OFFICE OF NAVAL RESEARCH

FINAL REPORT

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Electronic Transport in Semiconductor Heterostructures and in Mesoscopic Systems

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I. ACCOMPLISHMENTS AT THE TIME OF COMPLETION OF THE CONTRACT

Much of the work in the past three years has concentrated on creating a predictive simulation tool for edge emitting semiconductor quantum well laser diodes. This simulator (MINILASE II) has been completed and has been compared to modulation response experiments from the Santa Barbara group. Modulation response has been chosen because it is the most difficult characteristic to predict since nonlinearities enter in a crucial way. The close agreement between experimental and simulation results that is described in publication 15 has necessitated a careful treatment of the device physics:
(i) We have included an 8 band $k{\cdot}p$ bandstructure including the effects of strain. The effects of bandstructure are twofold. It had already been known that bandstructure determines the optical matrix element and therefore is crucial to obtain correct values for optical absorption, spontaneous emission and stimulated emission. Our self-consistent simulator has shown however, that of equal importance is the non-parabolicity which effects the location of the quasi-Fermi levels and therefore the gain. Only a complete simulator such as MINILASE II can show this with all its quantitative aspects.
(ii) We have resolved the energy distribution of charge carriers within the quantum well by numerically solving a Boltzmann equation. This energy distribution is key to the nonlinearities of gain in quantum well lasers. No other simulator has previously modeled the energy distribution of the charge carriers. Nevertheless modulation response cannot be quantitatively understood without it since the modulation response is influenced by minute deviations of the distribution function from the Fermi-type. The extreme sensitivity of the laser gain to the form of the distribution function f has been "automatically" shown by MINILASE II and can be understood from the following argument. The photon number S_ν in a given mode ν is proportional to

$$S_\nu \approx \left(G(f) - L\right)^{-1} \qquad (1)$$

The laser operating point is close to the pole $G(f)=L$. Thus minute changes of the distribution function f may cause large changes in S_ν. These changes in f arise from changes in the electron energy (raised electron and phonon temperature) and also from spectral hole burning which is of importance only at high power.

The precise calculations of the deviations from the Fermi distribution need to include deviations of the polar optical phonon occupation from equilibrium, heating of the charge carriers through phonons and carrier-carrier interactions, the rapid removal of carriers by stimulated emission, the carrier-carrier interactions, the rapid carrier-carrier capture, and charge carrier scattering to lower energies in the quantum wells. All this has been accomplished in MINILASE II and is described in detail in the referenced publications. It has been necessary for this purpose to develop a special scattering mechanism that simulates carrier-carrier interactions and at the same time permits ultrafast simulation that could be included in MINILASE II without creating impossible computational demands.

Our simulator is generally recognized as the most advanced and predictive laser simulator with respect to device physics. We have closely collaborated with Capasso's group at Lucent Bell Laboratories and have on several occasions transferred our technology and experiences to them. Their simulator is now extremely similar to MINILASE II, down to an identical treatment of quantum well capture, although their simulator still works with Fermi-distributions.

The work on laser diodes and nonlinearities in the modulation response has also inspired our most recent work on p-n junction capacitance which has proved all past work on the diffusion capacitance incorrect. This is described in [16]. One of the important results of this work is that diffusion capacitance exists only for short diodes. Long diodes in which all minority carriers have a chance to recombine do not show diffusion capacitance (in spite of the opposite notion in all textbooks).

Other important research results have been obtained for several quantum aspects of interface transport [1,2], and we have performed detailed simulations of quantum well capture [6]. A number of the most recent publications deals with the giant isotope effect in transistor lifetime [20,21,22] which was recently discovered in our group.

II. INDEX OF PUBLICATIONS

In the past grant period we have published (submitted) a total of 23 papers and have presented 15 invited lectures at international conferences as well as numerous contributed papers not included in this listing.

Publications

1)K. Hess, P. von Allmen, M. Grupen and L. F. Register, "Simulating Electronic Transport in Semiconductor Nanostructures," presented at NATO Workshop, Ile de Bendor, France, July 17-21, 1995, proceedings "Future Trends in Microelectronics," S. Luryi, J. Xu, and A. Zaslavsky editors, pp. 215-225.

2) V. L. Gurevich, V. B. Pevzner and K. Hess, "Phonon-Assisted Ballistic Resistance," Phys. Rev. B, 51, (8), pp. 5219-5226, 1995.

3) M. Grupen and K. Hess, "A Self-Consistent Calculation of the Modulation Response for Quantum Well Laser Diodes," Applied Physics Letters, 65, (19), pp. 2454-2456, 1993.

4) L. F. Register, R. Baca, G. Kosinovsky, M. Grupen and K. Hess, "Possibility of Off-Resonance Lasing in Vertical Cavity Surface Emitting Lasers." Appl. Phys. Lett., 66, (3), pp. 259-261, 1995.

5) M. Grupen, K. Hess and L. Rota, "Simulating Spatial and Spectral Hole Burning and the Modulation Response of Quantum Well Laser Diodes," presented at SPIE 1995 International Symposium, San Jose, CA, 2/6-9/95, proceedings "Physics and Simulation of Optoelectronic devices III," M. Osinski and W. W. Chow editors, pp. 468-479.

6) L. F. Register and K. Hess, "Simulation of Carrier Capture by Quantum Wells Due to Strong Inelastic Scattering," Superlattices and Microstructures, vol. 18, no. 3, pp. 223-228, 1995.

7) V. L. Gurevich, V. B. Pevzner and K. Hess, "Non-Ohmic Phonon-Assisted Landauer Resistance," in Quantum Transport in Ultrasmall Devices, edited by D. K. Ferry et al., Plenum Press, New York, pp. 457-460, 1995.

8) L. Rota, M. Grupen and K. Hess, "Spectral Hole Burning and Carrier-Carrier interaction in Semiconductor Quantum Well Lasers: A Monte Carlo Investigation," Published in Hot Carriers in Semiconductors, Eds. K. Hess, J. P. Leburton and U. Ravaioli, Plenum Press, New York, pp. 563-568, 1996.

9) M. Grupen, "Simulating Carrier Dynamics in Quantum Well Lasers," in Physics and Simulation of Optoelectronic Devices IV, edited by Weng W. Chow and Marek Osinski, Proc SPIE 2693, SPIE Bellingham, WA, pp. 374-385, 1996.

10) M. Grupen and K. Hess, "The Coupled Optoelectronic Problems of Quantum Well Laser Operation," Proceedings of the international Workshop on Computational Electronics, Tempe, AZ, October 28-November 2, 1995.
11) M. Grupen and K. Hess, "Simulating the Modulation Response of Quantum Well Laser Diodes," Proceedings International Symposium on Compound Semiconductors, St. Petersburg, Russia, Institute of Physics Conference Series 155, 641-647, 1996.
12) F. Oyafuso, P. von Allmen, M. Grupen and K. Hess, "Gain Calculation in a Quantum Well Laser Simulator Using an Eight Band k·p Model," Proceedings of the International Workshop on Computational Electronics, Tempe, AZ, October 28-November 3, 1995.
13) M. Grupen and K. Hess, "Severe Gain Suppression Due to Dynamic Carrier Heating in Quantum Well Lasers," Appl. Phys. Lett., 70, (7), 808-810, 1997.
14) J. W. Lyding and K. Hess, "Deuterium Treatment for Improved Hot Carrier Reliability of Integrated Circuit Transistors," Condensed Matter News, vol. 5, issues 3-4, pp. 8-10, 1996.
15) M. Grupen and K. Hess, "Simulation of Carrier Transport and Nonlinearities in Quantum Well Laser Diodes," IEEE Journal of Quantum Electronics, 34, pp. 120-140, 1998.
16) S. E. Laux and K. Hess, "New Quantitative Theory of p-n Junction Impedance: Analytical Resolution of Past Misconceptions" submitted to IEEE Transactions on Electron Devices.
17) K. Hess, I. C. Kizilyalli and J. W. Lyding, "Giant Isotope Effect on Hot Electron Degradation of Metal Oxide Silicon Devices," IEEE Transactions on Electron Devices, 45, 406-416, 1998.
18) F. Oyafuso, P. von Allmen, M. Grupen and K. Hess, "Inclusion of Bandstructure and Many-Body Effects in a Quantum Well Laser Simulator," Proceedings of the IWCE, Notre Dame, IN, 1997. (to be published)
19) B. Klein, L. Register, K. Hess and D. Deppe, "Theory and Modeling of Lasing Modes in Vertical Cavity Surface Emitting Lasers," Proceedings of the IWCE, Notre Dame, IN, 1997. (to be published)
20) D. A. Richie, P. von Allmen, K. Hess and R. Martin, "Electronic Structure Calculations Using an Adaptive Wavelet Basis," Proceedings of the IWCE, Notre Dame, IN, 1997. (to be published)
21) I. P. Ipatova, O. P. Chikalova-Luzime and K. Hess, "Effect of Localized Vibrations on the Si Surface Concentrations of H and D," Journal of Applied Physics, 83, pp. 814-819, 1998.
22) J. Lee, S. Aur, R. Eklund, K. Hess and J. W. Lyding, "SIMS Characterization of the Deuterium Sintering Process for Enhanced Lifetime CMOS Transistors," Journal of Vacuum Science and Technology, accepted (1998).
23) K. Hess, "High Field Transport," to be published in the Webster Encyclopedia of Electrical Engineering

III. INVITED PRESENTATIONS

I1) "Simulation of Quantum Well Lasers," presented at the 22nd Conference on the Physics and Chemistry of Semiconductor Interfaces, Scottsdale, AZ, January 8-12, 1995.
I2) "Simulation of Spatial and Spectral Hole Burning and Modulation Response of Edge- and Surface-emitting Quantum Well Lasers," presented at SPIE 1995 International Symposium, San Jose, CA, 2/6-9/95, Proceedings Physics and Simulation of Optoelectronic Devices III, M. Osinski and W. W. Chow editors, pp. 468-479.
I3) "Quantum Well Laser Diode Simulation," presented at International Symposium Heterostructures in Science and Technology, Wurzburg, Germany, March 13-18, 1995.

I4) "Simulations of Electronic Properties and Capacitance of Quantum Dots," presented at US-European Workshop on Nanostructures, Santa Barbara, CA, March 27/28, 1995.
I5) "Simulating Electronic Transport in Semiconductor Nanostructures," presented at NATO Workshop, Ile de Bendor, France, July 17-21, 1995, proceedings "Future Trends in Microelectronics," S. Luryi, J. Xu, and A. Zaslavsky editors, pp. 215-225.
I6) "The Coupled Optoelectronic Problems of Quantum Well Laser Operation," presented at the International Workshop on Computational Electronics, Tempe, AZ, October 28-November 2, 1995.
I7) "Role of Carrier Transport and Spectral Hole Burning in the Modulation Response of Semiconductors," presented at the 1995 International Semiconductor Device Research Symposium Charlottesville, Virginia, December 6-8, 1995.
I8) "Spectral Hole Burning and Carrier-Carrier Interaction in Semiconductor Quantum Well Lasers: A Monte Carlo Investigation," presented at the Ninth International Conference on Hot Carriers in Semiconductors, Chicago, IL, July 31-August 4, 1995, Proceedings Hot Carriers in Semiconductors, Eds. K. Hess, J. P. Leburton and U. Ravaioli, pp. 563-568.
I9) "Simulating Carrier Dynamics in Quantum Well Lasers," presented at SPIE, San Jose, CA, January 27-February 2, 1996.
I10) "Simulating Nonlinear Gain in Quantum Well Lasers," presented at the Workshop on Optical Properties of Semiconductor Nanostructures," Snowbird, Utah, May 6-11, 1996.
I11) "Simulating at the Modulation Response of Quantum Well Laser Diodes," presented at the International Symposium on Compound Semiconductors, St. Petersburg, Russia, September 23-27, 1996.
I12) "Carrier Capture in Narrow and Wide Quantum Wells: Simulation of the Transition from Weak to Strong Scattering," presented at 190th Meeting of the Electrochemical Society, San Antonio, TX, October 7-10, 1996.
I13) "Electronic Transport Between the Classical and Quantum Limits: Consequences for Device Speed," Advanced Heterostructure Workshop 1996, December 1-6, 1996, Kona, Hawaii.
I14) "Simulation of Carrier Transport and Nonlinearities in Quantum Well Laser Diodes," presented at The Second NASA Workshop on Device Modeling, August 7-8, 1997, Moffett Field, CA.
I15) "Impact of Nanostructure Research on Conventional Solid State Electronics: The Giant Isotope Effect in Hydrogen Desorption and CMOS Lifetime" in Frontier in Low-Dimensional Physics, 10th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria, February 19 to March 1, 1998.