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13. ABSTRACT *(Maximum 200 words)*

A brief summary of research accomplishments during the past three years is given, along with a list of 18 published papers that contain the details of this work. Also included is a list of invited presentations of ARO sponsored research. These accomplishments include: essential completion of our full band Monte Carlo simulator with the first principles derivation of deformation potentials from the same ionic potentials used to calculate the crystal band-structure; development of a powerful density functional based numerical method to calculate quantum capacitance in nanostructures including Coulomb, size-quantization and many-body contributions to the "charging" energy; and establishment of an entirely new "quantum Monte Carlo" method based on Schroedinger's equation for simulating dissipative quantum transport, a method that bridges the gap between phase-incoherent semiclassical transport and phase-coherent quantum transport.

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1 Progress over the Past Three Years

In the last three years we have essentially completed the basic development of our (semi-classical) full band Monte Carlo (FBMC) simulator, and we have established practical and powerful numerical and analytical methods for modeling capacitive charging, and resistive and *dissipative* quantum transport in nanostructures. Here we shall only briefly review this work; the details of this work are described in the 18 publications listed in the next section. The first two and one-half years also have been summarized previously in interim reports:

- Using a density functional theory of electron-phonon interactions, we derived deformation potentials for our FBMC from the same ionic potentials used to calculated the crystal band-structure. Previously, deformation potentials had been treated essentially as adjustable parameters in Monte Carlo simulations due to uncertainty in their values, particularly in silicon [1,2,3].

- As an initial step into true multi-scale simulations, we have combined our FBMC with pseudo-Hamiltonian-based calculations of transmission and reflection coefficients, again using the same pseudo-potentials, to model high energy electron transport over a GaAs/AlAs interface [4].

- We established an entirely new "quantum Monte Carlo" method for simulating dissipative quantum transport in mesoscopic systems, that we now refer to as Schrödinger equation (based) Monte Carlo (SEMC), and simulated polar-optical-phonon scattering of electrons in quasi-two-dimensional geometries with quantitative accuracy [5,6,7]. This particular scattering process, because it has a long range interaction potential, has proven to be the bane of many other methods of simulating dissipative quantum transport, even in one-dimensional simulations. This method allows us to bridge the gap between phase-incoherent semiclassical transport and phase-coherent quantum transport.

- In a primarily analytical approach to dissipative quantum transport, we showed that weak dissipation can be treated by introducing a position dependence to quasi-Fermi levels within mesoscopic structures [8,9].

- We identified the phenomenon of the "zero-bias anomaly" in the current of *p*-*n* tunnel diodes, known from experience in the 1960's, as a manifestation of Coulomb Blockade [10].

- We modeled a prototype atomic scale "single-electron" device to examine the requirements for achieving digital functionality in such a device within the "uncertainties" imposed by quantum mechanics [11]. This work was subsequently discussed in Science News 145, January 15, 1994.

- We developed a density functional theory to calculate "quantum capacitance" in nanostructure dots, including Coulomb, size-quantization and many-body contributions to the "charging" energy, and demonstrated significant deviations from classical theory [7,12,13, 14].

In recent months we have continued to build on this work:

- Continuing with the analytical method of References 8 and 9, we examined the onset of collision controlled transport and estimated the critical temperature interval that separates ballistic and fully collision controlled transport in a simple semiconductor structure [15]. This work demonstrated the possibility of a a novel oscillatory "phonon-assisted ballistic resistance".

- We extended the theory of quantum capacitance, establishing the atomistic connection between the capacitive energy, the ionization potential, the electron affinity, and the Kohn-Sham orbital energies of the charged system [16]. The tendency of the derived quantum capacitance to limit toward the classical electrostatic capacitance as the system becomes macroscopically large was also demonstrated in this work.

- We have begun optimizing a version of SEMC for structures that vary in only one dimension [17], such as resonant tunneling diodes and quantum well lasers. This version should be computationally quite efficient and allow for the ready incorporation of new physics while still allowing the simulation of most nanostructures of interest.

- In parallel with SEMC, we have also begun development of an "absorbing potential" based method for simulating dissipative quantum transport [17]. This approach is designed as a computationally efficient method of simulating the essential physics of such transport for inclusion in standard devices simulators. It also can be used in SEMC to simulate the effects of subsequent scattering on the initial scattering process, such as finite-lifetime broadening in energy in the "final" states of the initial scattering process.

- In a different project we reviewed the literature on real-space transfer effects with Dr. S. Gribnikov, encompassing literature on the subject from both the west and the former Soviet Union [18].

In conclusion, we believe that this ARO sponsored work of the last three years has significantly advanced the understanding of both semiclassical and quantum transport, and to bridge the gap between these two limits. Furthermore, we believe that FBMC, SEMC, along with the absorbing potential simplification, and our quantum capacitance calculations will be the building blocks of future integrated multi-scale simulations of nanostructure devices.

2 ARO Sponsored Publications

1. P. D. Yoder, V. D. Natoli and R. M. Martin, "Ab initio Analysis of the Electron-Phonon Interaction in Silicon," J. Appl. Phys. **73**, 4378 (1993).

2. P. D. Yoder, "First Principles Calculation of Electron-Phonon Scattering Rates in Si," in *Proceedings of the International Workshop on Computational Electronics*, Leeds, UK, August 11–13 1993.

3. P. D. Yoder and K. Hess, "First-Principles Monte Carlo Simulation of Transport in Si," in *Proceedings of the 8th International Conference on Hot Carriers in Semiconductors*, Oxford, UK, August 16–20, 1993.

4. P. D. Yoder and K. Hess, "Application of a New Multi-Scale Approach to Transport in a GaAs/AlAS Heterojunction Structure," in *Negative Differential Resistance and Instabilities in 2-D Semiconductors*, edited by N. Balkman et al. (Plenum, New York, 1993) pp. 99-107.

5. L. F. Register and K. Hess, "Numerical Simulation of Electron Transport in Mesoscopic Structures with Weak Dissipation," Phys. Rev. B **49**, 1900 (1994).

6. K. Hess and L. F. Register, "Modeling Nanostructure Devices," in *Proceedings of SISDEP 93, the 5th International Conference on Simulation of Semiconductor Devices and Processes* Vienna, Austria, September 7–9, 1993. Vol. 5, Selberherr, H. Stippel and E. Strasser editors, pp. 9–16.

7. K. Hess, L. F. Register and M. Macucci, "Toward a Standard Model in Nanostructure Transport Problems Including Dissipation," in *Proceedings of the 2nd International Symposium on Quantum Confinement: Physics and Applications*, edited by M. Cahay, S. Bandyopadhyay, J. P. Leburton, A. W Kleinsasser and M. A. Osman (The Electrochemical Society, 1994), Vol. 94-17, pp. 3–17.

8. V. L. Gurevich, V. B. Pevzner and K. Hess, "Phonon-Enhanced Landauer Resistance," J. Phys. **6**, 8363 (1994).

9. V. L. Gurevich, V. B. Pevzner and K. Hess, "Non-Ohmic Phonon-Assisted Landauer Resistance," in Proceedings of the NATO Advanced Science Institute on Quantum Transport in Ultrasmall Devices, Ciocco, Italy, July 17-30, 1994.

10. K. Hess, N. Holonyak, Jr. and T. A. Richard, "Photosensitive Coulomb Blockade in Semiconductor p-n Tunnel Diodes," Appl. Phys. Lett. **63**, 1408 (1993).

11. D. V. Averin, L. F. Register, K. K. Kikharev and K. Hess, "Single-Electron Coulomb Exclusion on the Atomic Level," Appl. Phys. Lett. **64**, 126 (1994).

12. M. Macucci and K. Hess, "Numerical Study of 2-D Quantum Dots," in *Proceedings of the International Workshop on Computational Electronics*, Leads, UK, August 11-13, 1993. ,

13. M. Macucci, K. Hess and G. J. Iafrate, "Electronic Energy Spectrum and the Concept of Capacitance in 2-D Quantum Dots," Phys. Rev. B **48**, 17354 (1993).

14. M. Macucci, K. Hess and G. J. Iafrate, "Simulation of Electronic Properties and Capacitance of Quantum Dots," J. Appl. Phys. **77**, 3267 (1995).

15. V. L. Gurevich, V. B. Pevzner and K. Hess, "Phonon-Assisted Ballistic Resistance," Phys. Rev. B. **51**, 5219 (1995).

16. G. J. Iafrate, K. Hess, J. B. Krieger, and M. Macucci, "Capacitive Nature of Atomic-Size Structures," accepted by Phys. Rev. B.

17. K. Hess, P. von Allmen, M. Grupen and L. F. Register, "Simulating Electronic Transport in Semiconductor Nanostructures" in *Proceedings of the NATO Workshop on Future Trends in Microelectronics*, Ile de Bendor, France, July 17-21, 1995, to be published.

18. Z. S. Gribnikov, K. Hess and G. A. Kosinovsky, "Nonlocal and Nonlinear Transport in Semiconductors: Real Space Transfer Effects," J. Appl. Phys. **74**, 1 (1995).

3 Invited Presentations of ARO Sponsored Research

1. "Numerical Approaches to Electronic Transport in Mesoscopic Structures Weak Dissipation," presented at the International Symposium on New Phenomena in Mesoscopic Structures, Hawaii, December 7–11, 1992.

2. "Approaching the Quantum Limit," presented at the 30th Annual International Nuclear and Space Radiation Effects Conference, Snowbird, Utah, July 20–23, 1993.

3. "Modeling Nanostructures Devices," presented at SISDEP 93, 5th International Conference on Simulation of Semiconductor Devices and Processes, Vienna, Austria, September 7–9, 1993.

4. "The Concept of Capacitance for Nanostructures," presented at the 21st Midwest Solid State Symposium, Detroit, MI, October 2 and 3, 1993.

5. "Electronic Transport in Silicon at High Energies: Recent Progress in Full Band Monte Carlo Simulations," presented at the SRC Topical Research Conference on Device Performance TCAD, October 23–28, 1993.

6. "Time Constant for an Atomic Relay Computed by Ab Initio Molecular Dynamics," presented at the Surfaces and Interfaces in Mesoscopic Devices Conference, Keauhou-Kona, Hawaii, April 24–29, 1994.

7. "The Electron-Hole Imbalance in the Active Region of QW Lasers, and its Effect on the Threshold Current," presented at the 3rd Annual International Workshop on Computational Electronics, Portland, OR, May 18–20,1994.

8. "Toward a Standard Model in Nanostructure Transport Problems Including Dissipation," presented at the 185th Society Meeting of the Electrochemical Society, Inc., San Francisco, CA, May 22–27, 1994.

9. "Simulations of Electronic Properties and Capacitance of Quantum Dots," presented at US-European Workshop on Nanostructures, Santa Barbara, CA, March 27 and 28, 1995.

10. "Simulating Electronic Transport in Semiconductor Nanostructures," presented at the NATO Workshop on Future Trends in Microelectronics, Ile de Bendor, France, July 17–21, 1995.

4 Degrees awarded to ARO supported students

Vadim B. Pevzner
Ph.D.: "Theoretical and Numerical Study of Nanostructures"
Current Employer: North Carolina State University

Paul D. Yoder
Ph.D.: "First Principles Monte Carlo Simulation of Charge Transport in Semiconductors"
Current Employer: Swiss Institute of Technology (ETH), Switzerland

5 Awards of Principle Investigator, Karl Hess

IEEE Electron Devices Society J. J. Ebers Award, 1993
University Scholar, University of Illinois, 1993
Fellow of the American Association for the Advancement of Science, 1994
Fellow of the American Physical Society, 1995
Sarnoff Award, 1995 IEEE Field Award
Tau Beta Pi Daniel C. Drucker Eminent Faculty Award University of Illinois, 1995