Computational Nano-Electronics Group (CNEG)

Microelectronics Division, EEE, NTU

An interdisciplinary group with a computational commonality

Our logo:

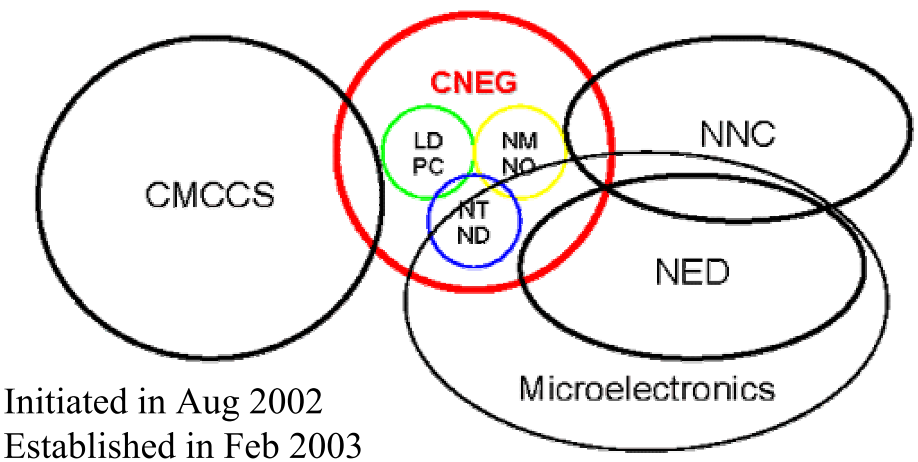
The integrated letter "**G**" comprising three prime colors (signifying originality) is showing the research focus on **C**omputational **E**lectronics of our **G**roup. The outlined (open) letter "**n**" is a modifier for our research direction in the *open* field of **N**ano-electronics. The spinning globe represents the letter "**i**" for our **I**nitiative on CNE, with *global* collaboration.

Computational Nano-Electronics Initiative

In collaboration with:

Website: http://www.ntu.edu.sg/eee/eee6/CNEI/

- Centre for Modeling and Control of Complex Systems (CMCCS), EEE, NTU
- Nanoelectronics and Devices (NED) Strategic Research Program, EEE6, NTU
- Nanoscience and Nanotechnology Corridor (NNC), MPE/EEE, NTU
- Computational Electro-magnetics & Electronics, IHPC, A*STAR



- Initiated in Aug 2002
- Established in Feb 2003

Computational Nano-Electronics Initiative (CNEI)

(http://www.ntu.edu.sg/eee/eee6/CNEI/)

Computational Nano-Electronics Group (CNEG) Staff:

Ast/P Ang Lay Kee, Ricky
A/P Au Yeung Tin Cheung
A/P Chen Tupei
Ast/P Fan Weijun
A/P Rusli
A/P Sun Chang Qing
A/P Yu Siu Fung
A/P Zhou Xing (*Program Director*)

Research Scope:

- Intense beam-nanostructure interaction (Ang LK)
- Transport in nanoscaled structure & quantum dots (Au Yeung TC)
- Semiconductor nanocrystals for novel applications (Chen TP)
- Band structures of quantum wells and quantum dots (Fan WJ)
- SiC device design, simulation, fabrication & characterization (Rusli)
- Nanosolid: functional materials design & characterization (Sun CQ)
- Photonic bandgap materials – ZnO thin film UV lasers (Yu SF)
- Nanoscale CMOS technology/device modeling (Zhou X)

Research Activities

Research Areas:
(within EEE *Centre for Modeling and Control of Complex Systems*)

- Low-dimensional physics and chemistry (Ang LY, Au Yeung TC, Sun CQ)
- Nano-materials and nano-optoelectronics (Fan WJ, Yu SF)
- Nano-technology and nano-devices (Chen TP, Rusli, Zhou X)

Research Projects / Manpower:

- A total of 11 funded projects whose PI or Co-PI are CNEG staff
- Funding sources: A*STAR, DSO, AcRF, NTU, CSM, SRC®
- Manpower: 3 Research Fellows, 1 Research Associate, 2 Project Officers, 14 PhD students

Research Collaboration:
- *Local*: IHPC, NUS, CSM, IME
- *Overseas*: U. Hong Kong, U. Michigan, Los Alamos Nat. Lab., Auburn U., LSI Logic, Hiroshima U., IIT-Bombay, U. Glasgow, Tsinghua U.

On-going Research Projects

- Modeling of Broadband Compact Vacuum Power Devices and Nano-electronics
- Reliability of Ultra-Thin Gate Dielectrics for ULSI Devices
- Characterization of Ultrathin Gate Dielectric Films for Sub-0.13μm Technology
- Semiconductor Nanocrystals and Their Device Applications
- Magnetic FeN Nanofilms
- Real Time Fabrication System for the Design and Fabrication of Semiconductor Lasers
- Quantum Confined Zinc Oxide Thin Film for UV Lasers Applications
- Nanostructured Zinc Oxide Films for UV Photonic Devices
- Development of Photonic True-Time-Delay Units for Phased-Array Antennas
- Project DOUST: Design and Optimization of Ultra-Small Transistors
- Technology-Based Predictive Compact Model Development for Next Generation CMOS

On-going PhD/MEng Projects

- Nanoscale strained-Si/SiGe MOSFET modeling
- Multi-level modeling of ULSI systems in the very-deep-submicron technology era
- Design III-V-N compound semiconductor devices
- Characterization and device/circuit modeling for current partition in sub-100nm MOS devices
- Analysis and simulation of miniature field emitter array
- Development of process technology for SiC devices for high power high frequency applications
- Semiconductor nanocrystals and their applications
- Current transport in SiO_2-based dielectric films with and without Si nanocrystals
- Band structures and optical properties of InGaNAs quantum well
- Optical and dielectric properties of passivated porous silicon
- Characterization of ultrathin gate dielectric films for sub-0.13μm technology
- Oxidation of SiC for devices application
- Size and catalytic effect on the magnetic properties of Fe-nitride thin films
- Design and fabrication of SiC devices

CNEG: 2003 Journal Publications

(http://www.ntu.edu.sg/eee/eee6/CNEI/publication.htm)

- Physical Review Letters: 1
- Applied Physics Letters: 5
- Journal of Applied Physics: 2
- IEEE Trans. on Electron Devices: 1
- IEEE Circuits & Devices Magazine: 1
- Thin Solid Films: 2
- Solid State Communications: 1
- J. Phys. Chem B: 3
- Mater. Sci. Eng. B: 1
- Prog. Mater. Sci.: 1
- ACTA Materialia : 1
- Diamond and related materials: 1

Total Journal: 20. Conference: 11

Interaction of intense electron beam with nano-structures

(by Ast/P Ang Lay Kee)

Fundamental Understanding (Theory):

- Beam limiting current and beam stability
- Beam loading and beam modulation
- Coupling between beam and input signal
- Detune and de-Q of nano-cavity

Applications of the theory/model:

- Simulation of field emitter array of nanotubes or nanotips
- Design of high-power, high-freq vacuum micro- & nano-devices

Simulation Code Development:

- Including quantum effects in typical PlC simulation codes

Facilities:

- 3 PIC simulation tools: PDP1D, OOPIC2D and MAGIC3D

Intense beam generation and interaction in nm regime

(Contact: Lay-Kee Ang, Email: elkang@ntu.edu.sg)

Objectives

- To obtain the fundamental understandings and useful scaling laws of intense electron beam generation and interaction in nm regime.
- Understand field emission (FE) process of carbon nanotubes (CNT)
- First principle + multiple scaled calculation for CNT's properties
- Innovative design of new vacuum nano-electronics – high power

Recent Accomplishments

- Develop a new quantum theory and scaling law to estimate the maximum current that can be transported across a nanosized gap [1,2]

  [1] *Phys. Rev. Lett.* ***91****, 208303 (2003)*

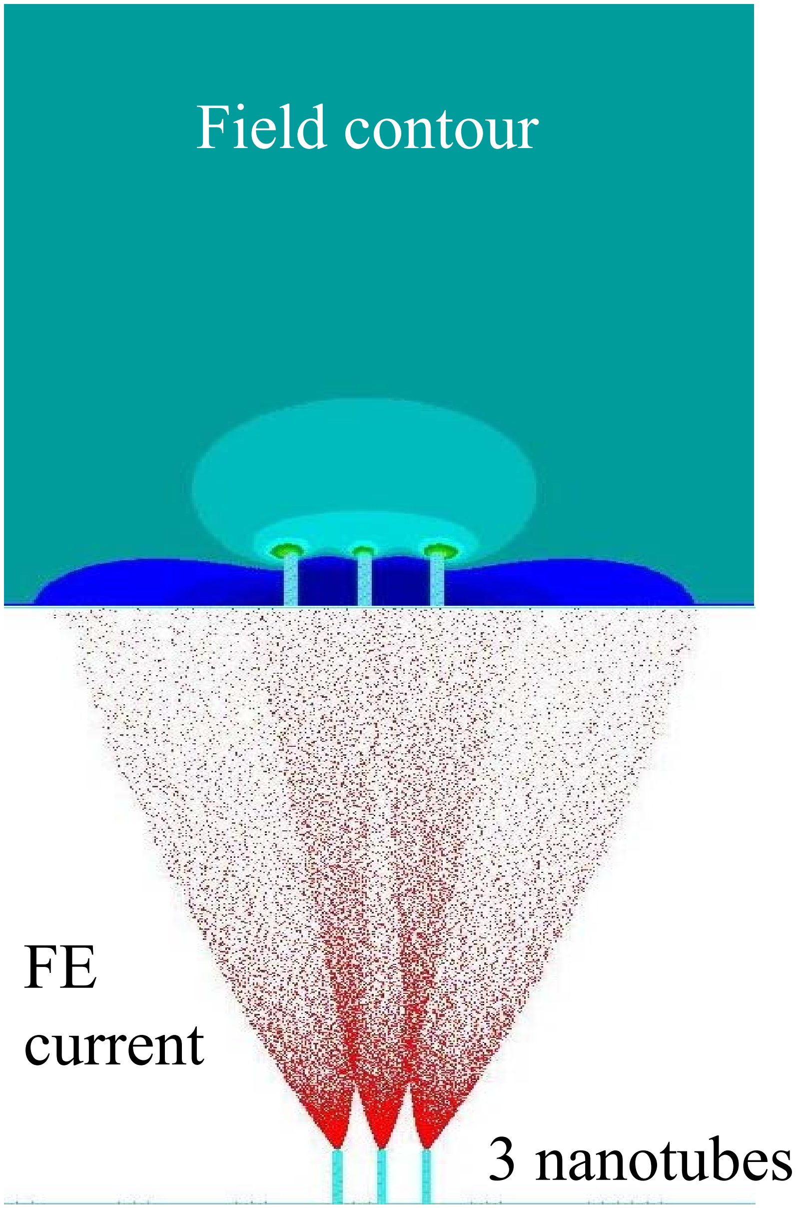
  [2] *IEEE Trans Plasma Sci. (in press, April 2004)*

- Using PIC technique, calculate the IV characteristics of field emission from multiple vertically aligned CNTs [3]

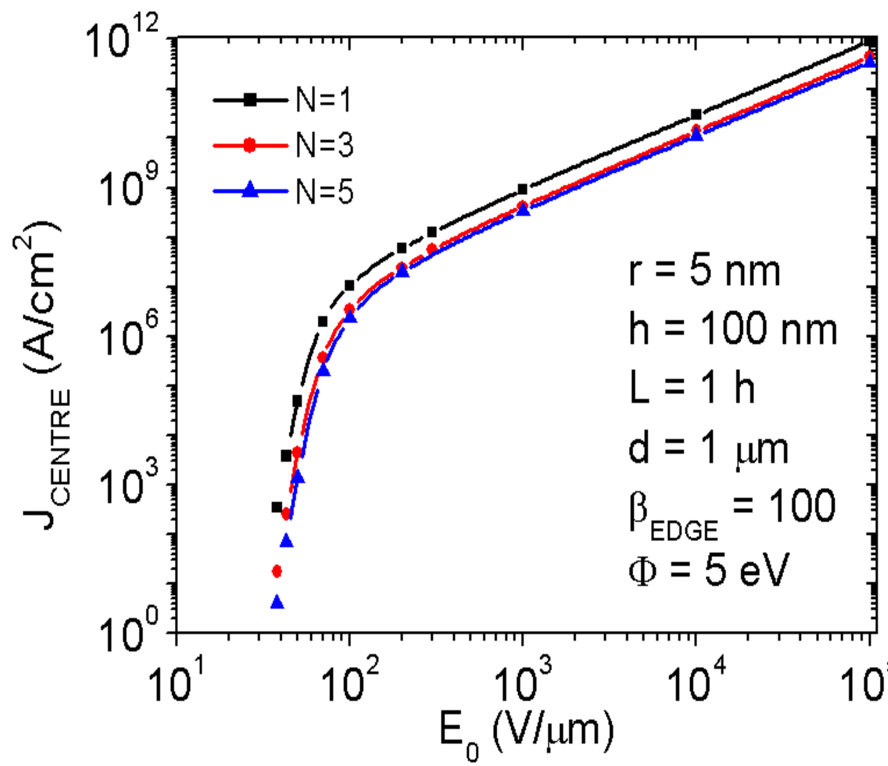
  [3] *International Journal of Nanoscience (accepted, 2004)*

Simulation of High Current Field Emission of Nanotubes

(By Ang LK and his student Koh WS)

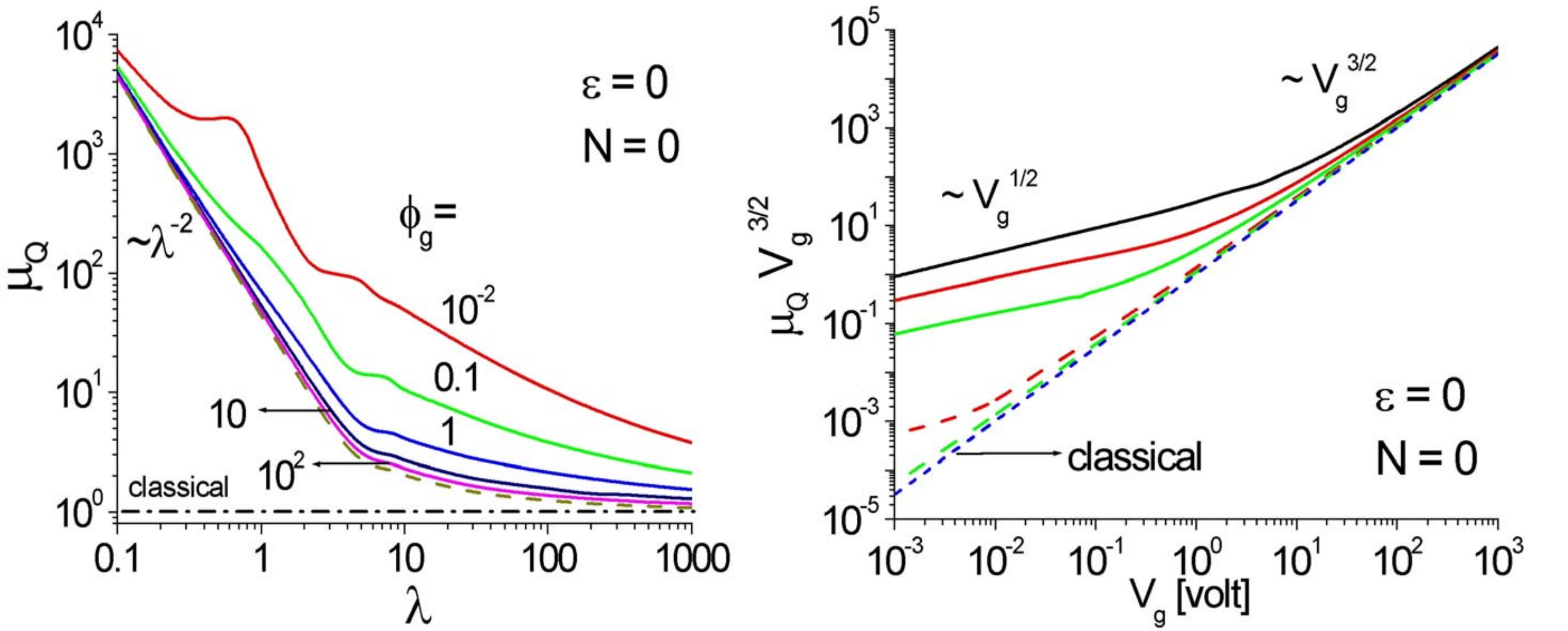


The objective is to calculate high current FE emission from multiple well-aligned carbon nanotubes. The calculation is self-consistent including the space charge field.



Intense electron beam interaction in nm regime

A quantum model is developed to calculate the maximum current that can be transported across a nano-diode [1]



[1] L. K. Ang, *et al*, New scaling of Child-Langmuir Law in Quantum Regime, Physical Review Letters (**91**, 208303, 2003)

<u>Transport in nanoscaled structure & quantum dots</u>

<u>(by A/P Au Yeung Tin Cheung)</u>

The effect of contacts on the ac transport in nanoscaled double-barrier resonant tunnelling structure:

- Calculation of the scattering matrix and density of states.
- Calculation of the ac conductance in the system.
- Investigation of the effect of contact on the ac transport.

The ac transport in coupled quantum dot system in the presence of coulomb interactions between the tunnelling and inter-dot capacitances:

- Investigate the gauge invariance of potential in the presence of coulomb interactions between tunnelling and inter-dot capacitances.
- Calculation of the ac conductance in the presence of the coulomb interactions between various capacitances.
- Investigation of the effect of the coulomb interactions between various capacitances on the ac transport in tunnelling-coupled quantum dot systems.

Semiconductor nanocrystals for novel applications
(by A/P Chen Tupei)

Potential applications of semiconductor nanocrystals (nc):

- Silicon-based optoelectronics:

  Strong room-temperature light emission of semiconductor nc embedded in SiO_2 thin films provides the possibility of integration of optoelectronic devices into Si circuits with mainstream CMOS process.
- Single electron devices:

  Coulomb blockade effect of semiconductor nc provides the possibility of single electron devices such as single electron memory cells and single electron transistors (SETs) operating at room temperature.

Research directions:

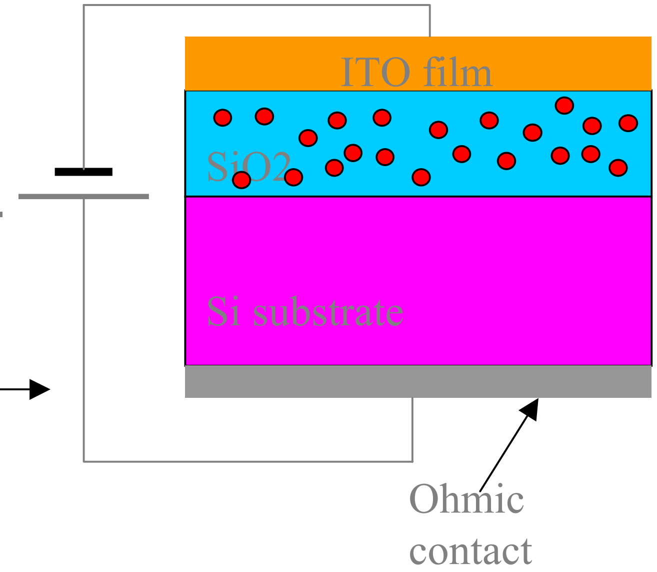
- Theoretical and experimental studies of size effect on physical properties
- Calculations of electronic structures of nc and nc/SiO_2 interface

Applications of Si nanocrystals (nc-Si) embedded in SiO2 matrix

1. Silicon-based light emitting devices

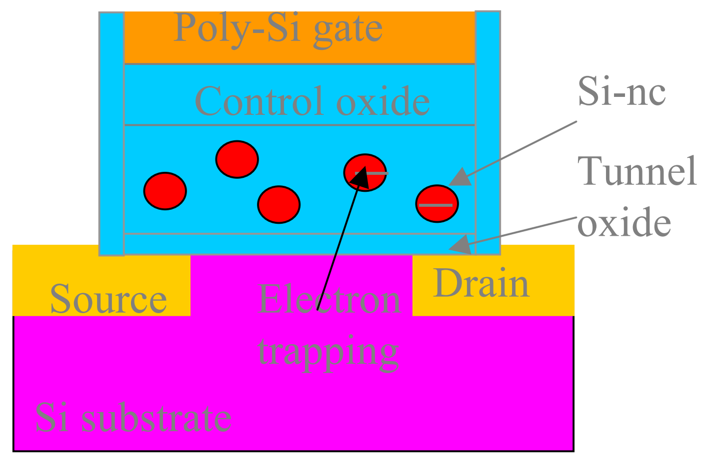
   for Si-based optoelectronic applications.

Basic structure of an EL device →



2. Single electron devices (SEDs):

   Coulomb blockade effect in the material system provides the possibility of SEDs (single electron memory cells and single electron transistors) operating at room temperature.

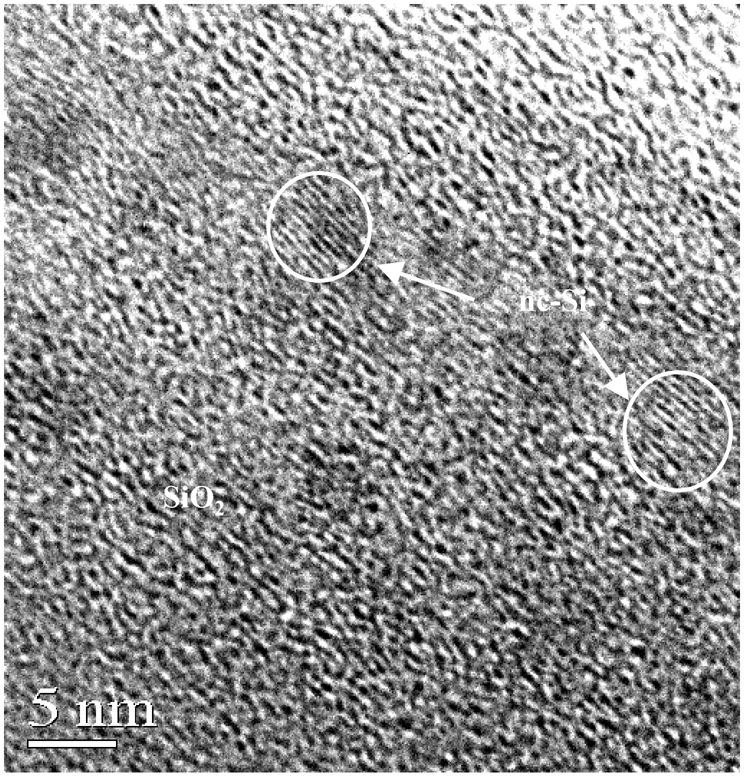


Basic structure of a single electron memory cell

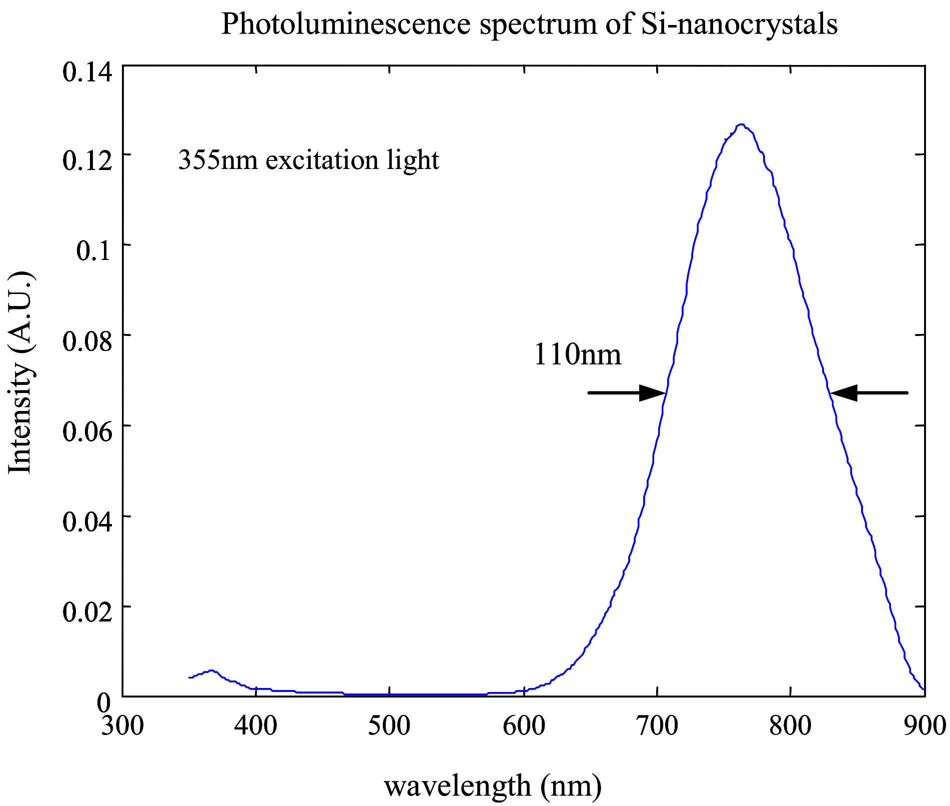
For more information, please contact T. P. Chen at echentp@ntu.edu.sg

Silicon Nanocrystals for Silicon-Based Light-Emitting Devices (LED) Application

T. P. Chen, O. K. Tan, S. F. Yu, M. S. Tse, and K. Pita
Division of Microelectronics, School of EEE, NTU



High resolution TEM image :
nc-Si of ~ 5nm embedded in SiO_2.



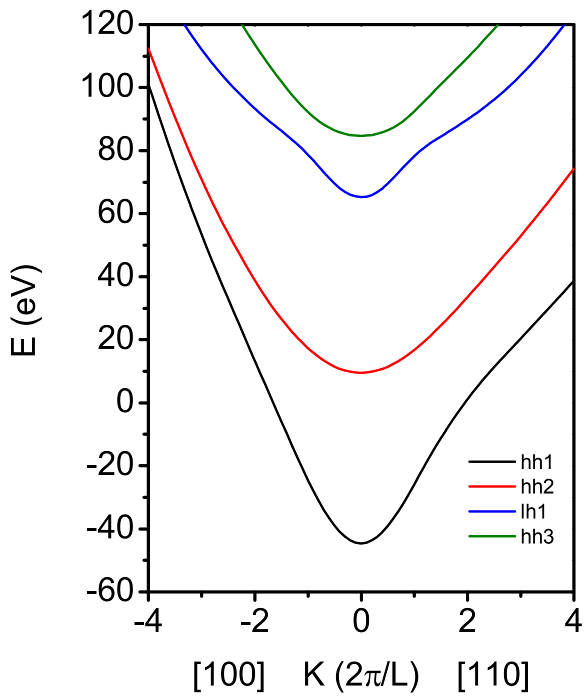
Photoluminescence of nc-Si embedded in SiO_2 synthesized with CMOS process.

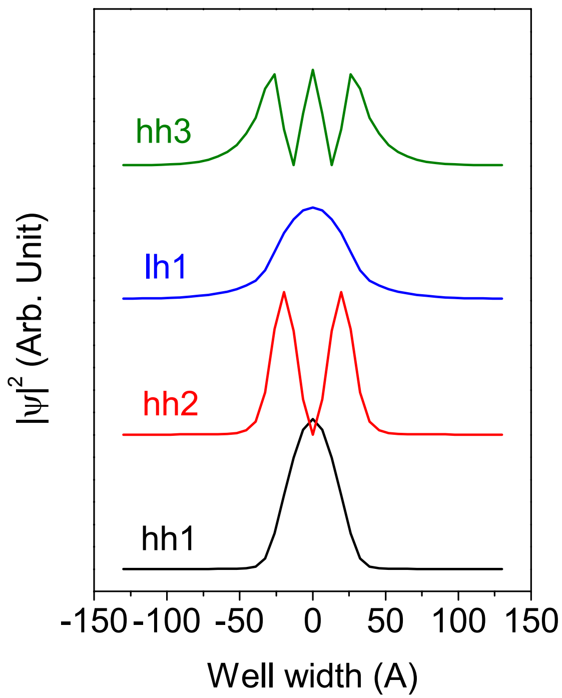
Band structures of quantum wells and quantum dots

(by Ast/P Fan Weijun)

1. The 6×6 k.p effective mass theory for QWs
2. Band structures of $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs compressively strained QWs
3. The squared optical transition matrix elements
4. The DOS of $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs QWs
5. The 6×6 k.p effective mass theory for QDs
6. Band structures of InAs/GaAs and InGaAs/GaAs QDs

Band Structures of GaInNAs/GaAs Quantum Wells





In-plane dispersion curves of the valence band of Ga0.7In0.3N1.3%As98.7%/GaAs QW with well width of 6 nm and barrier width 20 nm.

Wave functions of the valence band of Ga0.7In0.3N1.3%As98.7%/GaAs QW with well width of 6 nm and barrier width 20 nm.

(Contact: Dr Fan Weijun, ewjfan@ntu.edu.sg)

Development of Silicon Carbide Technologies

(by A/P Rusli)

Key Research Objective:

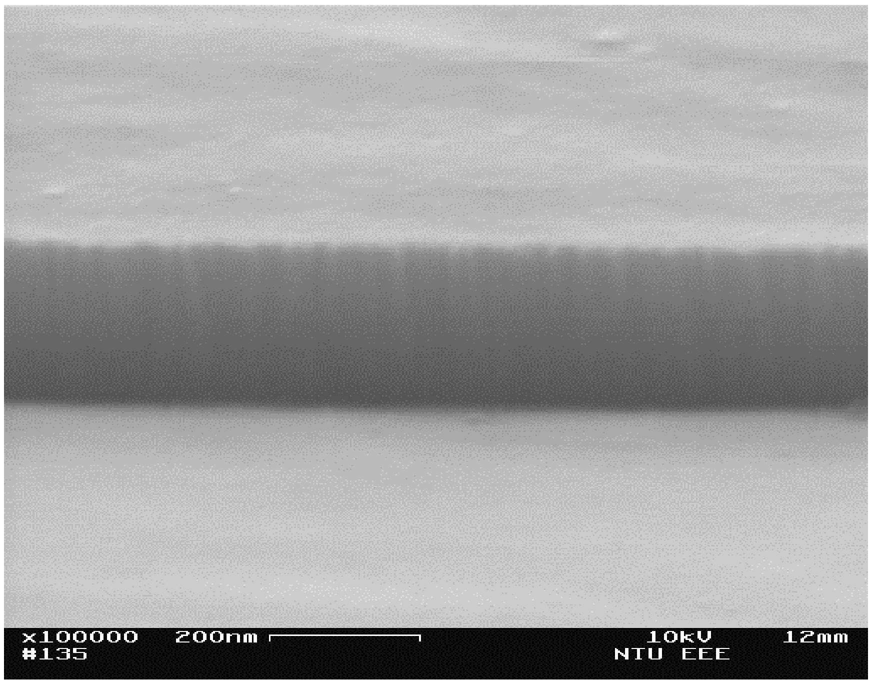
To develop SiC technologies for high temperature, high power and high frequency electronic devices and systems

Research Activities:

- **Study of thermally stable (> 300 ^{o}C) low resistance ohmic contacts and high blocking voltage (> 800 V) Schottky contacts**
- **Optimization of etching and thermal oxidation process technologies**
- **Explore alternative high quality dielectric films on SiC MOS devices**
- **Design and fabricate SiC MESFETs for operations at high temperatures (> 300^{o}C), high power densities (> 200W/cm) and high frequencies (f_T > 6 GHz)**
- **Develop SiC for sensing applications, i.e. UV photodetectors and Hall devices**

Silicon Carbide Research

(Contact: Dr Rusli, erusli@ntu.edu.sg)



The SEM picture of RIE process patterned SiC using a gas mixture of CHF_3 and O_2 at room temperature. The etch depth is 210 nm and the etch rate is 37.5 nm/min.

Silicon carbide (SiC) is the prototype of a new generation of wide bandgap semiconductors whose unparalleled combination of high breakdown voltage, high frequency operations, extreme temperature tolerance, mobility and radiation hardness enables whole new classes of commercial and military applications currently impossible or unaffordable with silicon or gallium arsenide, today's primary semiconductor materials. The unique and attractive characteristics of SiC devices have led to enhancement of numerous military and civilian systems. The SiC group in NTU aims to fully develop SiC process capability; and to design, fabricate and characterize SiC electronic devices. Our work will propel NTU to the frontier of material and device research on one of the most important wide bandgap semiconductor materials.

Nanosolid: functional materials design and characterization

(by A/P Sun CQ)

Modeling calculation

Shape and size dependency

Catalytic effect

Self-assembly and thermal stability

Room temperature super-plasticity

Design and fabrication

Photonics and dielectrics of passivated p-Si

Ferromagnetic nitride nano-films

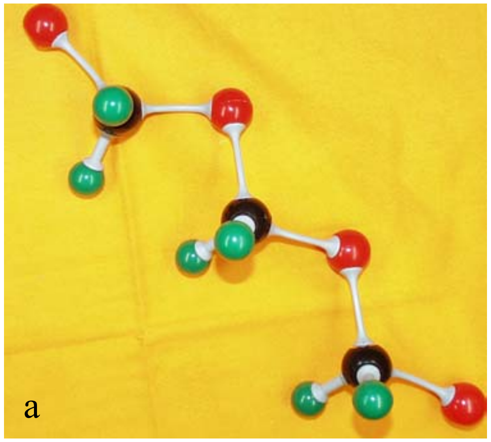
Oxide photonic crystal and photoluminescence

Characterization

Bond order-length-strength correlation

Single atomic bond and energy levels of an isolated atom

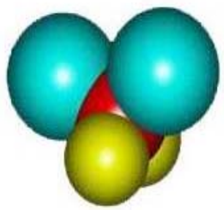
Nano-computation and atomic modeling drives out new concept that makes the dream into reality



(a) Nonbonding lone electron pairs zigzagged M-O-M monatomic chain derived from scanning tunneling microscopy/spectroscopy (STM/S) and low-energy electron diffraction (LEED) from the fcc (110) surface of Cu, Ni, and Ag. The primary tetrahedron consists two metal ions (M^+) and two metal dipoles (M^{dipole}). The former creates/widens the band gap, which is of use for photoemission, and the latter, lowers the work function for electron field emission. The lone pairs add localized mid-gap impurity states, which has littlie effect on the quantum efficiency of carrier recombination.

(b) Intense blue light (2.65 eV) emission of a synthetic metal oxide (bright spot) based on the model prediction. Photoluminescence was observed at room temperature under the UV light of Ar^+ excitation inside a glass chamber of film deposition.

Courtesy of CQ Sun, CNEG, [‘Oxidation electronics’ *Prog. Mater. Sci*. in press]



Basic oxide tetrahedron

Band & Barrier

Oxidation electronics: BBB correlation & its applications * (NSA-2003)

Sun CQ, Prog. Mater. Sci. 48 521 (2003)

Unification:

STM: atomic valences

PES/STS: valence DOS

TDS: bond nature & strength

LEED: Geometry & bonding kinetics

EELS/Raman: non-bond interaction

Discovery

Predictions

Applications

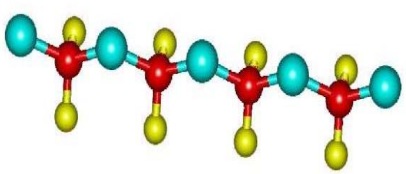
Quantification

- 4-stage Cu_3O_2 bonding kinetics

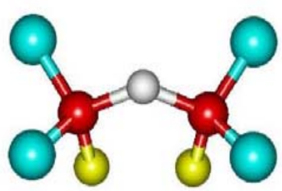
Generalization

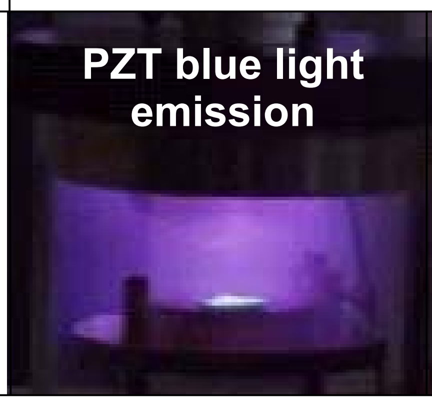
- **O-Cu{(001),(110)}**
- **O-(Rh, Pd)(110)**
- **O-(Co, Ru)(10-10)**
- **O-Rh(111)/Ru(0001)**
- **O-(V, Ag)(001)**
- **O-Rh(001)/(N, C)-Ni(001)**

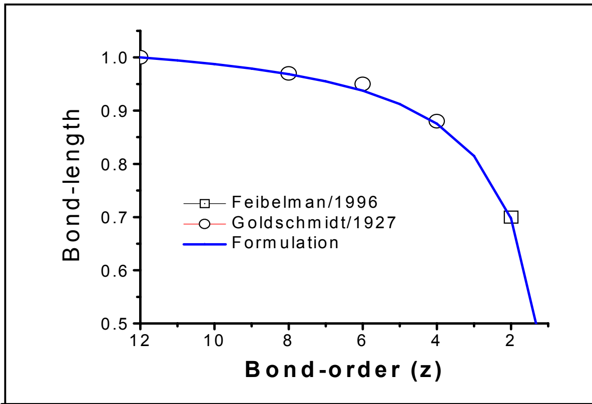
: O^{2-} : M^p: O^{2-} : chain

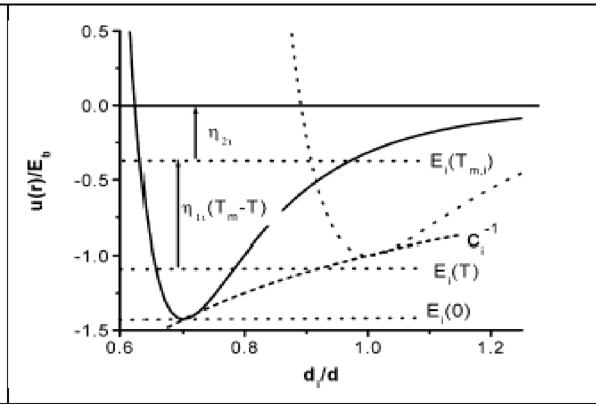


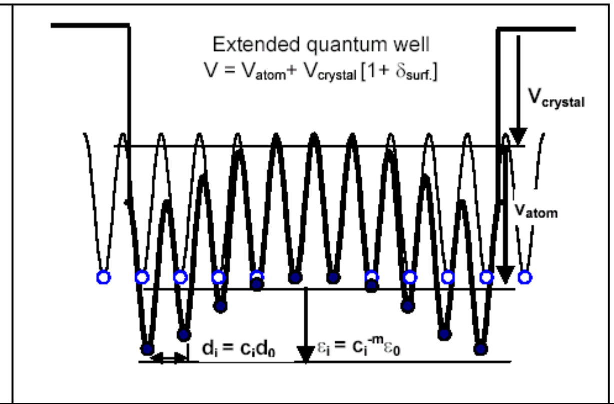
Cu_3O_2 molecule





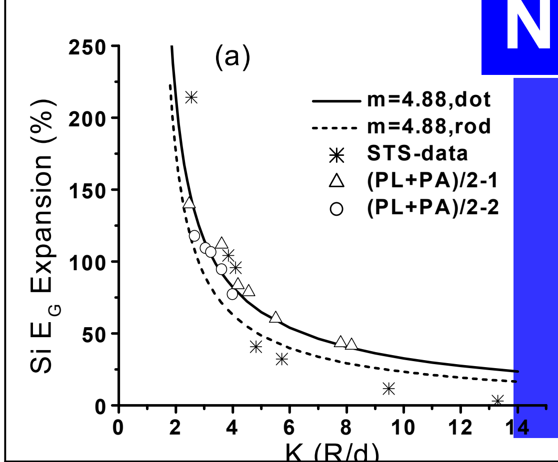


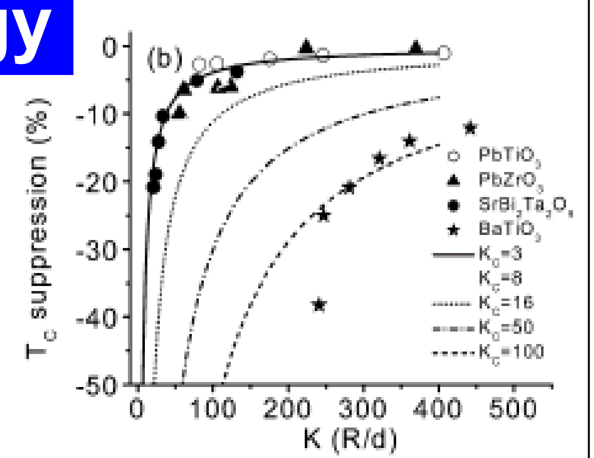


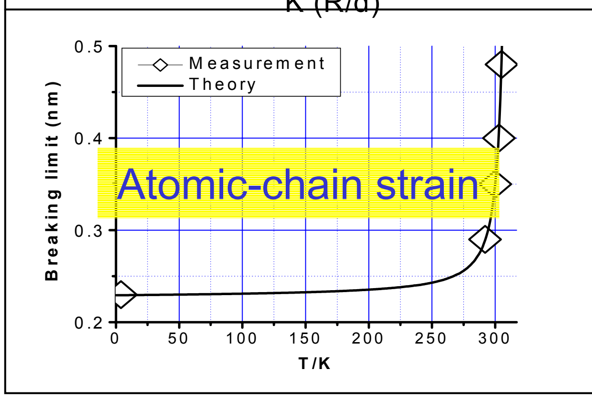


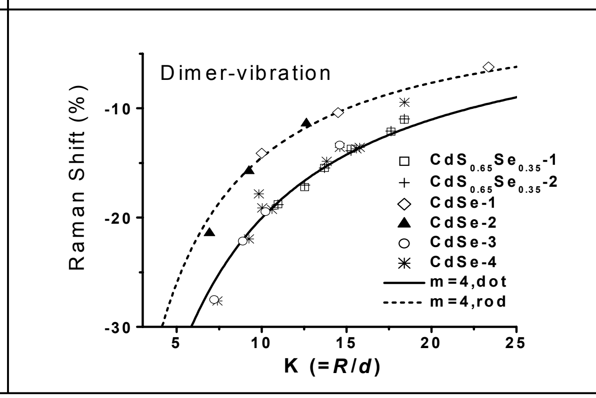
Nanosolid metrology

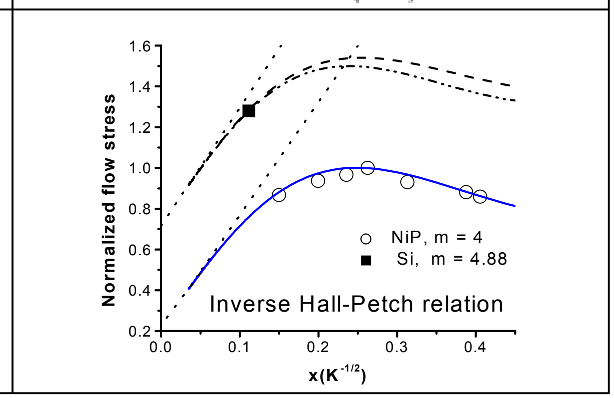
- Bond-order-length-strength
- Shape/size dependency
- Metrology
- Publications





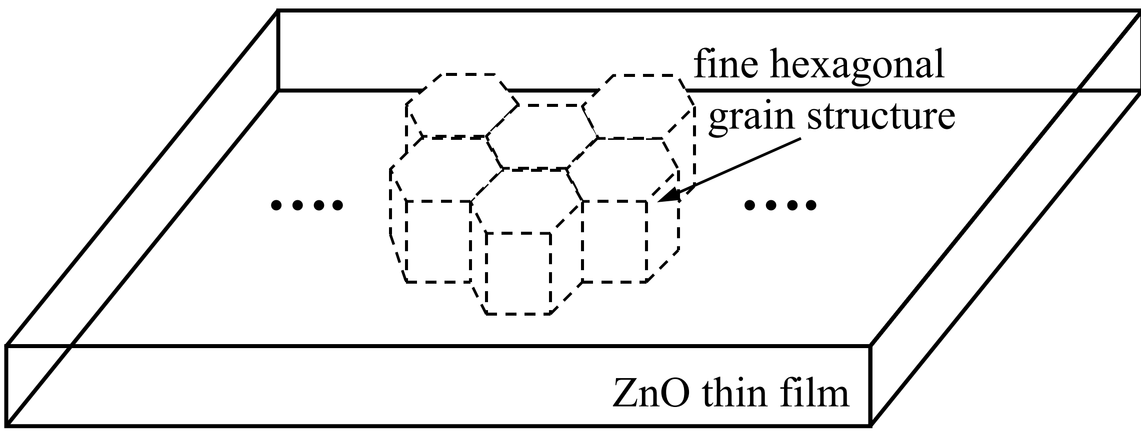






Investigation of Novel Photonic Bandgap Materials – ZnO Thin Film UV Lasers (application)

(by A/P Yu Siu Fung)



ZnO thin film with hexagonal grains

Experiments

Periodic hexagonal grain forms a 2D periodic structure – can be fabricate by FCVA in our IBP lab

Current Research/Investigation

- Design ZnO thin film with hexagonal grain structure as a high power and high efficiency UV laser cavity.
- Optimization of grain size and study the influence on the non-ideal periodic distribution of the hexagonal grains.

Nanoscale CMOS Technology/Device Modeling

(by A/P Zhou Xing)

Compact model for nanoscale CMOS technologies:

- Physics-based compact model (CM) (DC/AC/RF) for circuit simulation with geometry/bias/temperature scalability and predictability, characterized from given technology data

Numerical modeling and simulation of deep-submicron processes and devices:

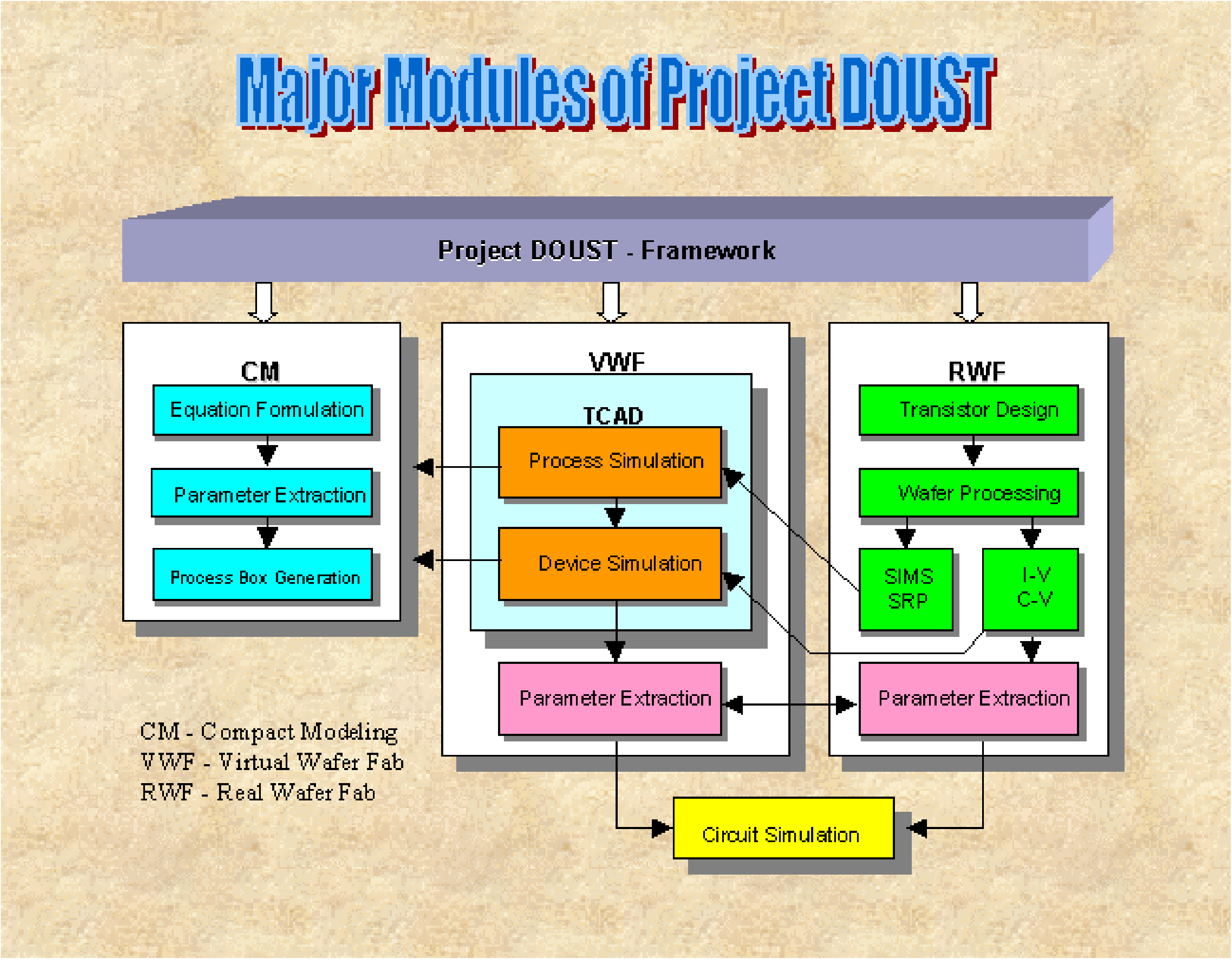
- Understanding of novel device structures and process effects
- Guidance to technology developers and feedback to CM development

Hierarchical modeling at the circuit/gate/block level:

- "Seamless integration of simulation modules with focus on the interplay and interfacing of the modules in order to enhance design effectiveness" [ITRS2001: difficult challenge beyond 2007 in complementing continuum tools with atomic ones]

Facilities: Complete suite of Synopsys (TMA) TCAD tools

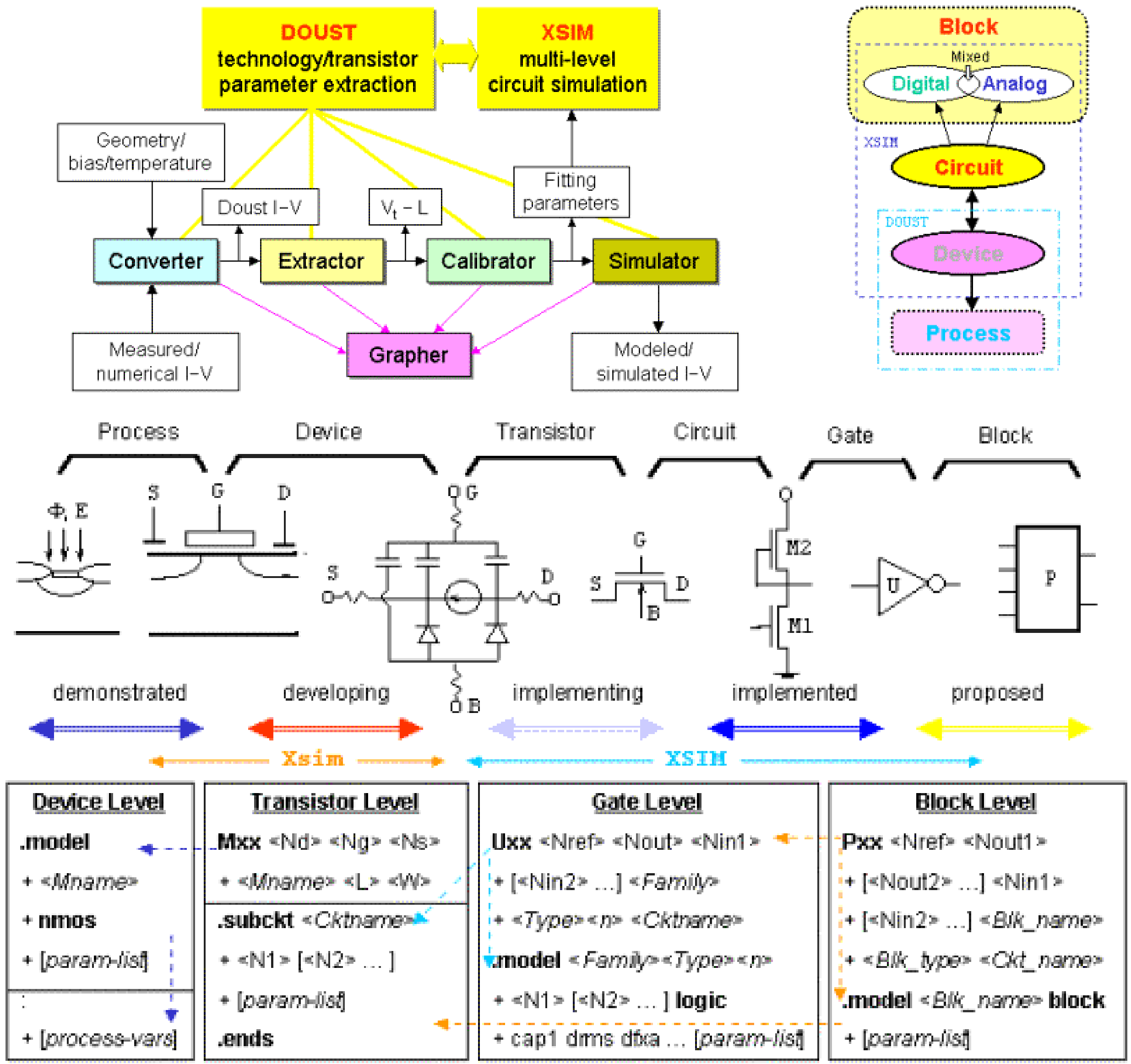
Project DOUST:
*D*esign and *O*ptimization of *U*ltra-*S*mall *T*ransistors

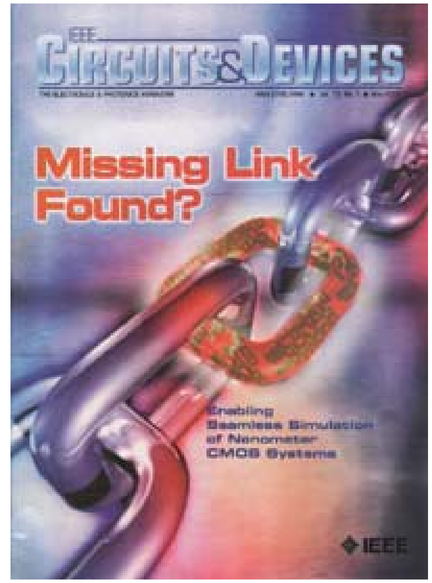


Dr Zhou Xing, http://www.ntu.edu.sg/home/exzhou/Research/DOUST/

Multi-Level Modeling of Nanoscale ULSI Technologies/Devices/Circuits/Systems

Invited feature article: ***IEEE Circuits & Devices Mag.***, vol. 19, no. 3, May 2003.





Dr Zhou Xing, exzhou@ntu.edu.sg, http://www.ntu.edu.sg/home/exzhou/

Technology-Based Predictive Compact Model Development for Next Generation CMOS

Funded by **Semiconductor Research Corporation**® through a Research Customization Program (RCP) supported by Chartered Semiconductor Manufacturing

Primary goal:

- A unified compact model for next generation CMOS circuit simulation that is accurate, continuous, symmetric, and scalable for a given (deep-submicron/ nanometer) technology, with minimum parameter set and easy extraction, and with predictive capability for the N+1 (and N+2) technology nodes

Main tasks:

- A predictive compact model that has minimum parameters and measurement data requirement and passes all major circuit tests: model equations and modeling approach
- A methodology to correlate compact model parameters to process variations: parameter extraction and algorithms
- A framework for predicting next generation N+1/N+2 CMOS technologies with the help of the compact model and TCAD: methodology and design of experiments

P.I.: http://www.ntu.edu.sg/home/exzhou/ | **SRC**®: http://www.src.org/ | **CSM**: http://www.charteredsemi.com/