Bridging Technology and Design for Beyond CMOS

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NANO-TEC has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° 257964
Outline

• Beyond Moore: devices and technology
  • Nanowires and nanotubes
  • Single Molecules
  • Nanomagnets

• Simulation and Design Beyond Moore
  • Device modelling
  • Novel architectures

• Conclusions
More Moore -> Beyond Moore

Transistor Scaling and Research Roadmap

90nm Node 2003
65nm Node 2005
45nm Node 2007
32nm Node 2009
22nm Node 2011

2015-2019 Research

Uniaxial Strain
SiGe S/D PMOS
1.2nm Ultra-thin SiO2

High-K & Metal-Gate Options
Non-planar Tri-Gate Architecture Option

Robert Chau, Intel, ICSICT, 2005
Beyond CMOS logic and memory device candidates:

- Nanowire transistors
- CNT transistors
- Resonant tunneling devices
- NEMS devices
- Single electron transistors
- Molecular devices
- Spintronic devices

All those candidates (some of which not yet demonstrated) still suffer from major reliability and stability problems
Nano-Device Structure Evolution

Source: Intel
Silicon nanowire transistors

$L_g = 1.3\mu m; \ \varnothing = 26 \ nm; \ \ t_{ox} = 300\text{nm SiO}_2$

-2 -1 0

+5V; 0V; -5V

200 nm

NiSi$_2$  Si  NiSi$_2$

source  $L_G$  drain

The CNTs behave like ideal p-type nanowires. The gate voltage modulates the transmission of the holes which are injected from the source contact.

The energy profile of the highest valence-subband in a (10,0) CNT for $V_{DS} = 0.2$ V and $V_{GS} = 0.6$ V.
**CNT quantum capacitance**

Gate is a Macroscopic metal Oxide

\[
\frac{1}{C_Q} = \frac{1}{C_E} + \frac{1}{C_D}
\]

\[
C_D = e^2 D(E_f)
\]

\[
C_E = \left(-\frac{\partial E_l}{\partial Q}\right)^{-1}
\]

In a classic MOS \(C_Q >> C_{ox}\) => modulation depends on \(C_{ox}\)

In a well-tempered MOS \(C_G >> C_s C_D\)

In 1D systems \(C_Q\) is small

\(V_{ds}\) can influence the channel charge and barrier
Molecular components

20 nm embedded GaAs layer after etching and deposition of 3 nm Ti and 7 nm Au.

5 nm embedded GaAs layer after etching and deposition of 2 nm Ti and 6 nm Au.

OPV11 molecules with simplified phenyl side chains synthesized by the group of Prof. Dr. E. Thorn-Csányi at the University of Hamburg.

In collaboration with G. Abstreiter, WSI, M. Tornow, TU Braunschweig
Molecular Conduction

Efficient Density Functional Theory codes

SIESTA (Soler et al.)
\[\rightarrow\text{Numerical basis functions, } O(n) \text{ scaling}\]

DFTB (Frauenheim et. al.)
\[\rightarrow\text{DFT parameterized tight-binding}\]

An electronic structure problem

Self-consistent solution

Transmission – electron flow

M. Reed et al., Scientific American 2002

TranSIESTA

gDFTB
A large variation is found in the IV characteristics between successive sweeps.

Reasons can be due to:

- Configurational changes in single molecules
- Variation in the number of molecules attached to the electrodes
- Changes in the bond of a single molecule to the metal contact
- ...

Such variability has to be dealt at a circuit/architecture level.
Cross bar non volatile memory

A crossbar memory – probably the simplest possible functional circuit – is one of the proposed application of single molecule electronics.

The current-voltage characteristics of molecules is typically hysteretic, with step-like nonlinearities and possibly non-symmetric (rectifying) behavior.
Computing with single molecules

Self-organized computation with unreliable, memristive nanodevices

G. S. Snider

Computing with hysteretic resistor crossbars

Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, CA 94304, USA
From modelling to design

We can simulate transport in molecular and semiconducting nanostructures quite reliably, accounting for charging effects, dissipation, screening as long as the molecular systems consist of a sufficiently small number of atoms,

but

the simulation of realistic systems, especially in terms of the contacts and in general the coupling with the external environment is still a problem
Multiscale modelling

DFTB + quantum-transport approaches using Non-equilibrium Green Functions.

Well-established drift diffusion simulator codes are used to simulate contacts and devices surrounding the molecules.

Ab initio models

Quantum-classical interfaces

Continuum-based and circuit models

Physics

Engineering

Paolo Lugli
TUM

Embedded Tutorial presented by the NANO-TEC Project: "BEYOND CMOS - BENCHMARKING FOR FUTURE TECHNOLOGIES"
Mixed-Mode Simulation

Atomistic information could be fed into the NanoTCAD simulator
Modelling a cross bar memory

We use SPICE circuit simulations to investigate such circuits. We built the model of the junction using published (molecular) I-V curves and then generated SPICE netlists of large circuits using a Matlab script.
Cross-point arrays

We have set up a circuit model for molecular cross bar arrays to address the performance and the scalability of such systems. The IV characteristics for the SPICE model taken from: E. Lortscher, J. W. Ciszek, J. Tour, H. Riel: Reversible and Controllable Switching of a Single-Molecule Junction, Small 2, No. 8-9, 973 (2006)

Nonlinearity of the molecule IV characteristics enhances read-out margin

Coupling molecular layer with solid-state diodes enables large-scale circuits
Coupled nanomagnets

Investigations of permalloy nanomagnets (thermally evaporated and patterned by electron beam lithography) confirm the simulation results

Courtesy of W. Porod, Notre Dame University
Working majority gate

SEM images

MFM images

Imre et. al. *Science* 2006
Logic with nanomagnets

The challenges:
- How to make signals propagating? → Integrated clocking
- How to write in the magnets? → Localized field from wires
- How to read out the magnets? → Hall sensor

In collaboration with M. Becherer and D. Schmit-Lansiedel (TUM), W. Porod (Notre Dame)
Conclusions

- Nanotechnology provides a variety of interesting and promising nanostructures.

- Critical issues such as reliability, stability and lifetime are going to become routine and will have to be addressed at a circuit/architecture level.

- Quantum mechanical device modelling must be matched to circuit simulations.

- Novel circuits and architectures are going to be needed for a full exploitation of nanocomponents.
Thanks for your attention!