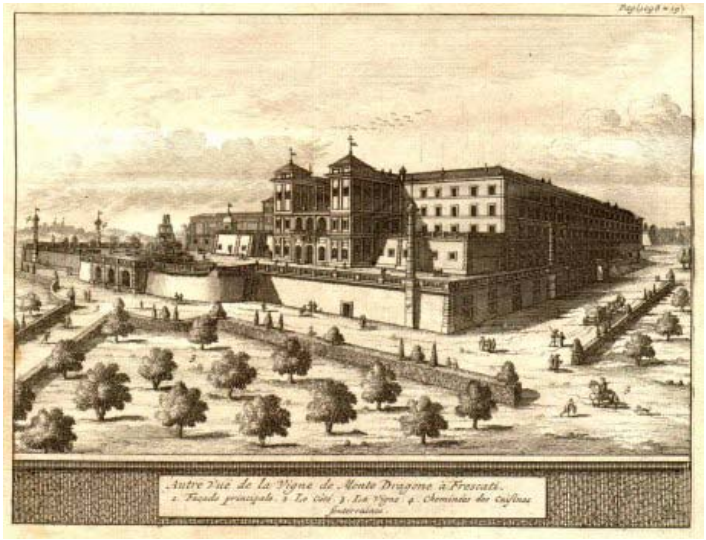
International Workshop on
Computational Electronics (IWCE-9)

Preliminary Program



Villa Mondragone

Monte Porzio Catone (Rome), Italy

25-28 May 2003

All relevant information are available at:

http://www.optolab.uniroma2.it/iwce9

Sunday, 25 May 2003	
Sun. 18.00-21.00	***Registration***
Sun. 19.00-21.00	**WELCOMING PARTY**

Monday, 26 May 2003 — **NanoMOS 1** — **Chairman: S. M. Goodnick**	
Mon. 8.45-9.00	**Prof. Alessandro Finazzi Agrò,** Rector of the University of Rome "Tor Vergata" **Prof. Nicola Vittorio,** Dean of the Faculty of Natural Science **Prof. Franco Giannini,** Head of the Department of Electronic Engineering ***Welcome address***
Mon. 9.00-9.30	**M. Fischetti (invited)** **IBM Research Division, Thomas J. Watson Research Center Yorktown Heights** ***Scaling MOSFETs to the limit: A physicist's perspective***
Mon. 9.30-9.45	F. M. Bufler, A. Schenk and W. Fichtner Institut fur Integrierte Systeme, ETH Zurich *Monte Carlo, Hydrodynamic and Drift–Diffusion Simulation of Scaled Double–Gate MOSFETs*
Mon. 9.45-10.00	G. Kathawala and U. Ravaioli Beckman Institute, University of Illinois at Urbana-Champaign *Comparison of Double-Gate MOSFETs and FinFETs with Monte Carlo Simulation*
Mon. 10.00-10.15	Hideaki Tsuchiya, Motoki Horino and Tanroku Miyoshi Department of Electrical and Electronics Engineering, Kobe University *Quantum Monte Carlo Device Simulation of Nano-Scaled SOI-MOSFETs*
Mon. 10.15-10.30	G. Fiori, G. Iannaccone Dipartimento di Ingegneria dell'Informazione, Università di Pisa *"Atomistic", quantum and ballisticeffects in sub-100nm "well tempered" MOSFET*
Mon. 10.30-11.00	**COFFEE BREAK**
Monday, 26 May 2003 — Quantum transport 1 — Chairman: M. P. Anatram	
Mon. 11.00-11.15	L. Bonci, M. Macucci, D. Guan, U. Ravaioli Dipartimento di Ingegneria dell'Informazione, Università di Pisa *Numerical analysis of tunneling between stacked quantum wires with the inclusion of the effects form effective mass discontinuities*
Mon. 11.15-11.30	Ting-wei Tang and Bo Wu Department of Electrical and computer Engineering, University of Massachusetts *Quantum Correction for the Monte Carlo Simulation via the Bohm Potential*
Mon. 11.30-11.45	Andrea Bertoni, Paolo Bordone, Giulio Ferrari, Nicoletta Giacobbi, Carlo Jacoboni S3 Research Center, Istituto Nazionale per la Fisica della Materia *Proximity effect of the contacts in electron transport in mesoscopic devices*
Mon. 11.45-12.00	R.Proietti Zaccaria, F.Rossi INFM e Dipartimento di Fisica, Politecnico di Torino *Generalized wigner function formulation for quantum systems with open boundaries*
Mon. 12.15-12.20	H. Kosina, M. Nedjalkov, and S. Selberherr Institute for Microelectronics, TU Vienna *A Monte Carlo Method Seamlessly Linking Quantum and Classical Transport Calculations*
Mon. 12.30-12.45	Gerhard Klimeck, Phillip Stout and R. Chris Bowen Jet Propulsion Laboratory, California Institute of Technology *Quantum and semi-classical transport in RTDs using NEMO 1-D*
Mon. 12.45-14.00	**LUNCH BREAK**

Monday, 26 May 2003 **Transport/devices 1** Chairman: C. Ringhofer	
Mon. 14.00-14.30	**Jason Ayubi-Moak, Shela Wigger, Stephen Goodnick and Marco Saraniti (invited)** **Department of Electrical Engineering, Arizona State University and Illinois Institute of Technology** ***Coupling Maxwell's Equations to Full Band Particle -Based Simulators***
Mon. 14.30-14.45	A. Wacker, S.-C. Lee, and M. F. Pereira Institut fur Theoretische Physik, Technische Universitat Berlin *Quantum Transport and Gain in Quantum Cascade Lasers*
Mon. 14.45-15.00	R. C. Iotti, F. Rossi Dipartimento di Fisica, Politecnico di Torino *Microscopic modelling of opto-electronic quantum devices: A predictive simulation tool*
Mon. 15.00-15.15	G.Csaba, W.Porod Center for Nano Science and Technology, Department of Electrical Engineering, University of Notre Dame *Restoration of magnetization distributions from joint magnetic force microscopy measurements and micromagnetic simulations*
Special Section: Web Based Simulations	
Mon. 15.15-15.45	*Phantoms HUB:* M. Macucci *ICODE:* F. Compagnone
Mon. 15.45-16.00	**COFFEE BREAK**
Mon. 16.00-18.30	**POSTER SESSION** **With wine tasting and traditional snacks**

Tuesday, 27 May 2003 Chairman: E. Molinari **Molecular and biological systems 1**	
Tue. 8.45-9.15	**A. Svizhenko, A. Maiti and M. P. Anantram (invited)** **NASA Ames Research Center** ***Modeling of the electro-mechanical response of carbon nanotubes: Molecular Dynamics and Transport Calculations***
Tue. 9.15-9.45	**T. van der Straaten, G. Kathawala and U. Ravaioli (invited)** **Beckman Institute, University of Illinois at Urbana-Champaign** ***A Transport Monte Carlo Simulation Model for Ionic Channels***
Tue. 9.45-10.00	Sheila Aboud, Marco Saraniti, R. Eisenberg Molecular Biophysics Dept., Rush University and Illinois Institute of Technology *Computation issues in modeling ion transport in biological channel: Self-consistent particle based simulations*
Tue. 10.00-10.15	R. Eisenberg Molecular Biophysics Dept., Rush University *Understanding BioMolecules by Reverse Engineering*
Tue. 10.15-10.30	C.Millar, A.Asenov and S.Roy Device Modelling Group, Department of Electronics and Electrical Engineering, Glasgow University *Brownian Ionic Channel Simulation*
Mon. 10.30-11.00	**COFFEE BREAK**

Tuesday, 27 May 2003 **NanoMOS 2** Chairman: W. Porod	
Tue. 11.00-11.30	**T. Ezaki (invited)** **Silicon systems research laboratories, NEC Corporation** ***Sub-100nm MOSFET simulation based on fully 2D quantization of electrons***
Tue. 11.30-11.45	S.E. Laux, A. Kumar and M.V. Fischetti IBM Research Division, Thomas J. Watson Research Center *Does Circulation in Individual Current States Survive in the Total Current Density?*
Tue. 11.45-12.00	Hiroshi Nakatsuji, Yoshinari Kamakura, Kenji Tanichi Department of electronics and information systems, Osaka University *Full band Monte Carlo simulation of two-dimensional hole transport in strained si p-MOSFETs*
Tue. 12.00-12.15	M. P. Anantram and Alexei Svizhenko Center for Nanotechnology, NASA Ames Research Center *Role of Phonon Scattering in Nanotransistors*
Tue. 12.15-12.30	C.Ringofer, D.Vasileska Department of mathematics, Arizona State University *Effective potential approach to modeling of 25nm MOSFET devices*
Tue. 12.30-12.45	H. Takeda, N. Mori, and C. Hamaguchi Department of Electronic Engineering, Osaka University *Quantum effects on transport characteristics in ultra-small MOSFETs*
Tue. 12.45-14.00	**LUNCH BREAK**

Tuesday, 27 May 2003 **Quantum transport 2** Chairman: P. Vogl	
Tue. 14.00-14.30	**M. Lundstrom (invited)** **Purdue University** ***Modal methods for Quantum Modeling of Semiconductor Devices***
Tue. 14.30-14.45	John R. Barker Department of Electronics and Electrical Engineering, University of Glasgow *Green function simulation study of non self-averaging scattering processes in atomistic semiconductor devices*
Tue. 14.45-15.00	M. Boriçi J. R. Watling, R. Wilkins, and J. R. Barker Department of Electronics and Electrical Engineering, University of Glasgow *A non perturbative model of surface roughness scattering for Monte Carlo simulation of relaxed silicon n-MOSFETs*
Tue. 15.00-15.15	C. Hamaguchi Dept. Electronic Engineering, Osaka University *High electron mobility limited by remote impurity scattering*
Tue. 15.15-15.30	E. Ciancio, R. C: Iotti, F. Rossi Dipartimento di Fisica, Politecnico di Torino *Gauge invariant formulation of Fermi's Golden Rule: Application to high field transport in semiconductors*
Tue 15.30-23.00	**EXCURSION AND SOCIAL DINNER**

Wednesday, 28 May 2003 — Chairman: C. Jacoboni	
Molecular and biological systems 2	
Wed. 8.45-9.15	**A. Fisher** (invited) **Department of Physics and Astronomy, University College** ***The role of phonons in molecular electronics: coherent and incoherent transport***
Wed. 9.15-9.45	**Otto F. Sankey[1] , Jun Li[1], Gil Speyer[2], and John Tomfohr[1,] (invited)** **[1]Department of Physics and Astronomy, [2]Department of Electrical Engineering** **Arizona State University** ***Theoretical aspects of tunneling current through single molecules***
Wed. 9.45-10.00	Alessandro Pecchia, Marieta Gheorghe, Luca Latessa, Aldo Di Carlo. Dipartimento di Ingegneria Elettronica, Universita` di Roma "Tor Vergata" *Coherent and incoherent transport through molecular devices*
Wed. 10.00-10.15	Christophe Adessi, Steven P. Walch and M. P. Anantram LPMCN, Universite Claude Bernard Kyon *DNA Conductance Modeling*
Wed. 10.15-10.30	A. Calzolari, R. Di Felice, and E. Molinari INFM - National Research Center on nanoStructures and bioSystems at Surfaces (S3) and Dipartimento di Fisica, Università di Modena e Reggio Emilia *Computer Simulation of Biomolecular Nanostructures*
Wed. 10.30-11.00	**COFFEE BREAK**

Wednesday, 28 May 2003 — Chairman: S. Laux	
Transport/devices 2	
Wed. 11.00-11.30	**S.Picozzi, R.Asahi, A.J. Freeman (invited)** **INFM - Dipartimento di Fisica, Università degli Studi L'Aquila** ***Accurate First Principles detailed balance determination of auger recombination and impact ionization rates in semiconductors***
Wed. 11.30-11.45	Y. Kazami, D. Kasai, Y. Mitani and K. Horio Faculty of Systems Engineering, Shibaura Institute of Technology *Simulation of Lag Phenomena and Pulsed I-V Curves of Compound Semiconductor FETs as Affected by Impact Ionization*
Wed. 11.45-12.00	N. J. Pilgrim, W. Batty, R. W. Kelsall Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds *Electrothermal Monte Carlo simulations of InGaAs/GaAs HEMTs*
Wed. 12.00-12.15	J. Branlard, S. Aboud, S. Goodnick, and M. Saraniti Electrical and Computer Engineering Department, Illinois Institute of Technology *Frequency analysis of 3D GaAs MESFET structures using full-band particle-based simulations.*
Wed. 12.15-12.30	A. Gehring, H. Kosina, and S. Selberherr Institute for Microelectronics, TU Vienna *Analysis of Gate Dielectric Stacks Using the Transmitting Boundary Method*
Wed. 12.30-12.45	M. Städele, F. Sacconi, A. Di Carlo, and P. Lugli Infineon Technologies AG and INFM-Università degli Studi di Roma Tor Vergata *Tunnel mass enhancement and oxide thickness corrections in ultrathin SiO2 layers*
Wed. 12.45-14.00	**LUNCH BREAK**

Wednesday, 28 May 2003 — Chairman: D. K. Ferry	
Quantum dots	
Wed. 14.00-14.15	T. Kuhn, M. Glanemann, and V.M. Axt Institut fur Festkorpertheorie, Westfalische Wilhelms Universitat Munster *Quantum control of carrier capture processes into localized states of a quantum dot*
Wed. 14.15-14.30	Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin*, R. Chris Bowen, and Paul von Allmen Jet Propulsion Laboratory, California Institute of Technology *Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots*
Wed. 14.30-14.45	M. Sabathil, D. Mamaluy, and P. Vogl 1Walter Schottky Institut, Technische Universität München *Efficient computational method for ballistic current and application to quantum dot RTD's*
Wed. 14.45-15.00	M. Povolotskyi, J.Gleize, A. Di Carlo, P. Lugli, S.Birner, P.Vogl INFM-Università degli Studi di Roma Tor Vergata and Walter Schottky Institute *Microscopic Description of Nanostructures grown on (N11) surfaces*
Wed. 15.00-15.15	R. Akis, J.P. Bird and D.K. Ferry Department of Electrical Engineering, ASU *Signatures of a Discrete Level Spectrum and Dynamical Tunneling in the Conductance of a Large Open Quantum Dots*
Wed. 15.15-15.30	Devis Belluci, Massimo Rontani, Filippo Troiani, Guido Goldoni and Elisa Molinari INFM - National Research Center on nanoStructures and bioSystems at Surfaces (S3) and Dipartimento di Fisica, Università degli Studi di Modena e Reggio Emilia *Spin-Spin Interaction In Artificial Molecules With In-Plane Magnetic Field*
Wed. 15.30- 15.45	**CLOSING REMARKS**

Poster Session

16.00 – 18.30 Monday, 26 May 2003

1	C.Alexander, J. R. Watling and A. Asenov Department of Electronics and Electrical Engineering Device Modelling Group, University of Glasgow *Mobility variations in ultra-small devices due to discrete charges*
2	Andrea Bertoni Dipartimento di Elettronica Informatica e Sistemistica, Università di Bologna *Simulation of electron decoherence induced by carrier-carrier scattering*
3	L. Boeri, G. Bachelet, E. Cappelluti, L. Pietronero Dipartimento di Fisica, Roma "la Sapienza" *Anharmonicity and non-adiabatic e-ph interaction in MgB2 and bad actors superconductors*
4	A. Bolognesi, A. Di Carlo Dipartimento di Ingegneria Elettronica, Universita di Roma "Tor Vergata" *Influence of carrier mobility and trap states on the transfer and output characteristics of organic thin film transistors*

5	L. Berletti, L. Demeio, O. Morandi, G. Frosali Dipartimento di Matematica, Università di Firenze *Numerical simulation of the Wigner-Kane model for a tunneling diode*
6	A. Caddemi, N. Donato, M.G. Xibilia Faculty of Engineering, University of Messina *Advanced Simulation of Semiconductor Devices by Artifical Neural Networks*
7	G. Curatola, G. Iannaccone Dipartimento di Ingegneria dell'Informazione, Università di Pisa *Ballistic transport in SiGe and strained Si Mosfet*
8	L. Demeio Dipartimento di Scienze Matematice, Università di Ancona *Splitting scheme solution of the collisionless Wigner equation with non-parabolic band profile*
9	Chris Duffy and Paul Hasler Department of Electrical and Computer Engineering, Georgia Institute of Technology *Modeling Hot-Electron Injection in PFET's*
10	G. Roy, A. R. Brown, A. Asenov, S. Roy Device Modelling Group, Department of Electronics and Electrical Engineering, Glasgow University *Quantum Aspects of Resolving Discrete Charges in "Atomistic" Device Simulations*
11	J. Shi, I. M. Gamba Dept. of Mathematics, University of Texas *A high order Wigner solver for quantum transport in nanostructures*
12	M.J. Gilbert, S.N. Milicic, R. Akis, and D.K. Ferry Department of Electrical Engineering and Center for Solid State Electronics Research, Arizona State University *Modeling of Fully Depleted Short Channel SOI MOSFETs in 3D using Recursive Scattering Matrices with Self-Consistent Potentials*
13	D. Guan, A. Godoy, U. Ravaioli and F. Gamiz Beckman Institute, University of Illinois at Urbana-Champaign *Comparison between non-equilibrium Green's function and Monte Carlo simulations for transport in a silicon quantum wire structure*
14	K. Kalna, L. Yang and A. Asenov Device Modelling Group, Department of Electronics and Electrical Engineering, Glasgow University *Simulation Study of High Performance III-V MOSFETs for Digital Applications*
15	W Ma, S Kaya and A Asenov SEECS, Russ College of Engineering & Technology, Ohio University *Study of RF Linearity in sub-50nm MOSFETs Using Simulations*
16	Z Ikonic, P Harrison and R W Kelsall Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds *Simulation of Carrier Transport in p-Si/SiGe Quantum Cascade Emitters*
17	G. Leuzzi, A. Mencattini, M. Salmeri Dipartimento di Ingegneria Elettronica, Università di Roma "Tor Vergata" *Physical based correction of extracted conductance parameters of nonlinear microwave semiconductor devices*

18	L. Yang, J. R. Watling, M. Boriçi, R. C. W. Wilkins, A. Asenov, J. R. Barker and S. Roy Department of Electronics and Electrical Engineering, Glasgow University *Simulations of scaled sub-100nm strained Si p-channel MOSFETs*
19	A. J. Garcıa-Loureiro, K. Kalna, A. Asenov and J. M. Lopez-Gonzalez Departmento de Electr´onica y Computaci´on, Universidad de Santiago de Compostela *3D Parallel Simulations of Alloy and Dopant Fluctuation Effects in PHEMTs*
20	A.Majorana, J.Carrillo, I.M.Gamba, Chi-Wang Shu Dipartimento di Matematica e Informatica, Università Degli Studi di Catania *A Direct solver for 2D non-stationary Boltzmann-poisson systems for semiconductor devices: a MESFET simulation by WENO-Boltzmann schemes.*
21	Alex Marchi, Susanna Reggiani, Andrea Bertoni, Massimo Rudan Advanced Research Center on Electronic System "E. DeCastro" and DEIS, Università di Bologna *Two-particle eigenfunctions of electrons propagating in two parallel quantum wires*
22	P.Marconcini, M.Macucci Dipartimento dell'Informazione Università Degli Studi di Pisa *Numerical techniques for the evaluation of conductance and noise in the presence of a perpendicular magnetic field.*
23	M.G.Pala, G. Iannaccone Dipartimento di Ingegneria dell'Informazione, Università di Pisa *Modeling decoherence effects on transport properties of mesoscopic devices*
24	A.Giorgio A. Perri Electron Devices Laboratory, Dipartimento di Elettrotecnica ed Elettronica, Politecnico di Bari *Modelling Photonic Band-Gap Structures having Multiple Defects*
25	A. Giorgio A.G. Perri Dipartimento di Elettrotecnica ed Elettronica, Politecnico di Bari, Laboratori di Dispositivi Elettronici *Design and Modelling of Phothonic Band-Gap Resonance Cavity*
26	S. Picozzi[1],A. Pecchia[2], M. Gheorghe[2], A. Di Carlo[2], P. Lugli[2], B. Delley[3], M. Elstner[4] [1]INFM and Dip. Fisica, Univ. L'Aquila, INFM and Dip. Ing. Elettronica, Univ. Roma Tor Vergata, [3]Paul Scherrer Institut, Villigen, [4]Dept. of Physics, University of Paderborn *A first-principles study of the Schottky barrier height at the organic/metal junctions in PTCDA/(Al,Ag) systems*
27	A.Reale, P.Lugli INFM e Department of Electronic Engineering, University of Rome Tor Vergata, Rome *Modeling nonlinear propagation of optical signals in semiconductor optical amplifiers*
28	V.Romano Dipartimento di Matematica e Informatica, Università degli Studi di Catania *Numerical Simulations of Electron Devices by the MEP hydrodynamical model of semiconductors*
29	M. Rosini, C. Jacoboni, S. Ossicini INFM-S3. Dept. Of Physics University of Modena *Semiclassical and quantum transport in Si/SiO2 Superlattices*
30	S.Roy, A.Lee, A.R. Brown, A. Asenov Device Modelling Group, Department of Electronics and Electrical Engineering, University of Glasgow *Applicability of quasi-3D and 3D MOSFET simulations in the 'atomistic' regime*
31	S.Roy, B.J.Cheng, G.Roy, A.Asenov Device Modelling Group, Department of Electronics and Electrical Engineering, University of Glasgow *A methodology for introducing 'atomistic' parameter fluctuations into compact device models for circuit analysis.*

32	M. Manenti, F. Compagnone, A. Di Carlo and P. Lugli Dipartimento di Ingegneria Elettronica Università di Roma Tor Vergata *Monte Carlo Simulations of Terahertz Emitting Quantum-Cascade Lasers*
33	F. Sacconi, A. Di Carlo, P. Lugli and M. Städele Dept. Electronic. Eng. University of Rome "Tor Vergata", Rome *Full-band tunneling currents in nanometer-scale MOS structures*
34	Santhosh Krishnan, Barry Zorman and Dragica Vasileska Dept. Electrical Eng. ASU *Self Consistent Subband Structure and Low Field Mobility calculation of Two Dimensional Holes in Si-SiGe Heterostructure FETs*
35	Johann Sée, Philippe Dollfus, Sylvie Galdin and Patrice Hesto Institut d'Électronique Fondamentale, Université Paris-Sud *Coulomb Blockade in Silicon Devices: Electronic Structure of Quantum Dots*
36	P.Shiktorov, E. Starikov, V. Gruzinkis, L. Regiani Semiconductor Physics Institute, Vilnius *Monte Carlo simulations of electronic nois in semiconductor materials an devices operating under cyclostationary conditions*
37	Constantinos Simserides Leibniz Institute for Neurobiology, Magdeburg *The Density of States and the pertinent Electronic Properties of the quasi two-dimensional-electron-gas in Simple and Diluted Magnetic Semiconductor heterostructures subjected to an in-plane magnetic field*
38	A. Sleiman, A. Di Carlo, P. Lugli Dipartimento di Ingegneria Elettronica, Università di Roma "Tor Vergata" *Monte Carlo Study of RF breakdown in HEMT's*
39	E. Starikov, P.Shiktorov, V. Gruzinkis, L. Regiani, L. Varani, J.C. Vaissiere Semiconductor Physics Institute, Vilnius *THz generation from dynamic free carrier superlattices in n+nn+ InN structures*
40	Alessandro Toscano and Lucio Vegni University "Roma Tre", Dept. of Applied Electronics *Advanced Electromagnetic Modelling of Multilayer Monolithic Microwave Integrated Circuits*
41	J. R. Watling, L. Yang, M. Boriçi, J. R. Barker and A. Asenov Department of Electronics and Electrical Engineering University of Glasgow *Degeneracy and high doping effects in deep sub-micron relaxed and strained Si n-MOSFETs*
42	Shinya Yamakawa, Shela J. Wigger, Marco Saraniti, and Stephen M. Goodnick Department of Electrical Engineering, Arizona State University *Fast Full-band Device Simulator for Wurtzite and Zincblende GaN MESFET using a Cellular Monte Carlo method*
43	Yiming Li and Hsiao-Mei Lu National Nano Device Laboratories, Taiwan *Effect of Shape and Size on Electron Transition Energies for Nanoscale InAs/GaAs Quantum Rings*
44	Yiming Li Ting-wei Tang, and Shao-Ming Yu National Nano Device Laboratories, Taiwan *A Quantum Correction Model for Nanoscale Double Gate MOS Devices Under inversion conditions*
45	R. Akis and D.K.Ferry Dept. Elect. Eng. And Center for Solid St*ate Electronic Research,* Arizona State University *Kinetic lattice Monte Carlo Simulations of Processes on the Silicon (100) Surface*