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Materials Integration: An All-of-the-Above Approach

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50 years of materials innovation

Materials Modeling in Industry

- Materials modeling is **maturing**
  - **Calls for an all-of-the-above approach**
- New capabilities being developed
  - Since 2000’s: metaGGA, LDA+U, HSE, GW, DFT-NEGF, Wannier, Grimme, etc.
- Developers not always focused on “right” problems
  - Seed commercial or academic development
- Cloud a viable alternative in some cases
- Commercial likely the “last-mile”
  - You can’t get a Ph.D. for some things!

Introduction: Me *(and Applied Materials)*

- Founding member Intel's Materials Modeling Team (in TCAD) – 15 years
- Exabyte.io: VP of Science – Materials Discovery on the cloud
- Property Vectors: materials modeling consulting
- ***Now:*** leading Applied Materials' Materials Modeling Team

World's #1

Semiconductor and display equipment company

$17.3 billion revenue

>12,750 patents

$2 billion R&D spending

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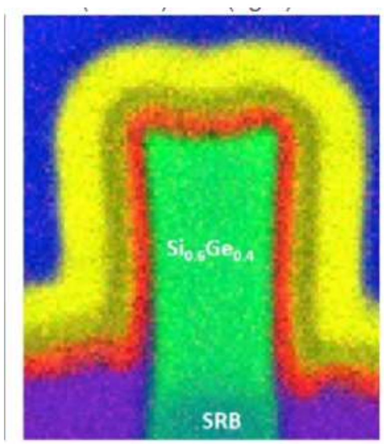
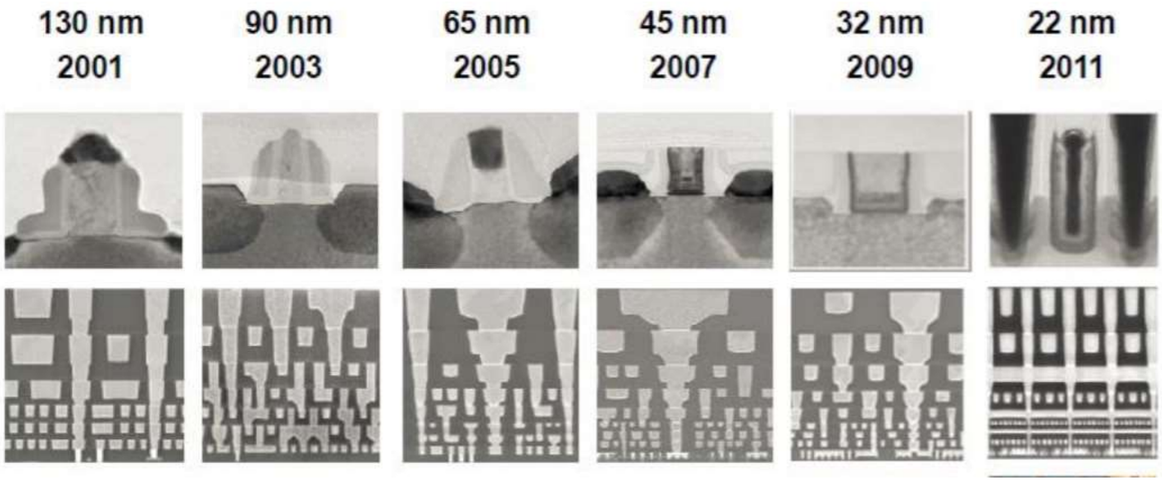
Every electronic device today is manufactured using Applied equipment

Scaling Requires New Materials Integration

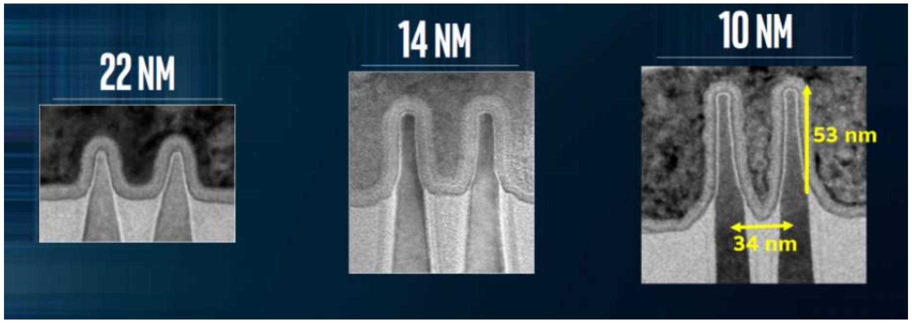
- Contrast changes = different materials, doping, crystal structure, composition
  - All must be designed/selected for:
    - Material properties (structure-property relationships)
    - Chemistry, electrical, mechanical, and thermal interactions with neighbors
- Wide variation in materials and properties = casting a wide net with software tool techniques



Src: GF/IBM IEDM paper EDX elemental map



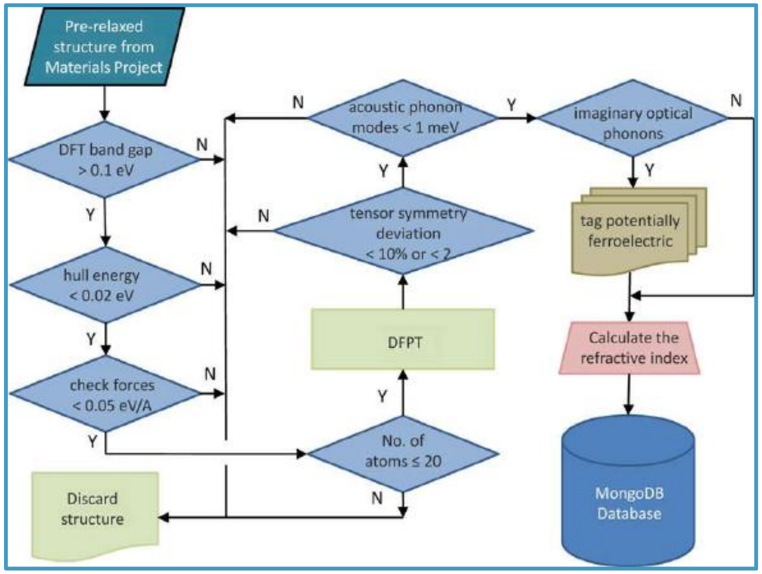
Src: M. Bohr Intel 2012 Press Release



Src: Intel TMG Day

Semiconductors: Typical Materials Modeling Projects

- Screening (closer to “pathfinding”):
  - Find subset of materials A to W with property X, Y, & Z
- Optimization (closer to development):
  - Material A_0 with property X_0 => find material A_1 with X_1
- Mechanism:
  - Understand why material(s) display a given property
- Parameterization:
  - Quantify a property for use in higher level models



Src: Nature (Pearson & Prinz)

Many Technical Challenges: Solved or “Good-enough”

- Electronic structure properties:
  - Band gaps
  - Dielectric constant
  - Work function
  - Barrier heights
  - Band offsets
- Mechanical properties:
  - Moduli
  - Stress vs. strain
- Chemistry properties:
  - Relative reaction barriers

Open Challenges

- Practical
  - Reliable and easy-to-use software *(workflows)*
  - Computational resources *(cloud democratizing)*
  - Realistic interface structures *(w/ passivation of defects)*
  - Bridging realistic time-scales
    - "Universal" MD fitting engines/workflows
- Technical *(most require 10x computing)*
  - Van der Waals
  - Plasma
  - Bridging realistic time-scales:
    - "Universal" MD potentials
    - General purpose accelerated dynamics and/or KMC
  - Computationally feasible electron-phonon interactions
  - Accurate reaction barriers *(including pre-exponential)*
  - Heavy elements/relativistic effects

Capability Sourcing Drivers: Varies Somewhat

- Commercial: core capabilities, GUI’s, and environment, *but slower to adapt*
  - Software provider purchase *(many similar providers)*
- Academic/National Labs: new bleeding edge capabilities, pre-test workflows, and generate learning, *but difficult to scale*
  - Cal-tech, U. Mich., U. Moscow, Oak Ridge, Iowa State, U. Washington, UCLA, Stanford, UT Dallas, Tyndall
- Open-source: standardized capabilities, modularity, automation, and databases*, but uncertainty*
  - LAMMPS, Quantum Espresso, NWChem, Ab-init, Materials Project, ASE, TS-ASE, git-hub *(pseudo open-source)*, viewers/GUI’s, AFLOW, Nomad, OCMD, ATAT
- Computing?

Cloud Computing

Vendor	Own Hardware	Corporate-level Security/IP Control	Core per Hour (w/ IB)	Pre-prepared FEA Workspace	Comments
Azure	Yes	Yes	$0.10	No	Focused on HPC
AWS	Yes	Yes	??? ($0.01 w/o IB w/ spot pricing)	No	Focused on Services and GPU's
Sabelcore	Yes	Yes	$0.10-$0.20	No	Boutique HPC
Altair/PBS Pro	No	Yes	$0.06	No	Reselling other resources (Azure, Swift, etc.)
TACC/OSCC	Yes	No	$0.03	No	Supercomputing Centers
NIMBIX	Yes	Yes	$0.08	Yes	Focused on FEA
Rescale	No	Yes	$0.08 (~$0.01 for spot pricing)	Yes	Reselling AWS with focus on FEA
Penguin	Yes	Yes	$0.08	Yes	Sells cloud and installed hardware
Exabyte	No	Yes	Varies	No	Materials Discovery Cloud
Kogence	No	Unknown	Unknown	No	Focused on community solutions
Rackspace	Yes				No engagement
Google	Yes				No engagement

- Data current as of EOY 2017 and based on $100k bulk purchases (Src: M. Haverty, Property Vectors)
- Oracle a new HPC cloud player as well as European options (1&1, OVH, Dimension Data, etc.)

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- Cloud computing competitive in some cases for burst usage
  - Sustained usage less cost effective
    - Perhaps competitive if staying within one node
- Security a big roadblock *(virtualization + cost may eventually win over concerns)*
- Potential value-added feature
  - Scalability an attractive aspect

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Materials Modeling: All-of-the-above

- Currently no commercial, academic, or open-source set of tools provides all that is needed
  - Future may involve hybrid supported open-source models (think Enterprise Linux RedHat/SUSE)
- <u>Ideal state/software:</u>
  1. Stable and comprehensive core engine(s)
  2. Simple automated workflows (for non-experts)
  3. Ability/flexibility to leverage open-source development
  4. Databasing and analysis
  5. Cloud + on-premises hybrid options

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