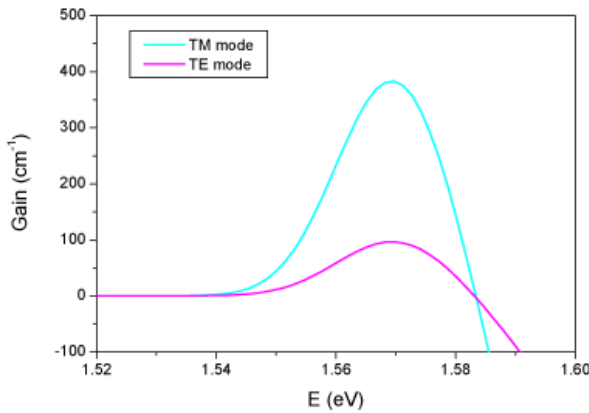
Hole subband dispersion in p-type **GaAs/Al_{0.5}Ga_{0.5}As** single heterojunction under applied in-plane uniaxial compression along [110] direction.



Momentum matrix elements

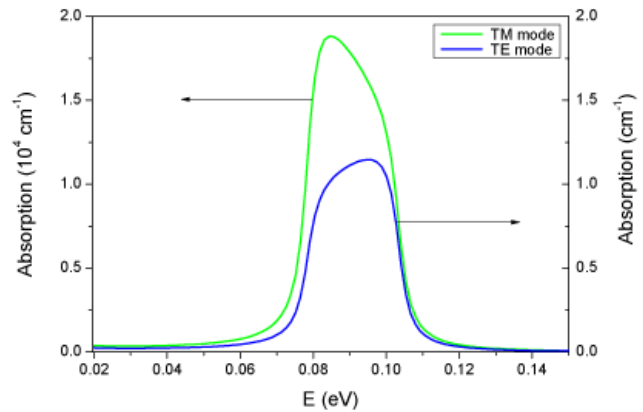


Optical absorption and gain



Optical gain in 140Å $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}_{0.84}\text{P}_{0.16}/\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ quantum well laser with $2 \times 10^{12} \text{cm}^{-2}$ concentration of injected electrons and holes at room temperature.

Intersubband optical absorption in 150Å $\text{AlSb}/\text{InAs}/\text{AlSb}$ heterostructure with electron sheet concentration of 10^{12}cm^{-2} at 4.2K.



Contacts

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