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13. ABSTRACT (Maximum 200 words)

This document describes the development of the Hydrodynamic Power Semiconductor Device Simulator (HPSDS), which solves the quantum mechanical hydrodynamic balance equations for the electrons and holes, along with the Poisson equation, for a two-dimensional device. The program will compute the electrostatic potential, electron and hole densities, recombination rate, electron and hole velocities, current densities, electron and hole temperatures, and other quantities of interest as functions of applied bias. The program allows extensive analysis of unipolar, bipolar, and heterostructure devices. Power devices such as thyristor and other four or five terminal devices are treated under all possible operating conditions. Both steady state and transient operating conditions can be considered. Because of the inclusion of energy balance equations and heat diffusion equation, accurate high-field characteristics can be obtained with this program. Silicon and Gallium Arsenide are the primary materials considered here, although other materials can be included if the user supplies the necessary material data file. In particular, wide band-gap materials such as Silicon Carbide and Gallium Nitride are included also.

In addition to the high-power aspects, high-frequency devices are also simulated. These include superlattice based negative differential resistance devices an resonant tunneling diodes.

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Power Semiconductor Simulation

Final Report

March 30, 2001

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Abstract

This document describes the development of the Hydrodynamic Power Semiconductor Device Simulator (HPSDS), which solves the quantum mechanical hydrodynamic balance equations for the electrons and holes, along with the Poisson equation, for a two-dimensional device. The program will compute the electrostatic potential, electron and hole densities, recombination rate, electron and hole velocities, current densities, electron and hole temperature, and other quantities of interest as functions of applied bias. The program allows extensive analysis of unipolar, bipolar, and heterostructure devices. Power devices such as thyristor and other four or five terminal devices are treated under all possible operating conditions. Both steady state and transient operating conditions can be considered. Because of the inclusion of energy balance equations and heat diffusion equation, accurate high-field characteristics can be obtained with this program.

Silicon and Gallium Arsenide are the primary materials considered in this program, although other materials can be included if the user supply the necessary material data file. In particular, wide band-gap materials such as Silicon Carbide and Gallium Nitride are being currently added to the materials library of the code. All materials related parameters are contained within a single subroutine, so that it is easily modified by the user to suit his own situation. For the theoretical basis and numerical implementation of the code, the reader is directed to the references. Materials parameters are also discussed in the references.

1. Introduction

1.1 Scope

This document reports on the project entitled "Power Semiconductor Simulation". The following paragraphs will identify a software system for accurate and computationally efficient codes for simulating high-power semiconductor devices. The codes were developed for use in any parallel-processing environment, which has the Massage Passing Interface (MPI), a de-facto standard of parallel programming model.

1.2 Objectives

The goal of this project was to develop a working simulation package for power semiconductor devices, such as large area thyristors, and high frequency devices, such as MESFETs, HEMTs for use in oscillators. Aside from the traditional materials to be simulated such as silicon and gallium arsenide, wide band gap semiconductors like silicon carbide will be simulated because of its good thermal and high voltage properties. The simulation code will be based on scaleable hardware and will be rapidly accessible to DoD researchers.

The project of large-scale numerical simulation of semiconductor devices involves computational tasks that are too demanding for single stand-alone computers and workstations. These tasks are best tackled with massively parallel computers. The numerical codes developed in this project will be specially tailored to suit massively parallel machines.

The code will enable users to perform full electrical and thermal analysis of semiconductor devices under high power/voltage/current operating conditions, thus making it a very useful design and simulation tool for power semiconductor applications as well as applicable to self-heating device studies and temperature dependent model generation.

1.3 Approach

Modeling of power semiconductor devices is more challenging than the modeling of ordinary semiconductor devices in that the former involves not only charge transport but also thermal transport in the devices. Further, the conduction of electricity is coupled with the conduction of heat. Thus the modeling/simulation of power devices depends upon the solution of a set of coupled nonlinear partial differential equations, the Poisson equation, the current continuity equations, and the semiconductor transport equations, as well as the heat diffusion equation, subject to the appropriate initial and boundary,conditions. The task of solving such a complicated system of equations entails extremely high demand for computing resources, both in terms of CPU cycles and memory. Massively parallel hardware and corresponding software will be needed to accomplish such a task.

1.4 Major Program Elements

The package contains several functional blocks, each of which is designed to perform a certain task. Each block is made of many program units, which perform sub-tasks. The program units have one or more subroutines or functions. In addition, a library consisting of commonly used tools are attached, along with several modeling drivers. The code is written in FORTRAN-90 language.

The blocks are:

Control (CF),
Definitions (DF),
Discretization (DS),
Devices (DV),
Local Quantities (LC),
Materials Parameters (MT).

The following is a complete list of the program units in each functional block. All the units are coded in FORTRAN-90 at the present time.

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The blocks are:

Control (CT);
Definitions (DF);
Discretization (DS);
Devices (DV);
Local Quantities (LC);
Materials Parameters (MT).

The following is a complete list of the program units in each functional block. All the units are coded in FORTRAN 90 at the present time.

CT_ADT
CT_DF
CT_ENERG
CT_PARTI
CT_POISS
DF_ENERG
DF_MOMEN
DF_PARTI
DF_POISS
DS_CARRIER_DENSITY

DS_CARRIER_TEMPR
DS_CHEMICAL_POTENTIAL
DS_CURRENT_DENSITY
DS_DOPEN_DENSITY
DS_ENERGY_DENSITY
DS_ENERGY_FLOW_DENSITY
DS_ENERGY_RATE
DS_EQUI_EQS
DS_INVERSE_MASS
DS_NPARA
DS_NPARA_CURRENT
DS_NPARA_POTENTIAL
DS_NPARA_TEMPR
DS_PARTICLE_RATE
DS_PHASE_VELOCITY
DS_POTENTIAL
DS_SCAT_RATE
DS_VELOCITY_RATE
DS_VELOCITY_TENSOR
DV_1D
DV_2D
DV_BOUND
DV_MyBOLISTIC_1D
GRID
HYSOLVER_UNITS
HyBE
LCEQ_UNITS
LC_CARRIER_DENSITY
LC_CHEMPOT
LC_CORR_FUNC
LC_CURRENT_DENSITY
LC_ENERGY_DENSITY
LC_ENERGY_FLOW_DENSITY
LC_ENERGY_RATE
LC_EQUI_EQS
LC_INVERSE_MASS
LC_NPARA
LC_NPARA_CURRENT
LC_NPARA_POTENTIAL
LC_NPARA_TEMPR
LC_PARTICLE_RATE
LC_PHASE_VELOCITY
LC_SCAT_RATE
LC_SINGLE_LT
LC_SINGLE_LT_IMP
LC_SINGLE_LT_PH

LC_VELOCITY_RATE
LC_VELOCITY_TENSOR
MT_ADT
MT_AlGAAS
MT_GENER
MT_KANE
MT_PARAB
MT_USER
WKSPACE
LIB_ELEMFUN
LIB_IE_POLATION
LIB_INTG
LIB_INTG_GAUSS
LIB_MATRIX
LIB_N_CONST
LIB_P_CONST
LIB_ROOT
LIB_VECP

2. Major Tasks

The following is a list of major tasks with the above observation in mind.

1. Parallelization of existing code for ballistic diode.
2. Single particle, time-independent code implemented
3. Modification of code to p-n diode and then power diode.
4. Single particle, time independent code parallelized
5. Single particle, time dependent code implemented
6. Modification of code for multilayer devices
7. Many-body, time independent code implemented
8. Single particle, time dependent code parallelized
9. Interface code development
10. Many-body, time independent code parallelized
11. Many-body, time-dependent code implemented
12. Single particle, time dependent, full band structure code implemented
13. Many-body, time dependent code parallelized.

3. Major Accomplishments

Schedule of Events

The following schedule reflects the schedule and status of the major tasks outlined above.

Module/Tasks	Expected Completion	Actual Completion
task 1	1/97	1/97
task 2	3/97	3/97
task 3	7/97	7/97

task 4	10/97	10/97
task 5	12/97	12/97
task 6	3/98	3/98
task 7	6/98	4/98
task 8	6/98	6/98
task 9	9/98	8/98
task 10	12/98	12/98
task 11	5/99	3/99
task 12	12/99	3/00
task 13	12/99	5/00

5. Alpha test summary

The following is a summary of the milestones and metrics demonstrated at the off-site CEN-2 Alpha testing conducted at Wright-Patterson AFB, on April 14, 1998.

- 63% speed-up achieved with 16 processors.
- MPI used on SGI Origin 2000 and SGI-PCA supercomputers.
- Now in process of moving parallel code to IBM SP-2.
- Reasonable load balance achieved.

Objective	Required	Observed
Scaled Speedup (16 nodes)	40 %	63%
% code in high level language	80 %	100 %
Number of HPC platforms software will run on.	2	2
# of validations per week	4 or more	4
User computer expertise required.(1-10)	Required = 2 (no GUI) 1=GUI, 5= need to modify source code each run.	2
Major error & % fixable per week.	10, 80 %	5, 100%
% Of software allows for interactive processing.	User specifies input and waits for output in a non real-time mode.	User specifies input and waits for output in a non real-time mode.
# of validations on full code	1 per 2 months	1 per 2 months
% of required external code interfaces completed	Greater or equal to 60%	60 %
% Of last validations that were accurate and valid.	60 %	100 %
# Of potential users exposed to new software capability through problems solved for	Greater or equal to 10	10

them.		

The parameters that can be calculated by computation method are summarized in the next table:

Carrier density	Yes
Carrier temperature	Yes
Electrostatic potential	Yes
Electric field	Yes
Current and current density	Yes

All outputs currently viewed with third party graphics visualization software.

6. Beta Test Results

Objective (CTP)		**Beta Test**
Scaled Speedup	REQ	50% on 32 processors
	OBS	
Scaled Speedup	REQ	Reduces clock time 16x or > on 32 processors
	OBS	
% code uses standard higher order languages, etc	REQ	90% or >
	OBS	
Number of HPC platforms software will run on with valid results.	REQ	2
	OBS	
4 or more validation testes on full code/month	REQ	Yes
	OBS	
Levels of users expertise software provides.	REQ	1
	OBS	
# major errors or < each week and % fixable	REQ	2, 100% within 2 workdays
	OBS	
# data/sets/user scenarios tested/week	REQ	4 or more
	OBS	
% of possible useful output parameters provided	REQ	90%
	OBS	

% of required external code interfaces completed	REQ	80% or greater
	OBS	
% of last 10 software runs produced accurate, valid output	REQ	80%
	OBS	
# of new users added to CTA's HPC community over last year.	REQ	15 or more
	OBS	

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