NAS Semiconductor Device Modeling Program

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Abstract

This document describes the research plans of the MRJ Semiconductor Device Modeling Program at NAS as of September 1997. The general motivation and approach for this work is presented first. Then, for each specific project in the program, the motivation, approach, and specific plans for the contract year are described.

1 Introduction (Bryan A. Biegel)

1.1 Importance of Information Technology

Information technology (IT) refers to any product used to create, store, retrieve, transmit, display, or process digital information. Thus, IT includes computer hardware, software, and peripherals; digital communications and networking equipment; and an increasing portion of many other products, including televisions, automobiles and airplanes, consumer electronics, medical electronics, mechanical control electronics, advanced weapons, and more. Since virtually every economic endeavor can benefit from the application of relevant information, IT has become fundamental to the efficient operation of nearly every business and government venture. Doing more business with less work, making more transactions with fewer errors, achieving higher quality in less time: all of these are hallmarks of the Information Revolution. Indeed, although it has been in progress for several decades, the effects of the Information Revolution are still accelerating. One of the latest accelerations has been through the Web, which has single-handedly, and in the space of only two or three years, given tens of millions of people better (easier, more reliable, cheaper, more democratic) access to desired information from more sources. The Web has also given these people new ways to communicate, learn, do research, work for social and political change, make purchases, and recreate.

The combination of developments like the Web and the rapidly increasing functionality per dollar of information technology (both hardware and software) have made IT both understandable and affordable by virtually everyone. As a result, IT now provides us with empowering technological innovations, enables us to address new challenges in our world, and allows us to tackle increasingly complex questions about our universe. IT has brought wider economic competition, faster technological advancements, and increased standards of living. Technology will continue to advance at an increasing rate due to an additional benefit of IT: that information can be (and increasingly is) comprehensively and cheaply stored, quickly retrieved, and expertly filtered. Knowledge (intelligently filtered information) is no longer lost or confined to a local research group, only to be rediscovered by many people with great cumulative effort and delay. With IT, knowledge can now be efficiently located and continuously developed and refined. The future advance of IT will continue these trends in the exponential growth of the knowledge base, allowing us to leverage the human intellect to make today's amazing discoveries and technologies seem neophyte by tomorrow. As a consequence, the effects of information technology, however profound they seem now, are just beginning to be felt.

1.2 Government/NASA Interests

Like businesses across the country, the government in general, and several of its agencies in particular (such as DoD, DoE, and NASA), have embarked on programs to "reinvent" themselves [1, 2]. That is, a stated policy goal is to accomplish more with less money, reduce administrative intrusiveness, while increasing reliability and reducing errors. The consistent application of advanced (but commercial, off-the-shelf) information technology will be a critical factor in the achievement of this goal. Thus, both the government and NASA have an interest in aiding the continued advancement of information technology as much as possible. The government has the additional interest that the information technology industry generates (directly and indirectly) a huge tax revenue, so that a declining IT industry would adversely affect the government's balance sheet.

The following are a few specific examples of government, DoD, and DoE uses of information technology.

- Government: Virtually free Web access, to democratize information access and education, increase tele-travel to reduce pollution, and make the economy (business and consumer transactions) more efficient. This will require dramatic increases in the gigaflops per dollar of server computers and gigabits per dollar of digital communications infrastructure, and similar decreases in the cost of Web access hardware.
- DoD: Advanced weapon systems (for aircraft, air defense, smart bombs, etc.) will require electronics (both digital and analog) to become more powerful, less expensive, smaller and lighter, and use less power. Detectors and transmitters will also have to become more sensitive and operate up to higher frequencies.
- DoD: Nuclear weapons safety simulation will require much larger supercomputer power than is available today.
- DoE: Nuclear power efficiency, safety, and waste storage modeling will also require huge computational power.

NASA needs for advanced information technology span the spectrum of applications, as is evident from the NASA Strategic Plan [2]. NASA plans include:

- Develop computational models consistent with observations of the formation and evolution of the universe, galaxies, stars, and planets. This will require much more powerful computational modeling capabilities.
- Develop predictive environmental, climate, natural disaster, and natural resource models to help ensure sustainable development and improve the quality of life on Earth. The Mission to Planet Earth (MTPE) will also require supercomputer computational modeling. Also needed for remote sensing are smaller, less expensive, and more accurate sensors, detectors, and scientific instruments, all of which will depend on advances in the associated electronics.
- Develop models of the effects of gravity and cosmic radiation in vital biological, physical, and chemical systems in space, on other planetary bodies, and on Earth, and apply this fundamental knowledge to the establishment of permanent human presence in space to improve life on Earth.
- Develop revolutionary technological advances to provide air and space travel for anyone, anytime, anywhere more safely, more affordably, and with less impact on the environment and improve business opportunities and global security. This will require numerical simulations to develop more efficient airframes and propulsion systems, lighter and stronger structural materials, and lighter and smaller components (such as computers and electronic instruments).
- For remote, robotic exploration, develop micro-scale, autonomous vehicles and instruments. The controlling electronics should be intelligent, small, light, and energy-efficient enough that the robot's functionality is never limited by the electronics.

The importance of information technology is not a national phenomenon, but an international one. U.S. leadership in information technology is arguably more important to our power and influence in the world than our status as the only military superpower. For example, the dominance of the U.S. on the Web and in the creation of state-of-the-art software have made English the de-facto universal language of information technology, something that no amount of military force could have accomplished. This points out that superior information technology, not weaponry, will win the biggest "battles" of the future, and will determine the new superpowers. It is for this reason that continued U.S. dominance in IT is considered vital to U.S. national security [3]. Obviously, the U.S. government will want to do what is necessary to maintain our status as the IT superpower as well. The only way to accomplish this by making sure that U.S. IT advances faster than that of other countries.

1.3 The Future

By extrapolating the progress of information technology into the future, some amazing and exciting applications seem possible. Here are a few examples:

- We will be able to (verbally) tell a water tap how hot and fast to dispense water, and when to stop. Want soap with that? Many functions of “smart” houses and buildings will operate in this manner.
- We will put on a virtual reality (VR) helmet and ride an exercise bike up and down the streets of San Francisco, with as much (or as little) VR as desired: visually perfect 360° reproduction of the scene, a bike that moves through the scene where you steer it and as fast as you pedal it, terrain feedback synchronized with the visual, cars, horns, pedestrians, and road hazards, but probably no exhaust fumes.
- Using VR technology, we will attend business meetings and school classes, meet with (not just talk with) family and friends, play interactive games, and visit interesting places around the world. VR technology will become so prevalent and useful that calling it “virtual” will be as meaningless as saying that talking on the phone is a virtual conversation. VR glasses will be the dominant visual interface to the digital world, because they will be an order of magnitude less expensive than previous CRT/LCD technology.
- It will be old-fashioned to buy a ready-to-bake meal that is not “electronically enhanced”. Embedded in the meal will be a smart sensor that provides dynamic feedback to the cooking appliance to produce desired (and safe) cooking results. The would-be diner will push the AutoCook button, and the meal will be defrosted, heated, cooked, and simmered using the optimal schedule for that meal.
- Through real-time computer translation, we will converse with people speaking languages we do not know.
- On a “real” nature hike, we will (verbally) ask our digital familiar what kind of bird we are seeing or whether a plant is poison oak. If the requested information can not be determined from the internal terabyte storage, the familiar will take a picture, send the query to the Web, and report (verbally) the conclusion.
- When “physical” travel is necessary, planes, trains, and automobiles will be automatically piloted via the quickest and safest route at the time. NASA will use similar technology to explore remote planets with autonomously piloted vehicles.
- Supercomputers will be so powerful that the relatively inefficient genetic algorithm method of developing artificial-intelligence models of physical systems will become much faster than traditional programming. Many new and powerful models will follow:
  - We will know what the weather will be weeks in advance, and what steps might be taken over those weeks to slowly modify conditions enough to mitigate damage from bad weather.
  - Earthquake prediction will improve dramatically, after a genetic algorithm develops a model of the Earth that accurately fits past earthquake data.
  - Safer and more effective medical drugs will be developed at an accelerating rate through more accurate simulations of the interactions of biological molecules.

All of these applications require innovation to achieve: faster processors, higher density memory and storage, lower power consumption, better human-computer interfaces, lighter weight, new materials, higher gigaflops per dollar and pound, much faster communications (wired and wireless), etc. However, none them are beyond the realm of science. Nevertheless, in some ways, science fiction writers just five years ago could not imagine some of the marvels information technology would bring. Five years from now, a similar conclusion may be reached in reference to the above predictions. The obvious questions are how long information technology will continue its rapid advance, what challenges might slow that progress, and how these challenges can be overcome as efficiently as possible. These questions are considered below.

1.4 Challenges Ahead

Progress in IT has largely been the result of advancements in three core technologies: semiconductor technology, integrated circuit technology, and software. The U.S. currently has world leadership in each of these areas. The most important of these technologies for IT advancement by any measure has been the orders of magnitude improvement in semiconductor technology. By removing this technology alone, the Information Revolution would never have happened. By extension, if semiconductor technology advancement falters, the technological achievements of the future, such as many of those listed above, will also never happen. The slowing of IT advancements would have serious repercussions for technology, the economy, and quality of life in the future. Obviously, there is a strong incentive to do whatever is necessary to allow and encourage IT advancement to continue for a long as possible. Further, the U.S. should try to remain at the forefront of this effort.

So how has semiconductor technology progressed in the past, and why won't this work in the future? Since the MOSFET is the dominant electronic device for information technology, and is expected to remain so for the near future, it is the focus in answering these questions. In the past, it was largely possible to extrapolate the design and operation of the next generation of electronic devices from the previous ones using relatively simple device scaling laws [4, 5]. Next generation devices were then produced through a process of experimental fabrication, device operation characterization, and educated guessing to try to change the process steps so as to change the device structure so as to hopefully converge to the desired device operation characteristics. This process of experimental iteration as guided by scaling laws has actually worked fairly well to date in maintaining an acceptable expense and time to develop each new electronic device generation.

In spite of the past success of the scaling laws as a means of developing improved electronic devices, there are several compelling reasons why this approach is quickly losing momentum. As a result, in the near future, it will not be possible to adequately extrapolate new device designs from previous ones, meaning that the cost of experimental iteration will become too high. The first reason is that it is becoming much more expensive to use experimental iteration to improve a device design, even if the number of experimental iterations were to remain the same. The second reason is that the number of experimental iterations necessary to produce the desired operation is increasing. The reason is that devices are becoming topologically very complex (structures do not have a single length, width, height, or doping density), so that scaling laws are difficult to apply, resulting in a less accurate initial design. Third, small geometry effects are not usually considered by the scaling laws. If these effects are included, the scaling laws become more complex, more uncertain, and more variable across device generations, again increasing experimental iterations. Small geometry effects include drain-induced barrier lowering, hot electron transport, punch-through, avalanche multiplication, oxide and junction breakdown, leakage currents, and more. Fourth, quantum effects such as gate oxide tunneling, inversion layer quantization, quantum transport, and transconductance degradation due to quantum exclusion of carriers from the near-oxide region are increasing in significance, and again the scaling laws do not account for these effects.

Through device modeling and measurement, it may be possible to quantify some of the small geometry and quantum effects in MOSFETs, and augment scaling laws to account for them to some extent. However, as MOSFET geometries shrink to 100 nm gate length and below, and scaling laws are continually modified to account of classical and quantum effects, it will become increasingly difficult (i.e., expensive) to use scaling laws to provide useful extrapolation rules for design of the next generation. The continual tweaking of scaling laws, the increased experimental iteration to produce a functional design, and especially the increase in quantum effects, are all indications that the MOSFET is finally approaching the end of its ability to be scaled. The Semiconductor Industry Association (SIA) roadmap [3] has predicted MOSFET gate lengths down to 70 nm, and individual versions of such devices have been demonstrated. However, as quantum effects begin to dominate classical effects at some length scale in the MOSFET, it will eventually be necessary to replace the MOSFET with a quantum functional device. Thus, the final, and perhaps most compelling, reason we must replace the past practice of using scaling laws and experimental iteration to advance electronic devices, is that scaling laws are not be applicable to, and give us no preparation for, making a transition to a new quantum device technology.

1.5 Importance of Simulation

Based on the above arguments, the combination of theory (distilled into scaling laws) and experimental iteration to advancing the state of the art in electronics technology are not adequate for future device generations. A new approach must be adopted which allows us to understand the physics of ultra sub-micron MOSFETs (and possible successor technologies) at a more fundamental level in order to keep R&D costs and delays down for future generations of electronic devices, and thus to maintain the present high rate of information technology progress. The remaining R&D approach is numerical simulation. This approach can provide the necessary detail of physics and device operation to reduce experimental iteration costs. In fact, simulation has many significant benefits over theory and experiment which can be exploited. In addition to much lower cost and turn-around time as compared to experiment, simulation can display internal device operation, isolate individual physical effects, and provide precise knowledge and ultimate control of device structures and environmental conditions. None of these features are provided by experiment, and all are needed for the best understanding of electronic device operation, whether for ultra-scaled MOSFETs or for even smaller quantum devices. If U.S. superiority in semiconductor technology is to be maintained, a strong program in semiconductor device modeling is clearly essential. In fact, the Semiconductor Industry Association Roadmap [3] explicitly states that “every technology roadmap calls for improved modeling and simulation”.

Having established a motivation for semiconductor device modeling, the important issue remains of establishing the most productive approach in this endeavor. That is, how should semiconductor device modeling be pursued so that it actually accomplishes the goal of reducing the cost and time of semiconductor technology R&D, and thus maintains the rate of progress in semiconductor technology as long as possible? The reality is that no single physical model is optimal in terms of efficiency and accuracy for all future electronic devices. Thus, a range of device models must be investigated. These models should span the technology range from existing electronics through purely quantum devices as the eventual successor to MOSFETs. They should also cover alternate and contributing technologies, such as optoelectronics, which may serve as switching devices or just provide an interface to fast interconnects in future electronics technologies. The NAS semiconductor device modeling program described herein manages to efficiently cover this technology range. Individual projects include adding quantum corrections to conventional electronic device models at the “large” scale of roughly 250 nm to 100 nm (Section 2.1), fully quantum models (Green’s function, Wigner function, and transfer matrix based) for mesoscale devices of roughly 100 nm to 10 nm (Sections 2.1 and 2.2), and even atomic-scale devices at sizes of 10 nm and smaller (Section 2.3). Finally, Section 2.4 describes an effort in optoelectronic device modeling.

Finally, although MOSFETs are by far the most commercially important semiconductor device technology, note that NASA’s needs for electronic device modeling cover a much wider range. In a recent presentation [6], Jet Propulsion Lab Director Carl Kukkonen described at least a dozen semiconductor device applications that NASA needs to develop or improve for the success of future missions, including the Mission to Planet Earth, Space Science, Human Exploration and Development of Space, and Aeronautics and Space Transportation Technology. These semiconductor device applications include infrared detectors, millimeter and submillimeter wave sensors, UV and x-ray CCDs, photonic devices, optoelectronic integrated circuits, micromagnetic devices, and electronic neural networks [7]. The ability to treat each of these semiconductor devices as case studies using one or more of our simulation approaches will serve as a direct measure of the comprehensiveness and capability of this semiconductor device simulation program.

1.6 References

[1] The National Performance Review Web page is http://www.npr.gov/.

[2] The NASA Strategic Plan can be found at http://www.hq.nasa.gov/office/codez/stratplan/cover.htm.

[3] The SIA Roadmap is available at http://www.sematech.org/public/roadmap/index.htm.

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2 Semiconductor Device Modeling Projects

2.1 Quantum Corrections to Conventional Electronic Device Models (Bryan A. Biegel)

2.1.1 Motivation

Electronic devices have decreased in size and switching time by many orders of magnitude over the past three decades. In spite of this, the drift-diffusion (DD) model of electronic device operation is still used in nearly all line-of-business device simulations [1]. The reason is that the DD model has adequately explained or predicted the behavior of commercially important electronic devices through this rapid technology advancement. However, the increasing significance of quantum effects such as oxide tunneling, inversion layer energy quantization, and wave-like transport of electrons over short distances has called into question the adequacy of the classical DD model (and other classical models) for near-future electronic devices as down-scaling continues. Technology leaders now very much want to know how significantly parasitic quantum effects will degrade electronic device operation with each future device generation, how long these effects can be suppressed and by what means, and how quantum effects might be used to actually improve device operation.

2.1.2 Approach

Experiment is not a suitable first line of attack in the investigation of these questions, since it can not view internal device operation or isolate particular physical effects, it has a very high (and increasing) cost, experimental structures and conditions are not precisely controllable, and turn-around time is very slow. Numerical simulation is a very viable alternative to experiment, since it does not suffer from these weaknesses. From the electronic device modeling community, two approaches are being followed in the attempt to answer these questions: the addition of quantum corrections to conventional device models such as DD, and the development of fully quantum mechanical models for electronic devices. However, existing simulation tools currently can not provide the needed information for two reasons: 1) converting a new device model (including quantum effects) into functioning simulation software is very time-consuming, and 2) the required computational resources are immense. Both of these difficulties are addressed by this project, the goal of which is the rapid and accurate investigation of quantum effects in near-future electronic devices.

This project addresses the first issue by advancing the trend in software development away from writing huge new software packages, and towards the re-use of existing software packages and modules to rapidly implement and investigate new electronic device models including quantum effects. In particular, this project will draw upon the wide array of highly functional numerical simulation software and expert personnel that NAS has accumulated in its pursuit of advanced aerospace simulation and parallel numerical code development, as well as emerging third-party numerical computation tools. Relevant NAS software resources include parallel equation solver routines (linear and non-linear systems), a 3-D Poisson equation solver, advanced dynamic gridding codes, and computational fluid dynamics codes. The goal of code reuse in this work is to maximize the time spent on the “high level” task of developing accurate and computationally feasible models of the physics of interest (quantum effects in electronic devices), while minimizing the “low level” work of writing code. The traditional approach to electronic device modeling of spending years writing monolithic, “vertical” simulation codes (which only implement a single physical model) line-by-line from the ground up usually results in the opposite distribution of effort, and correspondingly slow progress.

The second reason for the inability of device simulation tools to answer questions about quantum effects in electronic devices is that accurate simulation of quantum effects in commercially important devices requires huge computational resources, both in terms of memory and CPU cycles. This requirement is also addressed by this project by utilizing available resources at NAS. In fact, many of the NAS software resources mentioned above are designed specifically to take advantage of the large parallel computation systems at NAS. This combination of rapidly-developed software and very fast hardware will bring previously infeasible computations such as 2-D and 3-D quantum simulations within reach. In particular, it will finally allow the questions about quantum effects in current and future electronic devices to be answered.

2.1.3 Project Details

The two specific projects in this work each pursue one of the approaches being taken by the electronic device modeling community to answer the industry's questions about quantum effects in electronic devices. The first approach is to implement quantum corrections to classical electronic device models. For this project, a general PDE solver called PROPHET [2] (and possibly similar tools) will be used as a foundation for rapid implementation and investigation of electronic device models including quantum effects. Planned projects include adding quantum corrections to the drift-diffusion, hydrodynamic, and Boltzmann equation models of electronic transport in 1-D, 2-D, and 3-D. The first specific task will be to investigate the density-gradient quantum correction to the drift-diffusion model [3] in 3-D. In many cases, quantum corrections such as these have only been attempted in 1-D or under other severe limitations.

The second approach seeks to model quantum effects in electronic devices by using a fully quantum mechanical model for the system. For this project, an existing quantum device simulation tool called SQUADS [4] based on the Wigner function and transfer-matrix methods will be used to study quantum structures and effects in 1-D. This simulation tool has already produced new results in self-consistent and transient quantum device simulation. Future investigations with this package are planned into the use of very fine momentum gridding, new transport equation discretizations, and more accurate scattering models. Based on knowledge acquired from this work, a 2-D Wigner function code will be developed. A 2-D quantum device simulation of this accuracy (including open boundaries, scattering, self-consistency, and transient operation) has never been attempted. The computational requirements for such 2-D simulations will be several orders of magnitude higher than for the 1-D case, requiring that more sophisticated solution methods be employed. Where appropriate, NAS expertise and numerical code (which has successfully solved this scale of CFD computation) will be utilized. Note that the test device for most of this work will be the MOSFET, in which quantum effects are a great concern, due to the MOSFET's dominance in electronics and to the wide range of quantum effects which are increasing in significance in this device. However, quantum effect dominated devices such a resonant tunneling diodes and transistors will also be investigated for the longer-term.

2.1.4 References

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[3] M.G. Ancona and H.F. Tiersten, "Macroscopic physics of the silicon inversion layer", *Phys. Rev. B* **35**(15), p. 7959-65 (1987).

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2.2 Quantum and Mesoscopic Device Modeling (M.P. Anantram)

2.2.1 Motivation

The main avenues of experimental research being pursued in various laboratories to build the future generations of smaller/faster devices are (i) downsizing of conventional semiconductor devices and (ii) molecular devices. In a large number of these structures, the length scales and transit times are comparable to the wavelength of the electrons and the scattering times. Transport at these dimensions is not well described by semiclassical physics because quantum effects play an increasingly important role. The new generation of devices can either be similar to the present day devices, only that they are miniaturized or can be based on entirely new device physics. While, in the former case, it is desirable to annul the deviations caused by the quantum effects, in the later case, quantum effects will probably be exploited in designing the devices. So as to model and design the future generation of devices, it is essential to study transport at these dimensions and develop tools for this purpose. It is hoped that these tools will not only help in modeling the future generation of devices but will also help make progress in proposing new devices and device concepts.

2.2.2 Approach

Transport of electrons in devices with feature sizes in the nanometer regime is primarily quantum mechanical. Here, the well developed simulation tools based on the semiclassical transport equations are no longer directly applicable and often fail to describe the transport physics, and it is essential to use tools based on quantum transport equations. Such tools are however not readily available and our goal is to develop a comprehensive set of tools, which will aid us to study and analyze transport at these dimensions. These tools will be based on the Scattering Theory and Non-Equilibrium Green's function approaches.

2.2.3 Project Details

Some specific issues we are interested in are:

- Quantum effects in MOSFET-type structures: MOSFET is the single most important device in today's semiconductor industry. The Semiconductor Industry Association (SIA) road map envisions a channel length of about 500Å (250 or so atoms along the channel) and a width of about 1 micron. There is much ambiguity on the deviation of the device characteristics from its ideal value due to effects arising from the wave nature of electrons. The purpose of our study is to model the effect of altering the various device parameters on the current versus voltage characteristics and to investigate means of keeping the characteristics close to that ideally desired.

  Methods to include quantum effects in the present day semiclassical simulation tools have been proposed. It would be of great advantage if these tools could be used to simulate the future generation of MOSFETs by including appropriate quantum corrections, without significant increase in overhead. This leads to the second purpose of this project, which is to benchmark the semiclassical methods using the more detailed and thorough quantum simulations.
- Carbon nanotubes, a new class of materials, exhibit electronic properties which vary from that of semiconductors to metals. Individual tubes have dimensions in the nanometer regime, in at least one direction. Device concepts based on these materials have been proposed. More importantly, progress by experimental groups has been very encouraging. Methods to: isolate individual tubes, manufacture tubes with different electronic properties in a predictable manner and measure transport properties are underway. We have initiated an effort to study their transport properties. This study will both use and complement the study of mechanical and chemical properties of these structures, which is now being actively pursued at the Ames Research Center.

2.3 Theory and Modeling of Atomic-Scale Electronics (Toshishige Yamada)

2.3.1 Motivation

When electronic device size is reduced, there arise a lot of unwanted effects which will lead to malfunctioning of the devices. It has been pointed out [1] that the dopant spatial fluctuation would be a serious problem in the sub-0.07 micrometer gate length regime. In this dimension, the number of dopant atoms in the channel is typically a few dozen, and electrons see an ensemble of discrete dopant atoms. They are located randomly inside the channel, and this causes significant deviation in device characteristics, even though devices are designed to be the same, and places a serious limit for integration. It is quite impractical to develop process technology that controls the dopant positions precisely within atomic scale.

2.3.2 Approach

A fundamental solution is to create electronics only with simple but atomically precise structures by using current atom manipulation technology [2] or its developed version. In fact, we have already had technology to move individual Xe (rare gas) atoms, Fe (metallic) atoms, and Si (covalent) atoms and place them at desired positions by using an STM tip as tweezers [2]. This direction is consistent with the future NASA mission of demanding ultrasmall electronic devices. Here a completely new scheme is proposed that falls into this category - atomic-scale electronics [3]. Foreign atoms are placed as adatoms on an insulating substrate surface providing a two-dimensional periodic potential. Although only one lattice constant is possible in a natural crystal, we can assign an arbitrary lattice constant (typically much longer [4] than the natural one for mechanical stability reasons) and form artificial low-dimensional structures. By changing the lattice constant, the interaction between neighboring atoms can be controlled, so that we can design the energy band structure and the electronic properties. We then create electronic devices by forming junctions that will exhibit highly nonlinear I-V characteristics.

2.3.3 Project Details

As a preliminary evaluation, the energy band structures are calculated for simple structures with basic atoms using a tight-binding method with universal parameters. It has been shown that Si chains are metallic and Mg chains are semiconducting regardless of the lattice constant [3]. Obtaining metallic and semiconducting elements, we need to study how to dope semiconductors, and also how to form an Ohmic contact, both of which are keys in current semiconductor electronics. The doping method has been studied and a basic prescription to obtain p-type and n-type semiconductors is proposed [5], which can be called atomic modulation doping. The study of Ohmic contacts, which will be widely used for interconnection of devices, will be the next research topic. This requires a detailed analysis of electronic states at the atomic-scale heterojunction. Programs will be developed to calculate band structures self-consistently by solving a Poisson equation.

The work then will proceed to the study of electronic transport properties of a simple metallic chain, a semiconductor-metal junction, and a p-n junction. As is the case with mesoscopia, the existence of electrodes feeding current to the structure will significantly modify the electronic and transport properties. The study of Ohmic contacts will clarify this physics and give an engineering prescription for how to control the modification. It has to be examined whether the transmission coefficient picture [6] that has been quite successful in mesoscopia can still be useful in this atomic scale. After clarifying the relevant physical properties of these atomic chains, we will propose three-terminal devices, which are much more desirable than two-terminal ones.

2.3.4 References

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2.4 Comprehensive Modeling and Simulation of Optoelectronic Devices (Cun-Zheng Ning)

2.4.1 Motivation

With the increasing demand for high speed and high efficiency processing (computing), transmission, and reception of information, semiconductor optoelectronic devices and systems are becoming more and more important. In optoelectronic devices and systems, this ever increasing demand is being fulfilled by combining the established knowledge and technology of electronics with the advantage of optics. Optical interconnects offer a paradigm for this emerging technology. In a typical optical interconnect using optoelectronic integrated circuits (OEICs), optical devices (such as lasers or modulators) are integrated monolithically with electronic devices (such as transistors) to perform functions of signal conversion, reception, or amplification. Obviously modeling and simulation of such devices are critically important for understanding the device physics and performance limits, and for devices and system designs. The situation of optoelectronic device modeling and simulation (OEDMS) is very similar to that of semiconductor electronic device simulation about 20 years ago. Just as electronic device simulation is critical to today's micro-electronics industry, so will be the optoelectronic device simulation to the future optoelectronic industry.

2.4.2 Issues and Approach

In general, OEDMS involves complicated interacting processes of electronic, optical, and thermal nature. Depending on the specific device size, it could be necessary to describe one or several of these processes at the quantum mechanical level. The detailed interactions of optical and electronic processes in semiconductors require a microscopic theory with possible inclusion of many-body interactions. Space and time domain resolution is very often desired and this increases the degree of complexity quite dramatically. Obviously optoelectronic device simulation and modeling represent an almost infinite complexity in many respects.

The complexity of optoelectronic modeling and simulation demand both sophisticated model development based on fundamental physics principles and a significant computational capability. NASA Ames' unique resources in computational machine power, manpower, and expertise in algorithms and methods accumulated with the CFD activities place us in a unique position to perform such challenging tasks.

At present OEDMS is in its very initial stage of research and development. Currently there is not much effort in OEDMS. There are however, more and more experts who realize the increasing importance of OEDMS. Most of the present models for the optoelectronic device simulation are very rudimentary and very often involve unjustified simplification of the physical reality. In contrast, our approach will be based on the fundamental microscopic theory of underlying processes as much as possible and feasible.

2.4.3 Project Details

Our OEDMS activity will adopt a stepwise approach. In the initial stage of development we will concentrate on microscopic foundation of individual physics processes that play important roles in affecting the device performances. This type of research will not only lead to a more complete understanding of the underlying processes, it will also lead to a simplification and a systematic and controllable approximation to be used in the overall simulation. These processes include carrier-carrier and carrier-phonon scattering, plasma heating, carrier capture by and escape from quantum wells, and other many-body interaction processes.

Our next stage is to combine those individual processes (after possible simplification and parameterization) into a single environment for optical device simulation. As a prototype devices, vertical cavity surface emitting lasers (VCSELs), which are now being adopted in increasingly many OEICs, will be used for developing comprehensive and reliable modeling and simulation tools for the optics part of the problem. We begin by studying the transverse mode and temporal dynamics of the VCSELs. The detailed band structure information of underlying semiconductor quantum wells and microscopic theory with many-body interaction will then be incorporated. The intermediate goal of this project is to develop a comprehensive modeling package for optical devices (both active and passive) including optical, electronic, and thermal processes in a self-consistent fashion. The final goal is to integrate electronic devices with optical devices, achieving a truly optoelectronic modeling and simulation capability for OEICs.

2.5 National TCAD Environment (Bryan A. Biegel)

2.5.1 Motivation

The effort to make TCAD lead the development of future electronics faces several challenges. First, many device models need to be implemented and applied, sometimes multiple models in a single computation. These models include advanced classical models (including drift-diffusion, energy-balance, hydrodynamic, and BTE), particle-based models (Monte-Carlo), quantum-corrected classical models (e.g., density-gradient correction to drift-diffusion, quantum hydrodynamic), full quantum models (including transfer matrix, density matrix, Wigner function, and Green's function), and optical and optoelectronic models. No single physical model is optimal in terms of efficiency and accuracy for all future electronic device simulation needs. The second challenge is that for an device simulator to have significant impact, it must not only function correctly, but must also be easy to use, flexible (in terms of model changes and output views), computationally efficient and robust, and platform independent. The third challenge is to find sufficient computational power to produce accurate answers with the models of interest. Finally, the fourth challenge is that TCAD tools (process, device, circuit, and system) must be coupled, to maximize efficiency and accuracy of information transfer, and to permit global optimization. As the cost of experimental iteration to perfect new devices and technologies rises, a virtual semiconductor fab must replace the physical fab for all but the final verification steps, just as is done for circuit verification today. The relatively slow progress of TCAD in the past, and the critical role it must play in the future in order to maintain the rate of electronics advancement, clearly indicate that a fundamentally new approach to TCAD tool development is necessary in the future. In particular, Each research group can no longer afford to develop numerous huge, single model, single purpose simulation codes for a few users per code. Each group also can not afford to purchase supercomputers to run accurate simulations. These two conclusions define the approach in this project.

2.5.2 Approach

Based on the two conclusions above, two interdependent technologies are proposed to solve the challenges facing future TCAD. First, a national TCAD environment (NTE) is proposed, which will provide a foundation for modular implementation and enhancement of a fully-coupled (process, device, circuit, system models), Web-based TCAD simulation system. This system will include an intuitive GUI, high-quality graphics, upgradeable functionality (including gridding, matrix computations, linear and non-linear solvers, and graphics). Very importantly, the model will be independent of the numerical code, and can be specified in the input file at run time (like ALAMODE [1] and PROPHET [2]). The second technology is the Information Power Grid (IPG) [3], which is a proposed national network of supercomputers and scientific workstations that will act like the electric grid in supplying CPU power to whomever needs it from where ever it is available at a given time. The NTE will be implemented as an application for the IPG, which will provide inexpensive and transparent access to the computation resources necessary to make many of the advanced device (and other) models computationally feasible.

2.5.3 Project Details

This project is in the early formation stage, so that the direction in which it will progress is currently uncertain. The Stanford TCAD group has been formulating and championing a concept much like the NTE described above [4], but without the IPG component. Therefore, as far as conceptual work, we will likely find much to draw on from Stanford's work on the NTE, and make our biggest conceptual contributions in adding the IPG to this effort, a component which we consider crucial to the NTE's success. NAS has a number of unique resources to bring to this project. NAS supercomputing and parallel computation hardware, advanced numerical computation software, and numerical and parallel computation experts will allow in-house prototyping of both the IPG and NTE. NASA also has a unique interest in the NTE/IPG. Although industry may not see a compelling short-term business case, and academia will require some organizing force (and funding), NASA can clearly justify support for these technologies. As stated in Section 1.2, the computational power of the IPG and the advanced technology that the NTE will make possible are both critical to NASA and U.S. government missions. It is with this understanding that this project is pursued as part of our SDM program.

2.5.4 References

[1] The top ALAMODE web page is http://gloworm.stanford.edu/tcad/programs/alamode.html.

[2] The top PROPHET web page is http://gloworm.stanford.edu/~conor/prophet/guide.html.

[3] The top IPG web page is http://science.nas.nasa.gov/Groups/Tools/IPG/.

[4] The top Computational Prototyping web page is http://www-snf.stanford.edu/ComputationalPrototyping/.