Thursday June 3, 1999 - Afternoon
Jeudi 3 juin 1999 - Après midi

L-V.1 14:00-14:40 Invited

THEORY OF ELECTRON TRANSPORT IN SMALL SEMICONDUCTOR DEVICES USING THE PAULI MASTER EQUATION, **M.V. Fischetti,** IBM Research Division, Thomas J. Watson Research Center, P.O.Box 218, Yorktown Heights NY 10598, USA

Drift-diffusion, hydrodynamics, and even Monte Carlo sbnulations are entirely based on the semiclassical 'billiard ball' description of the electrons, i.e., objects of well-defined position and velocity. But in semiconductor structures whose dirJensions are small enough to approach the wavelength of the electrons in the 'contacts' (40 nm or so for Si), we can instead use a complementary view, regarding the contacts as injecting 'pure plane waves'. Therefore, by solving the self-consistent Poisson/Scllroedinger problem with open boundary conditions (to account for the presence of the contacts), and by accounting for scattering among the eigenstates using Fermi golden rule, we obtain a first-order kinetic (Master) equation which describes electron transport in these tiny devices. When written in a basis of suitable wavefiJnctions and with the appropriate open boundary conditions, this transport equation removes some of the approximations which render the Boltzmann equation unsatisfactory at small length-scales, permitting the inclusion of tunneling, interference effects, arbitrary'steep' potentials, and intra-collisional field effects. . Here the master equation is derived emphasizing the irreversibility. After a discussion on the validity and limitations of this approach, three one-dimensional examples Ian n+-i-n+ diode, an MOS tunneling structure, and a resonant tunneling diode) will be described to illustrate the merits and faults of this scheme. The talk will close with a brief summary of work in progress: Extensions to 2-dimensions and the inclusion of full-bandstructure effects.

L-V.2 14:40-15:00

AB-INITIO CALCULATIONS OF OPTICAL PROPERTIES FOR THE DESIGN OF THERMOPHOTOVOLTAIC DEVICES, W. Wolf*, C.B. Geller**, T.S. Blazeck** and E. Wimmer*; *Molecular Simulations (MSI), Orsay, France, **Bettis Atomic Power Laboratory, West Mifflin PA, USA

An accurate and efficient ab initio methodology is presented for the prediction of optical properties of a wide range of semiconductors and other solids. Building on the work by Massidda et al. [1], the chosen implementation is based on a screened non-local exchange formulation [2] and the all-electron, full-potential linearized augmented plane wave (FLAPW) program [3]. This methodology includes spin-orbit relativistic effects. It predicts energy band gaps for a wide range of semiconductors with an absolute accuracy of a few tenths of one eV and describes relative changes with even higher accuracy. Optical spectra can be calculated for doped as well as pure semiconductors including subtle effects at the band edges (e.g. Moss-Burstein shift). The capabilities of this approach are illustrated for systems including pure GaAs, Zn and Se-doped GaAs, and co-doped semiconductors. The calculated absorption coefficient curve for In0.75Ga0.25As is compared with that interpolated from InAs and GaAs and the resulting changes in predicted quantum efficiency are shown for a typical thermophotovoltaic device geometry.

[1] S. Massidda, M. Posternak, and A. Baldereschi, Phys. Rev. B 48, 5058 (1993); S. Massidda, A. Continenza, M. Posternak, and A. Baldereschi, Phys. Rev. B 55, 13494 (1997)
[2] D. M. Bylander and L. Kleinman, Phys. Rev. B 41, 7868 (1990); A. Seidl, A. Görling, P. Vogl, J. A. Majewski, and M. Levy, Phys. Rev. B 53, 3764 (1996)
[3] H. J. F. Jansen and A. J. Freeman, Phys Rev. B 30, 561 (1984)

L-V.3 15:00-15:20

A TEMPERATURE DEPENDENT MODEL FOR THE SATURATION VELOCITY IN SEMICONDUCTOR MATERIALS, R. Quay, C. Moglestue, Fraunhofer-Institute of Applied Solid State Physics, Tullastr. 72, 79108 Freiburg, Germany, V. Palankovski, S. Selberherr, TU Vienna, Gusshausstr. 27-29, 1040 Vienna, Austria

Precise modeling of the saturation velocity is a key element for device simulation, especially for advanced devices such as e.g. High Electron Mobility Transistors (HEMTs) where the saturation velocity vsat is directly related to the available gain of the device. We present a model implementing the temperature dependence of the saturation velocity vsat into the two-dimensional device simulator MINIMOS-NT.

The new model covers all relevant materials such as the elementary semiconductors Si and Ge, and the binary III-V group semiconductors GaAs, AlAs, InAs and InP. Furthermore, a composition dependent modeling for alloyed semiconductors such as e.g. SiGe, Al(1-x)GaxAs or In(1-x)GaxAs is included. The implementation reflects a significant literature survey on available experimental data and Monte Carlo simulation data. The work is completed by new Monte Carlo simulations, especially for material compositions, where no experimental data are available. The effects of the temperature dependence of vsat for devices such as e.g. AlGaAs/InGaAs/GaAs HEMTs are demonstrated by device simulation results.