

# Modeling and simulation of strained quantum wells in semiconductor lasers

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Many modern optoelectronic devices, in particular semiconductor lasers, essentially rely on Quantum Well structures which need to be properly designed. Based on the Envelope Function Approach for heterostructured materials and the **kp**–theory, a model has been developed which allows to simulate such structures consistently. The model is based on matrix–valued **kp**–Schrödinger operators. Effects such as confinement, band mixing, spin–orbit interaction and strain can be treated for different material systems, e.g. cubic and wurtzite crystallographic structures. Important information provided by the model are the non parabolic band structure, the quantum confined states, their respective transition matrix elements, carrier densities and the optical response function, which is crucial for semiconductor laser modeling. The impact of prominent Coulomb effects has been considered by including the Hartree interaction via the Poisson equation and the bandgap renormalization via exchange–correlation potentials, resulting in generalized matrix–valued Schrödinger–Poisson systems. Based on these results, comprehensive device simulations have been performed. These simulations include the interaction between the electronic behaviour of the device and the optical field, i.e., they account for carrier transport, optical wave wave guiding, and generation and transport of thermal energy. The bandstructure information enters parametrically via the density of states, or alternatively by a capture–escape mechanism, and the optical response function. The simulation results

are in good agreement with experiments, demonstrating their applicability for designing modern optoelectronic devices. Indeed, the described simulations of semiconductor lasers now can be routinely performed in an development environment. e.g. at the “Heinrich–Hertz–Institut für Nachrichtentechnik” (HHI), Berlin. where they are used for optimizing multi quantum well laser structures.

## Publications within the Project

### Publications in Journals and Books

- U. Bandelow, H.-Chr. Kaiser, T. Koprucki, and J. Rehberg. Modeling and simulation of strained quantum wells in semiconductor lasers. In *Mathematische Verfahren zur Lösung von Problemstellungen in Industrie und Wirtschaft*. Springer Verlag, in press. Weierstrass Institute for Applied Analysis and Stochastics Preprint No. 582, Berlin 2001.
- U. Bandelow, M. Radziunas, J. Sieber, and Matthias Wolfrum. Impact of gain dispersion on the spatio-temporal dynamics of multisectio lasers. *IEEE Journal of Quantum Electronics*, 37(2):183–188, 2001.
- U. Bandelow, H. Gajewski, and H.-Chr. Kaiser. Modeling combined effects of carrier injection, photon dynamics and heating in Strained Multi-Quantum Well Lasers. In Marek Osinski Rolf H. Binder, Peter Blood, editor, *Physics and Simulation of Optoelectronic Devices VIII*, volume 3944 of *Proceedings of SPIE*, pages 301–310, 2000.
- U. Bandelow, M. Radziunas, V. Tronciu, H.-J. Wünsche, and F. Henneberger. Tailoring the dynamics of diode lasers by dispersive reflectors. In Marek Osinski Rolf H. Binder, Peter Blood, editor, *Physics and Simulation of Optoelectronic Devices VIII*, volume 3944 of *Proceedings of SPIE*, pages 536–545, 2000.
- H.-Chr. Kaiser and J. Rehberg. About some mathematical questions concerning the embedding of Schrödinger–Poisson systems into the drift–diffusion model of semiconductor devices. In B. Fiedler, K. Gröger, and J. Sprekels, editors, *Equadiff 99 Proceedings of the International Conference on Differential Equations*, volume 2, pages 1328–1333. World Scientific, 2000.
- U. Bandelow, H.-Chr. Kaiser, T. Koprucki, and J. Rehberg. Spectral

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- H.-Chr. Kaiser and J. Rehberg. On stationary Schrödinger–Poisson equations modelling an electron gas with reduced dimension. *Mathematical Methods in the Applied Sciences*, 20:1283–1312, 1997.

## Congress Communications

- U. Bandelow and T. Koprucki. Calculation of electronic states in quantum structures. Talk at European Semiconductor Laser Workshop, Heinrich-Hertz Institut f. Nachrichtentechnik, Berlin, September 1, 2000.
- Th. Koprucki. Efficient simulation of electronic states in semiconductor quantum wells. 16th GAMM–Seminar Leipzig on Numerical techniques for Schrödinger equations, February 3–5, 2000.
- U. Bandelow, H. Gajewski, and H.-Chr. Kaiser. Modeling combined effects of carrier injection, photon dynamics and heating in Strained Multi-Quantum Well Lasers. Photonics West (SPIE) at San Jose Convention Center, San Jose, California USA, 22 to 28 January 2000.
- U. Bandelow, M. Radziunas, V. Tronciu, H.-J. Wünsche, and F. Henneberger. Tailoring the dynamics of diode lasers by dispersive reflectors. Photonics West (SPIE) at San Jose Convention Center, San Jose, California USA, 22 to 28 January 2000.
- H.-Chr. Kaiser and J. Rehberg. About some mathematical questions concerning the embedding of Schrödinger–Poisson systems into

the drift–diffusion model of semiconductor devices. *Equadiff 99, International Conference on Differential Equations*, Freie Universität Berlin, Germany, August 1–7, 1999.

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- H. Stephan, U. Bandelow, and H. Gajewski. Lateralmodendynamik in Halbleiterlasern. Symposium Analysis und Simulation nichtlinearer Muster, Fritz Haber Institut, Berlin, Mai 28 1999.
- Th. Koprucki, U. Bandelow, H.-Chr. Kaiser, and J. Rehberg. A finite-element approach to the eigenvalue problem arising from kp–Hamilton operators for quantum wells. 11th III-V Semiconductor Device Simulation Workshop, IEMN, Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France, May 10-11, 1999.
- O. Mayrock, H.-J. Wünsche, F. Henneberger, O. Brandt, U. Bandelow, and H.-Chr. Kaiser. Calculation of localized multi-particle states in (Zn,Cd)Se and (In,Ga)N quantum wells. International Conference on the Physics of Semiconductors (ICPS 24) 2 – 7 August, 1998, Jerusalem, Israel. Proceedings of the ICPS24, Art. IXB29 (1344.pdf), edited by D. Gershoni.
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- H. Gajewski and H.-Chr. Kaiser. Transversal modeling of semiconductor lasers. Workshop "Scientific Computing in Electrical Engineering" Berlin, Germany, September 30 – October 2, 1998.

- J. Rehberg and H.-Chr. Kaiser. A hybrid semiconductor device model including nanostructures. International Congress of Mathematicians Berlin, Germany, August 18–27, 1998. Poster in Section 11. Mathematical Physics.
- H.-Chr. Kaiser and J. Rehberg. Modeling of QW-lasers including Schrödinger–Poisson systems. International Congress of Mathematicians Berlin, Germany, August 18–27, 1998. Poster in Section 16. Applications.
- U. Bandelow, H.-Chr. Kaiser, and J. Rehberg. 2d multiband kp modeling of nanostructures. 10<sup>th</sup> III–V Semiconductor Device Simulation Workshop, Torino, Italy, October 16–17, 1997.
- H.-Chr. Kaiser and J. Rehberg. Matching the phenomenological and the quantum mechanical description of semiconductor devices. Workshop on Phase Transitions: Microscopic and Mesoscopic Theory, Berlin, Germany, 2–7 June , 1997.

## Seminar Communications

- U. Bandelow. Einbeziehung von Quantisierungseffekten in WIAS–TeSCA. Research Seminar on Semiconductor Lasers, WIAS Berlin, November 16 2000.
- U. Bandelow. Lasermodellierung - Beiträge des WIAS zum Projekt "Terabit-Optics-Berlin". Talk at session of scientific committee of WIAS, WIAS, Berlin, oct 13 2000.
- Uwe Bandelow, Herbert Gajewski, Hans-Christoph Kaiser, Thomas Koprucki, and Joachim Rehberg. Modeling and simulation of strained quantum wells in semiconductor lasers. Statusseminar 2000 des BMBF–Förderschwerpunktes “Neue Mathematische Verfahren in Industrie und Dienstleistungen”, Frankfurt am Main.
- U. Bandelow. Modeling of active optoelectronic components. Invited talk at Intel Corp., Santa Clara, CA, USA, march 25 2000.
- U. Bandelow. Modellierung von  $1.55 \mu\text{m}$  MQW-Kantenemittern II. Joint seminar of HHI and PDI Berlin on Photonik Crystals, Paul–Drude–Institut, Berlin, 7 March 2000.

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- U. Bandelow. Modellierung und Simulation von Halbleiterlasern. Kolloquium des Weierstraß–Institutes für Angewandte Analysis und Stochastik (WIAS), Berlin, 21 February 2000.
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- Th. Koprucki. Numerische Verfahren zu kp–Operatoren. Methode und Beispiele. Seminar “Funktionalanalytische Methoden” von Prof. Dr. Arno Langenbach am Weierstraß–Institut für Angewandte Analysis und Stochastik Berlin, 11. November 1998.
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- H. Gajewski and H.-Chr. Kaiser. Mathematische Modellierung und Simulation von Halbleiterstrukturen. Kolloquium, Paul–Drude–Institut für Festkörperelektronik, Berlin, Germany, December 12, 1998.
- U. Bandelow. Mode Degeneracy and Self-Sustained Pulsations. Research Seminar on Semiconductor Lasers, HU-Berlin, Inst. f. Mathematics, December 11 1997.
- U. Bandelow. Modenentwicklung und Dynamik. Research Seminar on Semiconductor Lasers, HU-Berlin, Inst. f. Mathematics, December 4 1997.
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