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13. ABSTRACT (Maximum 200 words)
A brief summary of research accomplishments during the past three years is given. Details are covered by the six submitted technical reports and twenty papers published in refereed journals.

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**SIMULATION OF ELECTRONIC TRANSPORT IN
SEMICONDUCTOR HETEROLAYER DEVICES**

FINAL REPORT

KARL HESS

October 10, 1992

U. S. ARMY RESEARCH OFFICE

**PROPOSAL NUMBER 26711EL
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**Beckman Institute and
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Progress Over the Past Three Years and ARO Sponsored Publications

Work in the three years of the grant was aimed at both improving and generalizing the full band Monte Carlo approach and at developing numerical methods to simulate transport in nanostructures. Our emphasis has been to understand transport in wide energy ranges away from the band edges. This goal can be achieved easier with the aid of computer visualization since the complexity of transport at high energies is such that visualization techniques appear indispensable. Below a brief description of the major progress is given. Details are described in 20 publications which are listed also.

- We have developed techniques of visualization in 3-dimensional geometric space and k-space with the possibility of animated sequences.

A summary of this work was described in Phys. Today [1].

In the area of Monte Carlo Transport we have:

- Developed a complete theory of impact ionization including the intracollisional field effect and collisional broadening [2-5].
- Applied Monte Carlo methods to field effect transistors and Real Space Transfer devices [6].
- Generalized the full band Monte Carlo method to include \vec{k} -dependent scattering (instead of energy dependent) and a generalized treatment of phonon scattering using a unified pseudopotential approach [8-10].

In the area of quantum transport (mesoscopic systems) we have:

- Developed numerical approaches to calculate transmission coefficients in complex nanostructures [11,12].
 - Simulated transient response in mesoscopic devices [13,14].
 - Included the effects of weak dissipation in nanostructures and mesoscopic systems [16].
 - Investigated electron-electron interactions in nanostructures by a direct numerical approach including two electrons in an exact formalism [17].
 - Developed criteria for the additivity of conductance in parallel mesoscopic channels [18,19].
- and
- Given a review of various numerical approaches that can efficiently be used to describe transport *in mesoscopic systems* [20].

ARO Sponsored Publications 1989 - 1992

- [1] K. Hess, "Supercomputer Images of Electron Device Physics," *Physics Today*, Feb. (1990).
- [2] J. Bude, K. Hess and G. J. Iafrate, "Field Assisted Impact Ionization in Semiconductors," *Proceedings of the Workshop on Computational Electronics*, K. Hess, J. P. Leburton and U. Ravaioli editors, Kluwer Academic Publishers, pp. 131-136 (1990).
- [3] J. Bude, K. Hess and G. J. Iafrate, "Impact Ionization: Beyond the Golden Rule," *Proceedings of the 7th International Conference on Hot Electrons, Semicond. Sci. Technol.*, Vol. 7 pp. B506-B508, March, 1992.
- [4] J. Bude, K. Hess and G. J. Iafrate, "Impact Ionization in Semiconductors: Effects of High Electric Fields and High Scattering Rates," *Phys. Rev. B.*, Vol. 45, No. 19, pp. 10958-10964, May 1992.
- [5] J. Bude and K. Hess, "Thresholds of Impact Ionization in Semiconductors," *JAP* accepted for publication.
- [6] I. Kizilyalli and K. Hess, "Monte Carlo Simulations of Submicron Devices," Chapter III.2, "Hot Carriers in Semiconductor Microstructures: Physics and Applications," Jagdeep Shah, Ed., Academic Press, pp. 235-275.
- [7] J. M. Higman, J. Bude, and K. Hess, "Electronic Transport in Semiconductors at High Energy," *Computer Physics Comm.* 67, pp. 93-104, 1991.
- [8] P. D. Yoder, J. Bude, J. M. Higman and K. Hess, "Monte Carlo Simulations of Electronic Transport in Semiconductors at High Energies," *Proceedings of the Seventh International Conference on Numerical Analysis of Semiconductor Devices and Integrated Circuits*, Copper Mt., CO (1991), Front Range Press, pp. 47-48 (1991).
- [9] P. D. Yoder, J. M. Higman, J. Bude and K. Hess, "Monte Carlo Simulation of Hot Electron Transport in Si Using a Unified Pseudopotential Description of the Crystal," *Proceedings of the 7th International Conference on Hot Electrons, Semicond. Sci. Technol.*, UK, Vol. 7, pp. B357-B359, 1992.
- [10] K. Hess (editor), "Monte Carlo Device Simulations: Full Band and Beyond," Kluwer Academic publishers, chapters 2,10.
- [11] V. Pevzner, F. Sols and K. Hess, "Approaches to Transport in Semiconductor Nanostructures," *Proceedings of the NATO ASI in Il Ciocco, Italy*, D. K. Ferry, editor, Plenum, New York pp. 223-254, 1991.

- [12] F. Sols and M. Macucci, "Circular Bands in Electron Waveguides," *Phys. Rev. B*, **41** pp. 11887-11891 (1990).
- [13] L. F. Register, U. Ravaioli and K. Hess, "Numerical Simulation of Mesoscopic Systems With Open Boundaries Using the Multidimensional Time-Dependent Schrödinger Equation," *J. Appl. Phys.* **69** (10), pp. 7153-7158 (1991).
- [14] L. F. Register, U. Ravaioli and K. Hess, "Transient Response in Mesoscopic Devices," *Proc. of the Workshop on Computational Electronics (Urbana, IL., May 21-23, 1990)* 235-238 (1990).
- [15] L. F. Register, U. Ravaioli and K. Hess, "A Numerical Method for the Calculation of Transient Response in Mesoscopic Devices," *Proceedings of the NATO ASI*, D. K. Ferry, Editor, Plenum New York, pp.547, 1991.
- [16] F. Sols, "Dissipative Scattering and Transport in Mesoscopic Systems", *Proceedings of the International Symposium on Nanostructures and Mesoscopic Systems*, Santa Fe, New Mexico, 1991, Edited by W. Kirk and M. Reed, Academic Press, Inc., pp. 417-423 and F. Sols, "Scattering, Dissipation, and Transport in Mesoscopic Systems," *Annals of Physics*, Vol. 214, pp. 386-438, 1992.
- [17] L. F. Register and K. Hess, "A Two-Particle Model of Electron-Electron Interactions in Quantum Structures," *Proceedings of the International Symposium on Nanostructures and Mesoscopic Systems*, Santa Fe, New Mexico, 1991, Edited by W. Kirk and M. Reed, Academic Press, Inc., pp. 369-378, 1992.
- [18] M. Macucci and K. Hess, "Numerical Study of Mesoscopic Structures with Multiple Channels," *Proceedings of the International Workshop on Computational Electronics*, Beckman Institute, Urbana, May 28/29 (1992) pp. 245
- [19] M. Macucci and K. Hess, "Conditions for the Additivity of Conductance for Parallel Mesoscopic Constrictions," *Phys. Rev. B*. accepted for publication.
- [20] M. Macucci, V. Pevzner, L. F. Register and K. Hess, "Numerical Approaches to Transport in Mesoscopic Systems," *Proceedings of the Winterschool*, Mauterndorf, Austria, February 1992, to be published.

Invited Presentations

"Monte Carlo Simulation of Electron Transport in Semiconductors at High Energies," IMACS 1st International Conference on Computational Physics, University of Colorado at Boulder, Boulder, Colorado, June 11-15, 1990.

"Approaches to Transport in Semiconductor Nanostructures," (with V. Pevzner and F. Sols) NATO Advanced Study Institute on "Granular Nanoelectronics" Il Ciocco, July 23-August 4, 1990. (see paper #11)

"Monte Carlo Simulation of Impact Ionization in Semiconductors," presented at the IBM Summer Institute on Monte Carlo Simulation on Supercomputers," Oberlech, Austria, August 13-17, 1990.

"Electronic Transport in Semiconductors at High Energy," presented at Supercomputer Symposium, University of Minnesota, Minneapolis, Minnesota, November 19-20, 1990.

"Integration Technologies of the Future: The Ultrafast, Ultrasmall, and the Ultradense," presented at the National Engineering Consortium ComForum, Phoenix, Arizona, March 14-15, 1991.

"Monte Carlo Simulations of Electronic Transport in Semiconductors at High Energies," presented at Seventh National Conference on Numerical Analysis of Semiconductor Devices and Integrated Circuits, Copper Mt., Co., April 8-12, 1991. (see paper #8)

"Numerical Approaches to Transport in Mesoscopic Systems," presented at International Conference on Mesoscopic Systems, Mauterndorf, Austria, February 24-28, 1992. (see paper #20)

"Electronic Transport in Semiconductors at High Energies," presented at NATO Workshop on Hot Electron Instabilities," Il Ciocco, September 22, 1992.

Ph.D. Thesis Finished

J. Bude Ph.D. (1992)

V. Pevzner Ph.D. (1992)