materials design

Atomistic Simulations as a Driver of Industrial Innovation

Ray Shan
Materials Design

August 5th, 2020

Outline

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- Industrial value of materials research
- The *MedeA* software of Materials Design
- Examples
  - Device optimization with **Infineon**
  - Battery research with **Toyota**
  - Gate-stack control with **Texas Instruments**
  - Ultrahard materials
  - Polymers and Fluids
- Conclusions

Value of Materials Research

Creation of products which are

- Valuable for customer
- Innovative
- Safe and reliable
- Efficient to manufacture
- Environmentally responsible
- Meeting regulations

Value of Modeling and Simulation

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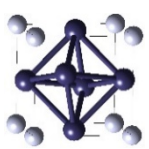
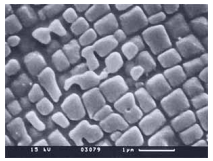
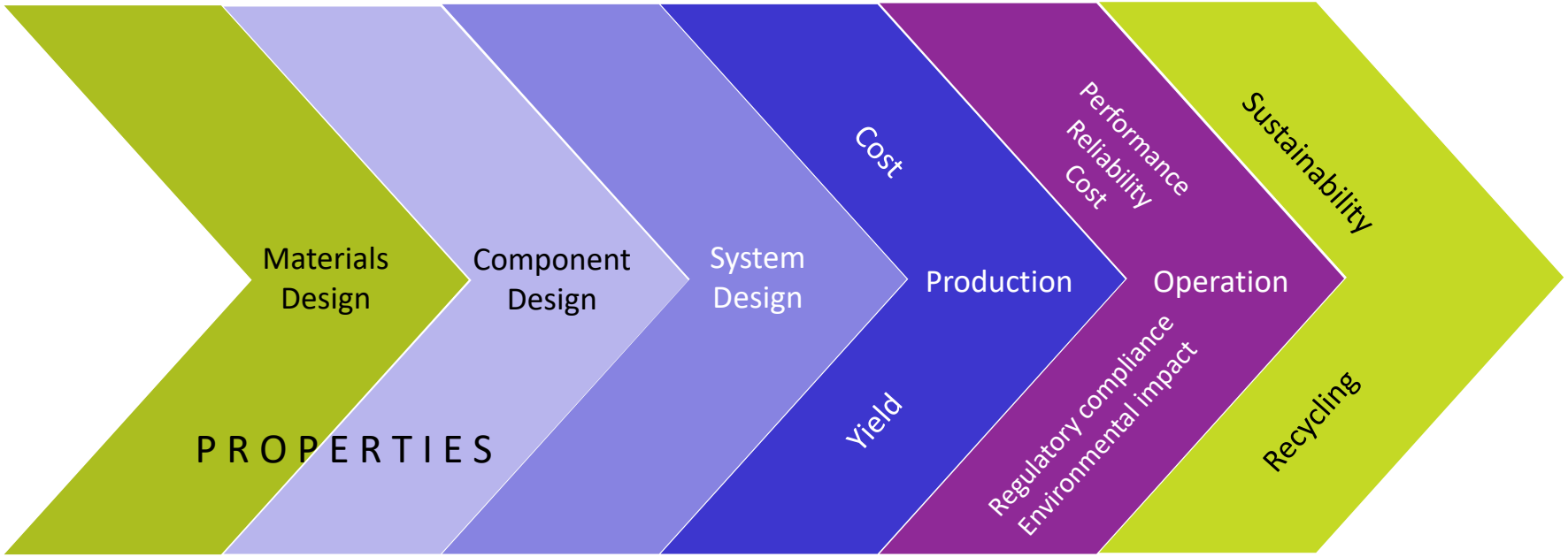
- Prediction of properties
- Understanding mechanisms

Optimal design and processing

Innovation Process

- Improvement of industrial products is a long-term iterative process
- Materials modeling and simulation are catalysts of this process

Purpose of Atomistic Modeling

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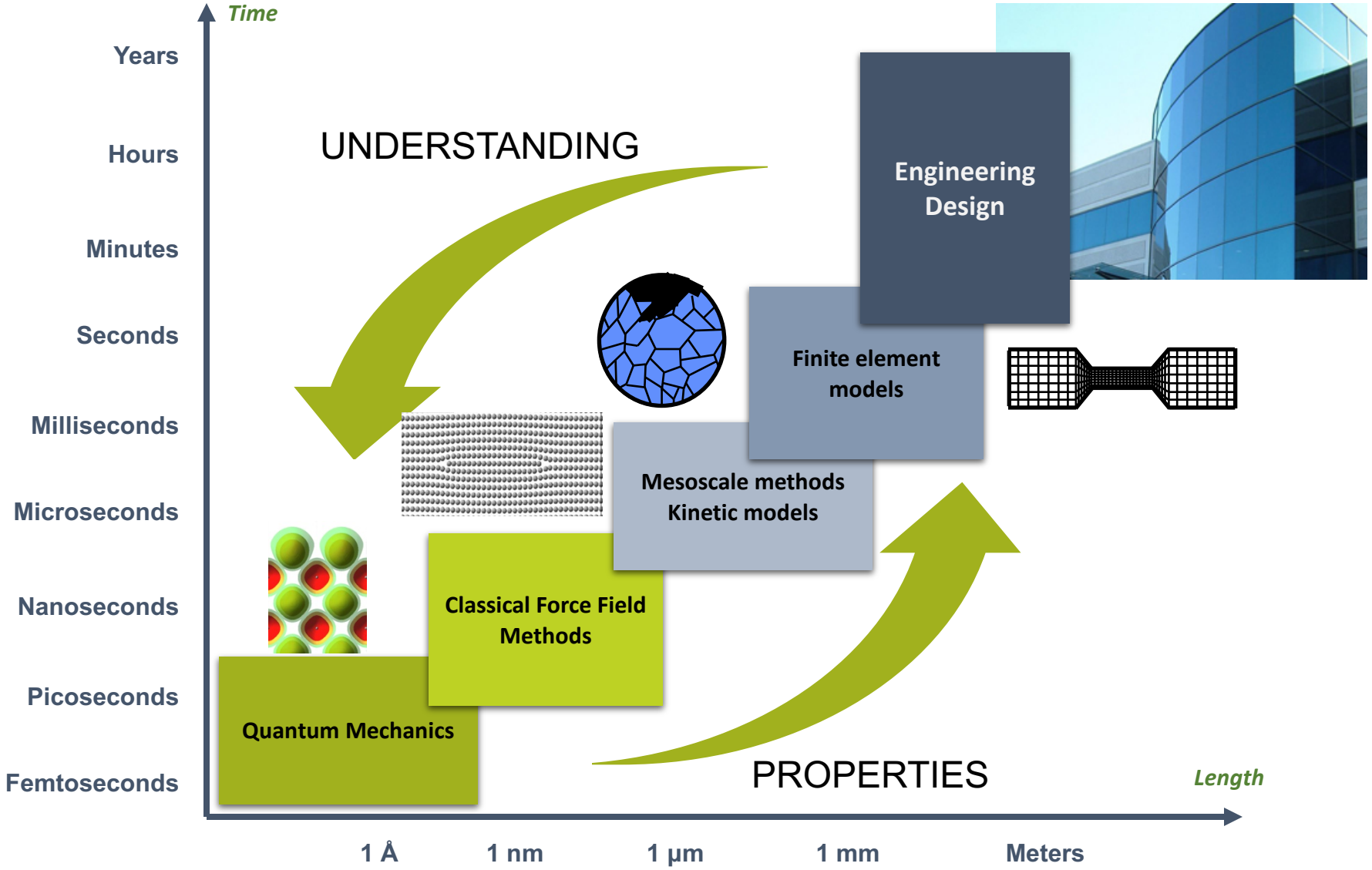

MedeA Software Environment

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GUI

BUILDING & ANALYSIS

Builders: crystals, defects, interfaces, surfaces, molecules, nanostructures, amorphous materials, polymers

Analysis: geometry, band structures and DOS, electron and spin density, potential, Fermi surface, phonons, transition states, dynamics trajectories

DATABASES

Experimental and Computed Structure and Property Data

ICSD | NIST | COD | Pearson

Job Server

Local or remote

Job submission & control

Task Servers

Mechanical Thermal Chemical Kinetic Electric Optic Magnetic

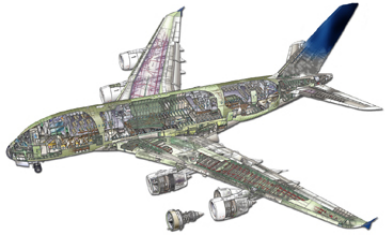
COMPUTATION OF PROPERTIES

ab initio QM - VASP | Quant. Chem. - Gaussian | Semi-empirical - MOPAC | Mol. dynamics - LAMMPS

Monte Carlo - GIBBS

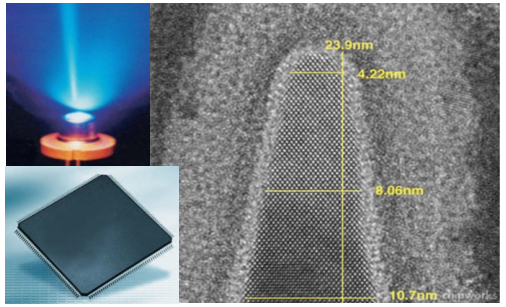
Breadth of Applications

Automotive

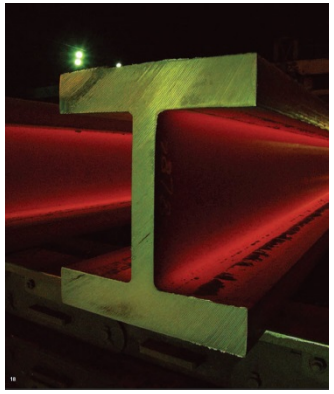


Aerospace

Polymers



Electronics



Metals and Alloys

Glass and Ceramics

Batteries and Energy Storage

Molecular Crystals

Oil & Gas

Minerals

Catalysts

Fluids

Materials Properties from MedeA

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Structural properties

- Molecular structures
- Crystal structures
- Surface structures
- Structure around defects
- Morphologies
- Adsorption geometries
- Structures of interfaces
- Liquids and amorphous systems

Thermo-Mechanical properties

- Density
- Elastic moduli
- Thermal expansion coefficients
- Fracture

Thermodynamic properties

- DU, DH, DS, DG, heat capacity
- Binding energies
- Solubility
- Melting temperature
- Vapor pressure
- Miscibility
- Phase diagrams
- Surface tension

Chemical properties

- Chemical reaction mechanisms and rates
- Reactivity on surfaces
- Solid-solid reactions
- Photochemical reactions

Transport properties

- Mass diffusion coefficient
- Permeability, diffusivity, solubility
- Thermal conductivity
- Viscosity
- Electrical conductivity

Electronic, optical, and magnetic properties

- Electron density distribution - electrical moments
- Polarizabilities, hyperpolarizabilities
- Optical spectra
- Dielectric properties
- Piezoelectric properties
- Electrostatic potential
- Spin density distribution, magnetic moments
- Energy band structure - metal, semiconductor, insulator
- Band gaps, band offsets at hetero-junctions
- Ionization energies and electron affinities
- Work function

Embrittlement of Cu Micro-Structures

Materials Science & Engineering A 618 (2014) 398–405

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Temperature dependent transition of intragranular plastic to intergranular brittle failure in electrodeposited Cu micro-tensile samples

A. Wimmer [a], M. Smolka [b], W. Heinz [a], T. Detzel [c], W. Robl [d], C. Motz [e], V. Eyert [f], E. Wimmer [f], F. Jahnel [g], R. Treichler [g], G. Dehm [h,*]

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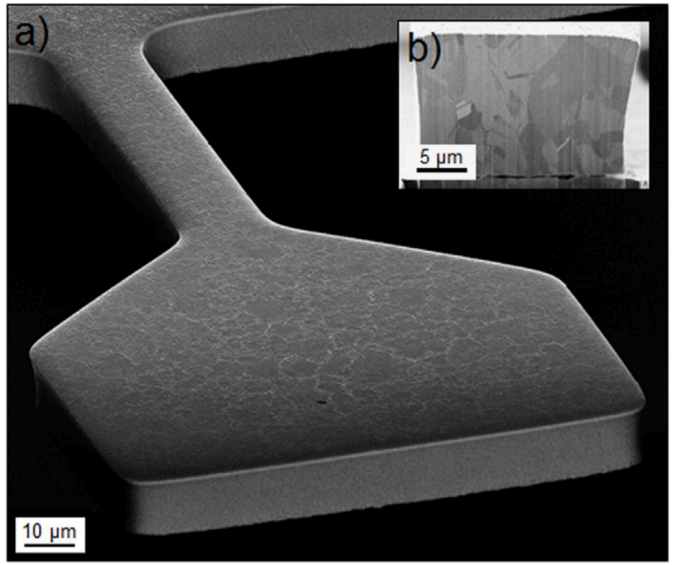
ABSTRACT

Smaller grain sizes are known to improve the strength a
Consequently, metallic thin films and structures which
deposited under processing conditions that lead to a fi
temperatures as low as 473 K the failure mode of 99.99 a
ductile intragranular to brittle intergranular fracture. The
strength and elongation to fracture. Chemical analyses
impurities detected at grain boundaries. *In situ* microme
microscope and atomistic simulations are performed to



- Objective: Improve strength and ductility of Cu microstructures
- Approach: Introduce additives to reduce grain size (Hall-Petch effect)
- Challenge: Additives cause embrittlement at elevated temperatures

Sample Characterization

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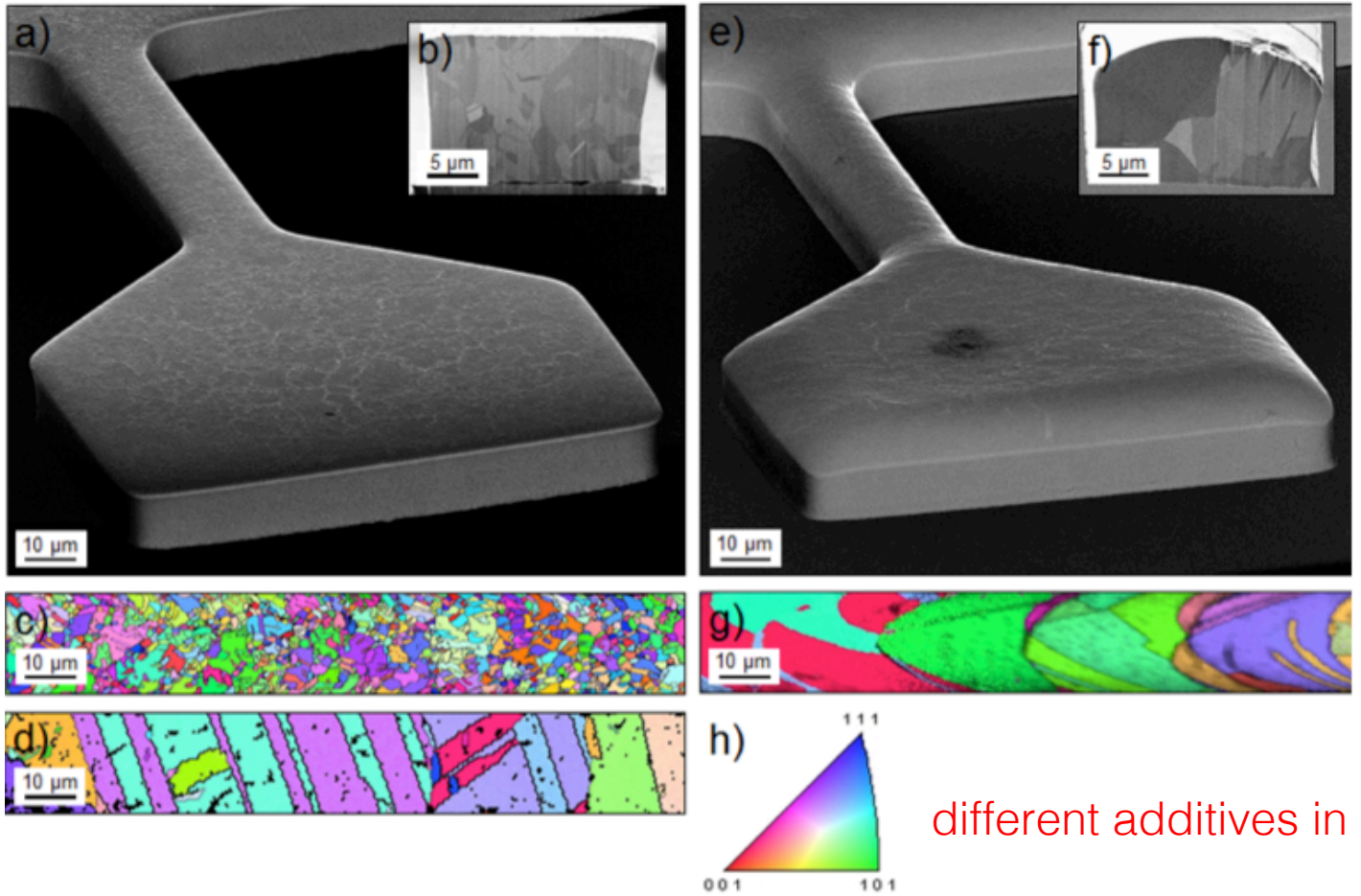
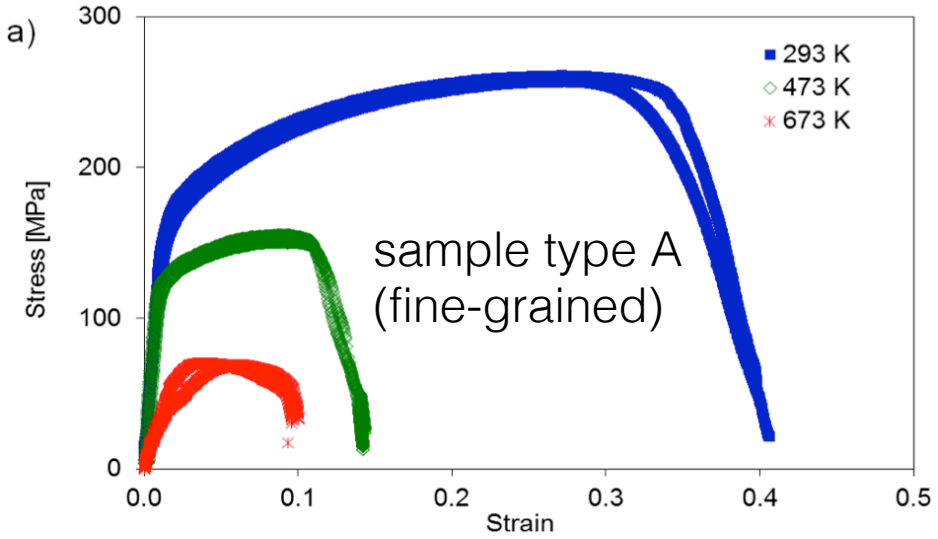
EBSD/
SEM

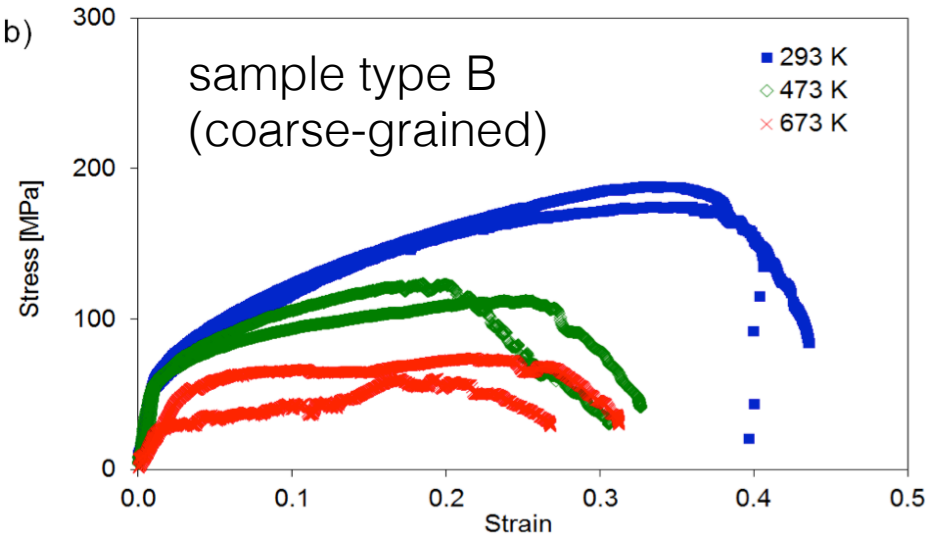


different additives in samples (a) and (e)!

- (a, b, c) sample type A (medium grain size: 2.7 ± 0.6 µm)
- (e, f, g) sample type B (medium grain size: 10.1 ± 2.6 µm)

Stress-Strain Behavior





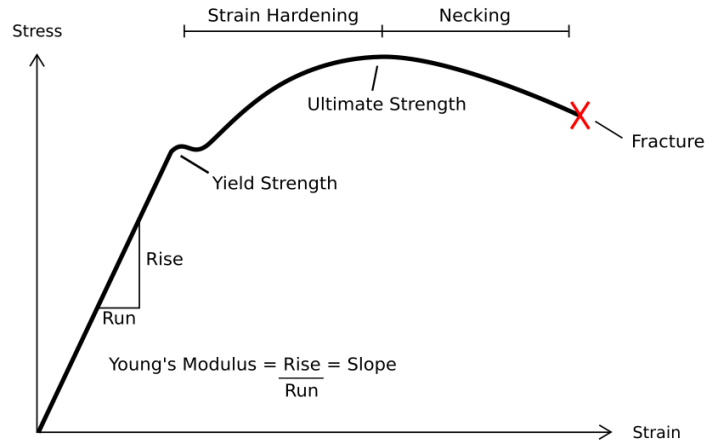
different additives in samples A and B!

293 K: coarse-grained → fine-grained

- yield stress and ultimate stress increase
- changes explained by Hall-Petch effect

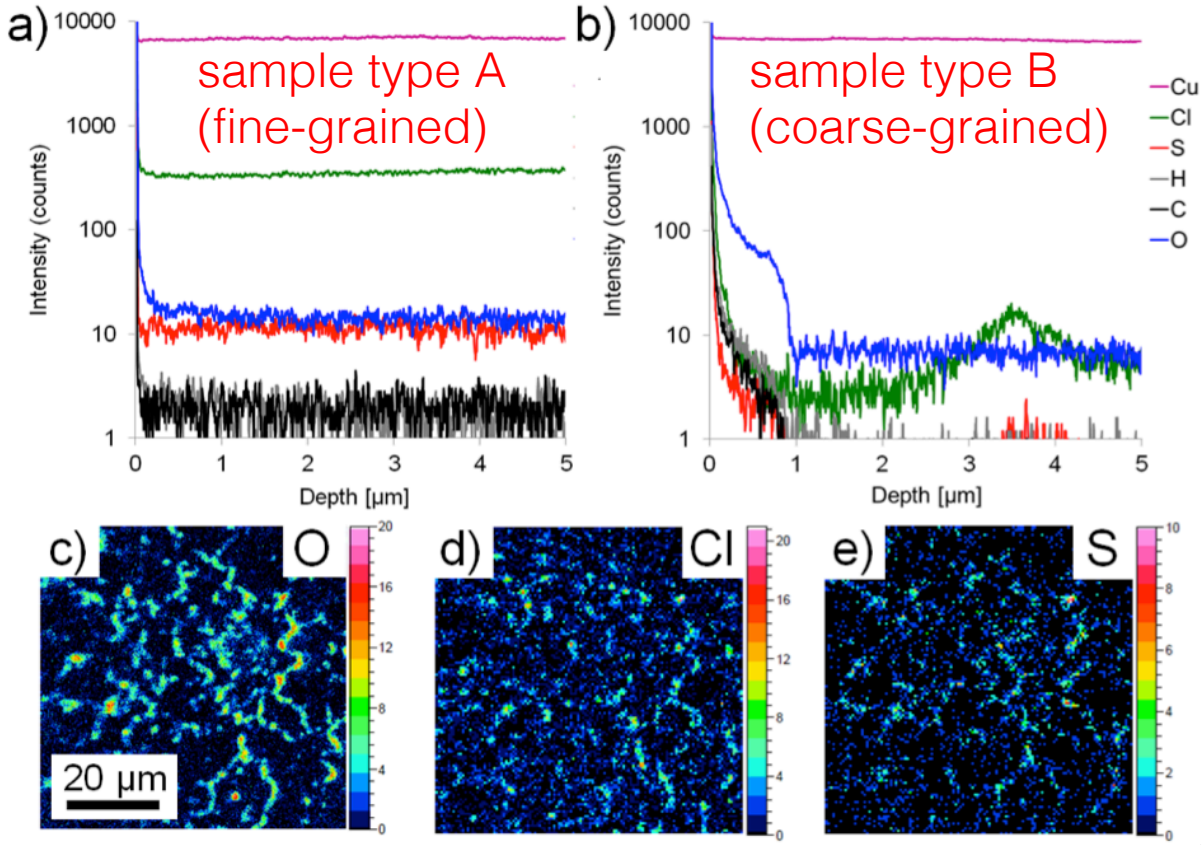
473 K and 673 K:

- drastic reduction of elongation to fracture for fine-grained samples
- scattering of results for coarse-grained structures due to small number of grains



Chemical Analysis

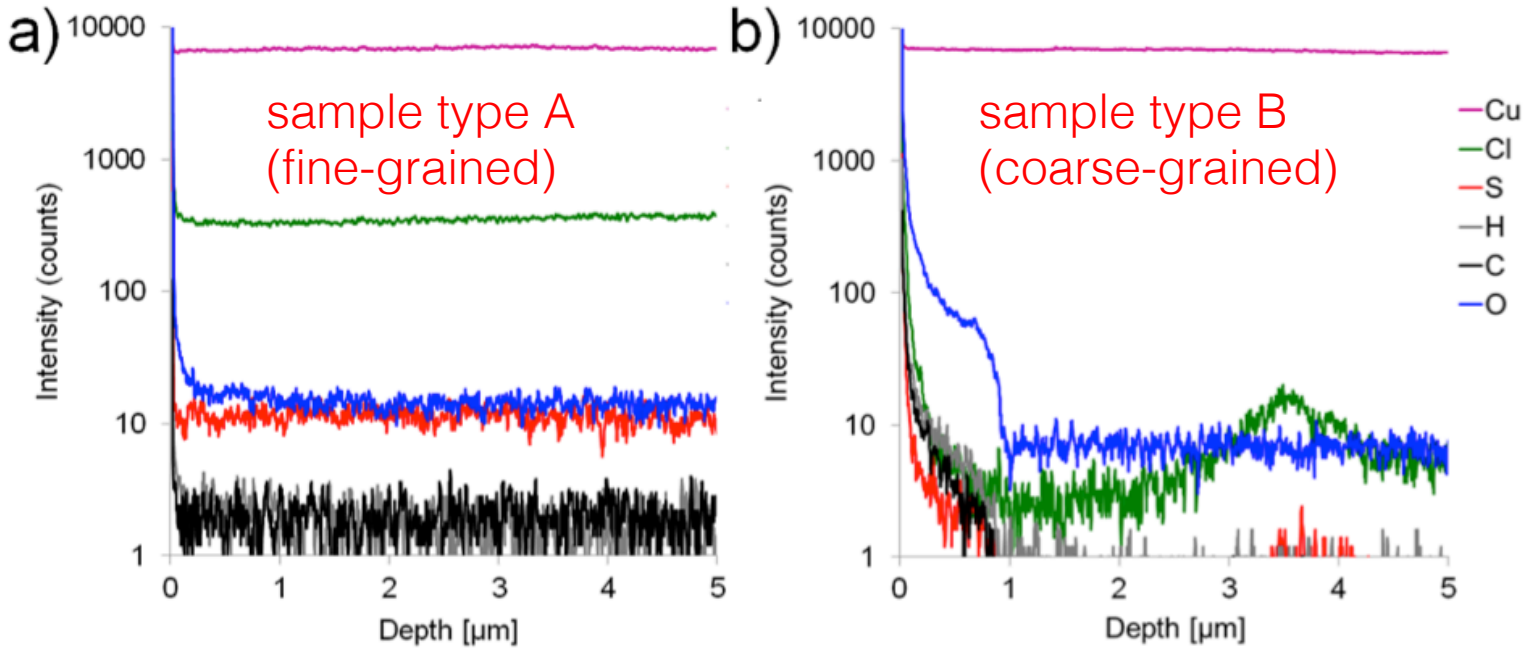
TOF-SIMS



- higher S, Cl content in fine-grained samples (additives)
- O, S, Cl enrichment at grain boundaries
- segregation of O, S, Cl to grain boundaries and surfaces

Strategy of Atomistic Simulations

- Create models of surfaces and grain boundaries
- Understand grain boundary and surface segregation; compute segregation energies
- Understand grain boundary weakening due to S and Cl; compute cleavage energies
- Find elements which could compensate the detrimental effect of S and Cl but maintain the electronic and thermo-mechanical properties of Cu



Model of Grain Boundary

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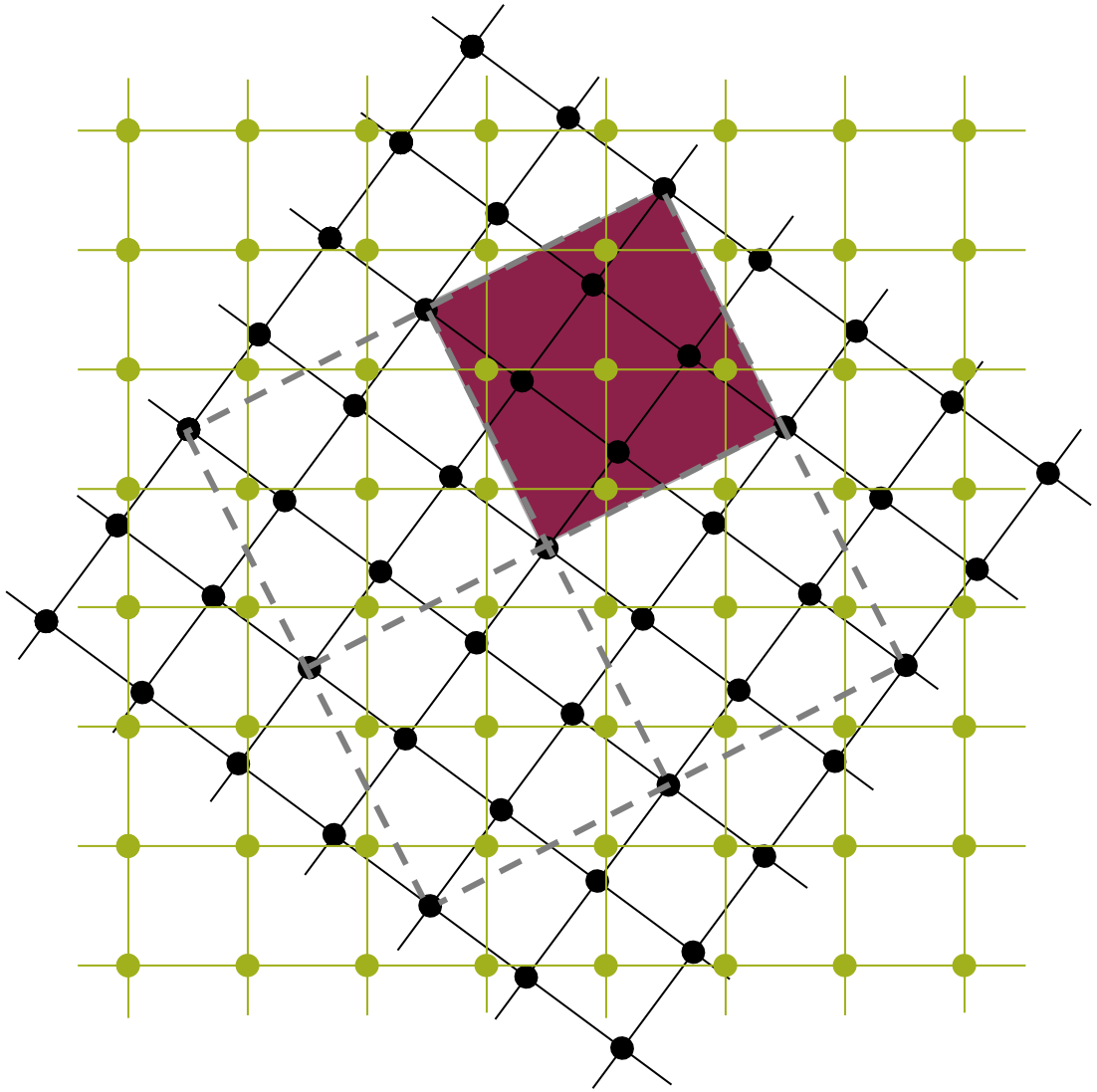
Σ5(001) Twist
Grain Boundary



MedeA-Surface Builder
MedeA-Interface Builder

Coincident Site Lattice Theory:

- minimize grain boundary energy
- maximize number of points common to original and rotated lattice

Grain Boundary and Surface

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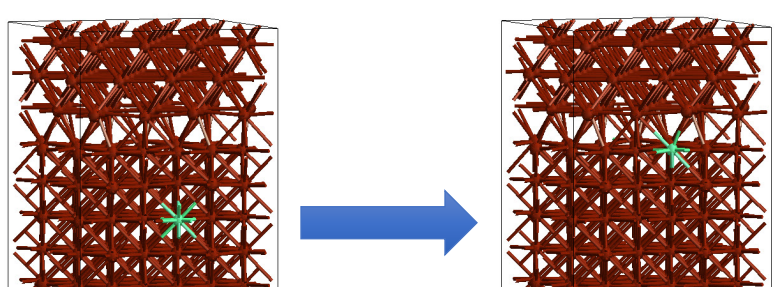
MedeA-Surface Builder, MedeA-Interface Builder



grain boundary segregation

surface segregation

- Understand grain boundary and surface segregation; compute segregation energies for Σ5(001) and Σ7(111) twisted grain boundaries
- Understand grain boundary weakening due to S and Cl; compute cleavage energies
- Find elements which could compensate the detrimental effect of S and Cl but maintain the electronic and thermo-mechanical properties of Cu

Grain-Boundary Segregation

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MedeA-VASP

Calculated energy release during segregation ΔE_{seg} of Cl and S in Cu.

	ΔE_{seg} [kJ/mol]	
	Cl	S
GB segregation, ∑5 (001)	−69.9	−54.3
surface segregation, (001)	−321.5	−145.3
GB segregation, ∑7 (111)	−53.5	−56.3
surface segregation, (111)	−272.0	−129.9

- S and Cl have strong tendency to segregate from the bulk to the grain boundary
- Tendency to segregate to the surface is even more pronounced

Grain-Boundary Cleavage

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MedeA-VASP

Calculated work of separation E_{sep} of $\sum 5$ and $\sum 7$ grain boundaries of pure Cu and Cu contaminated with Cl and S with planar impurity concentration c_{imp} in atoms per nm^2.

	c_{imp} [$1/nm^2$]	E_{sep} [J/m^2]		
		Pure Cu	Cl	S
$\sum 5$ (001)	0.77	1.08	0.82	1.01
$\sum 7$ (111)	0.62	1.13	0.89	1.04

- S impurities, and even more so, Cl impurities cause pronounced reduction of the work of separation at the grain-boundaries

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MedeA-Interface Builder
MedeA-Surface Builder
MedeA-VASP

- Embrittlement caused by S and Cl impurities
  - S and Cl segregate from the bulk to the grain boundary
  - S and Cl reduce the work of separation at the grain-boundaries
- Challenge: Find elements which compensate the detrimental effect of S and Cl but maintain the electronic and thermo-mechanical properties of Cu

Grain boundaries
Fracture
Plasticity

Strength of Ni Grain Boundaries

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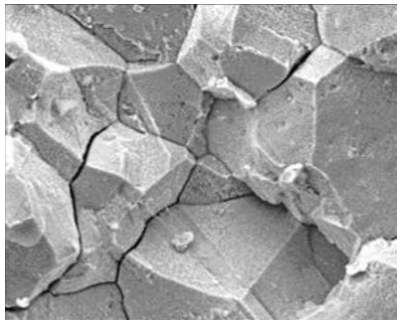
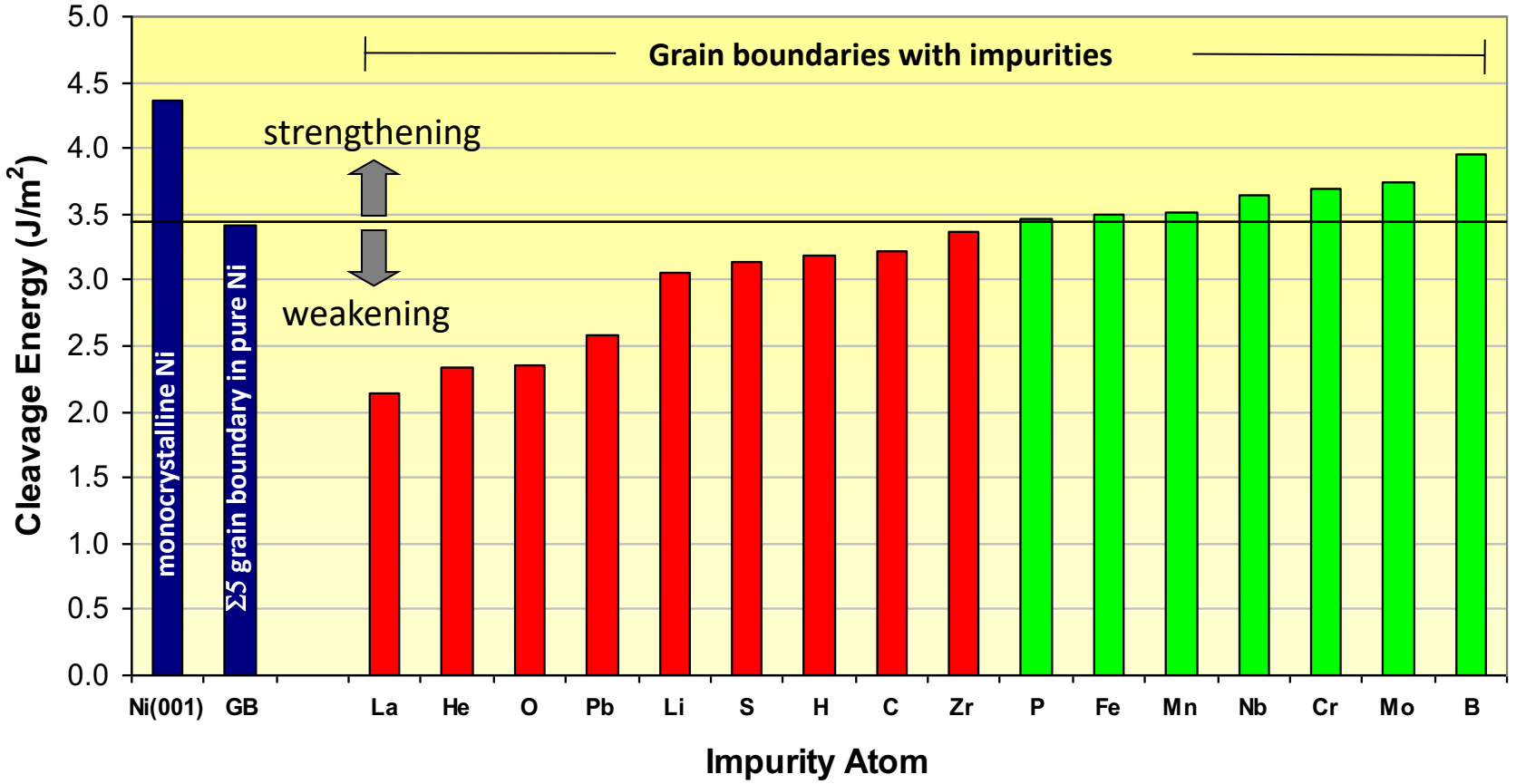
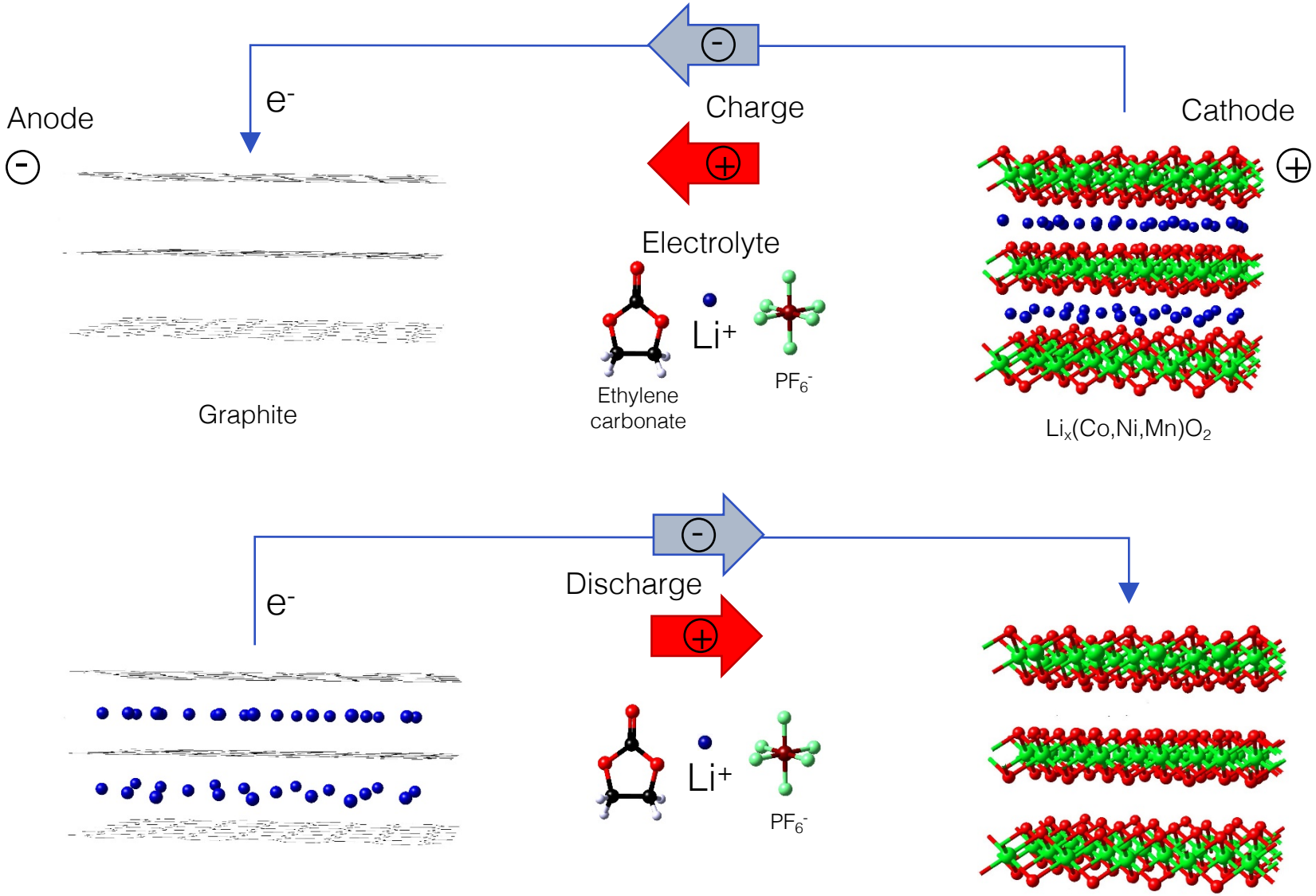
- Which impurities are dangerous?
- Which alloying elements improve performance?





Low-Strain Cathode Materials for Solid-State Li-Ion Batteries

Li-Ion Battery



Issues

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- Limited capacity: Li_xCoO_2 is unstable if more than half of Li is removed. In practice, operation is restricted to $0.5 \leq x \leq 1$; half of the capacity is not used.
- Li_xCoO_2 expands when Li is removed and contracts when Li is inserted. This causes degradation.
- The liquid electrolyte is flammable.
- Each cell behaves differently, which is a serious issue in battery packs.

Low-Strain Cathode Materials

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Computational Design and Experimental Verification of Zero- and Low-strain Cathode Materials for Solid-State Li-ion batteries

Fabio Rosciano[1], Mikael Christensen[2], Volker Eyert[2], Alexander Mavromaras[2], Erich Wimmer[2]

[1]Toyota Motor Europe, Advanced Technology 1, Hoge Wei 33, Zaventem, Belgium
[2]Materials Design S.A.R.L., Montrouge, France

TOYOTA

ALWAYS A BETTER WAY

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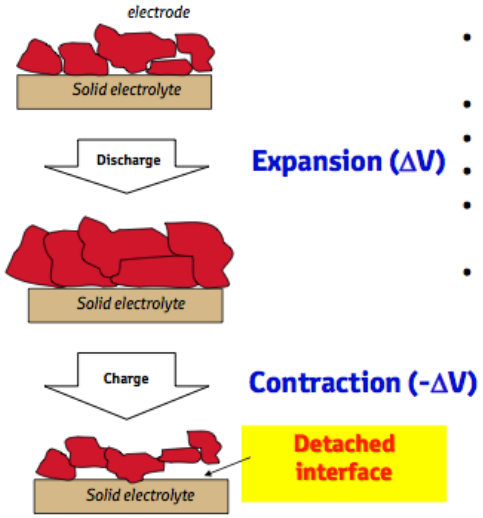
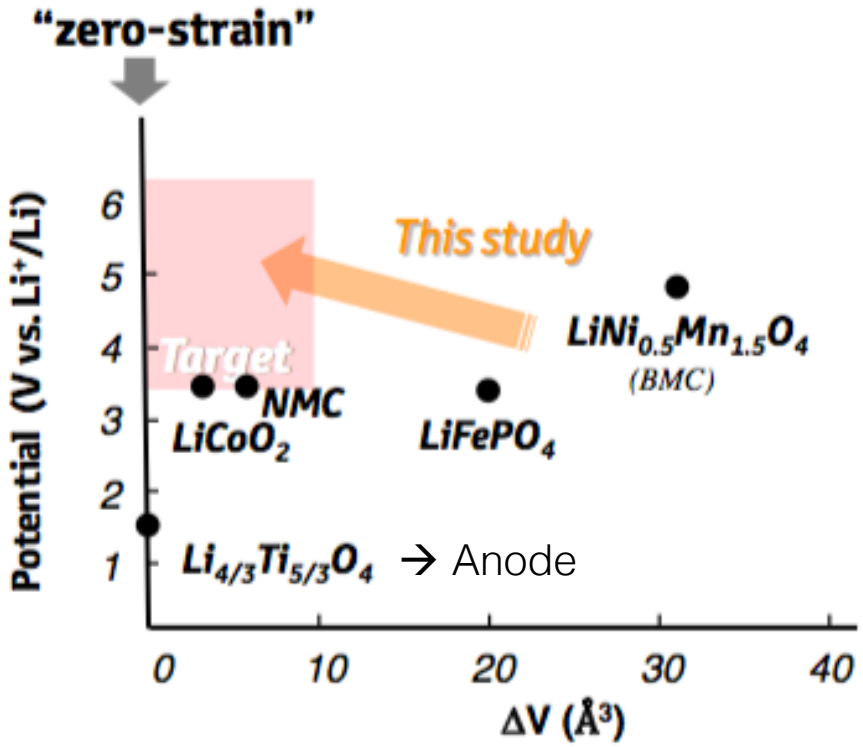
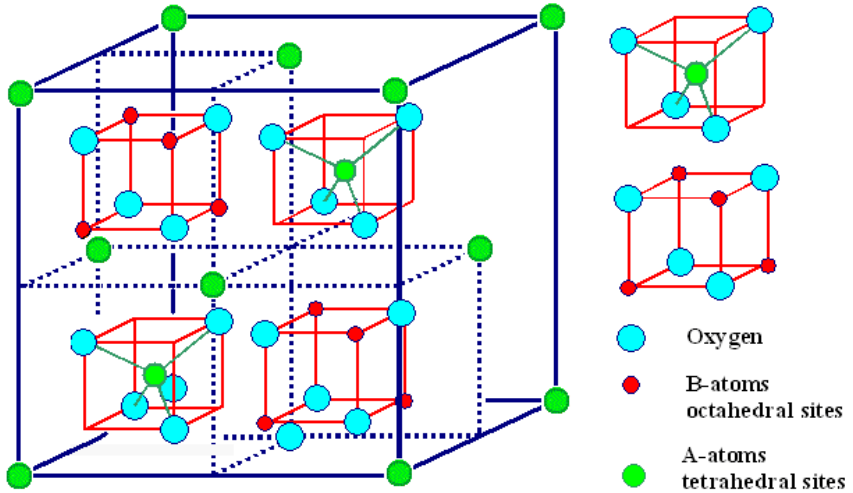


- Volume change of electrodes on charge/discharge is major cause of degradation of Li-ion batteries
  - stress generated at grain interfaces leads to destruction of solid-state batteries
- Use atomistic simulations to find high-voltage, zero-strain cathode materials for use with solid-state electrolytes

F. Rosciano et al., International Battery Association, Brisbane March 2014

Target and Optimization Strategy





AB_2O_4 **spinel** The red cubes are also contained in the back half of the unit cell

- Use atomistic simulations to find high-voltage zero-strain cathode materials
  - Improve on spinel-type $LiNi_{0.5}Mn_{1.5}O_4$ ($\Delta V = 30$ Å^3)
  - Start from $LiMn_2O_4$ and replace Mn

$$x\,LiM^1{}_2O_4 + y\,LiM^2{}_2O_4 + z\,LiM^3{}_2O_4 = Li(M^1{}_xM^2{}_yM^3{}_z)O_4$$

M = Mg, V, Cr, Mn, Fe, Co, Ni, Cu, Al

only configurations with three metals

Optimization Strategy

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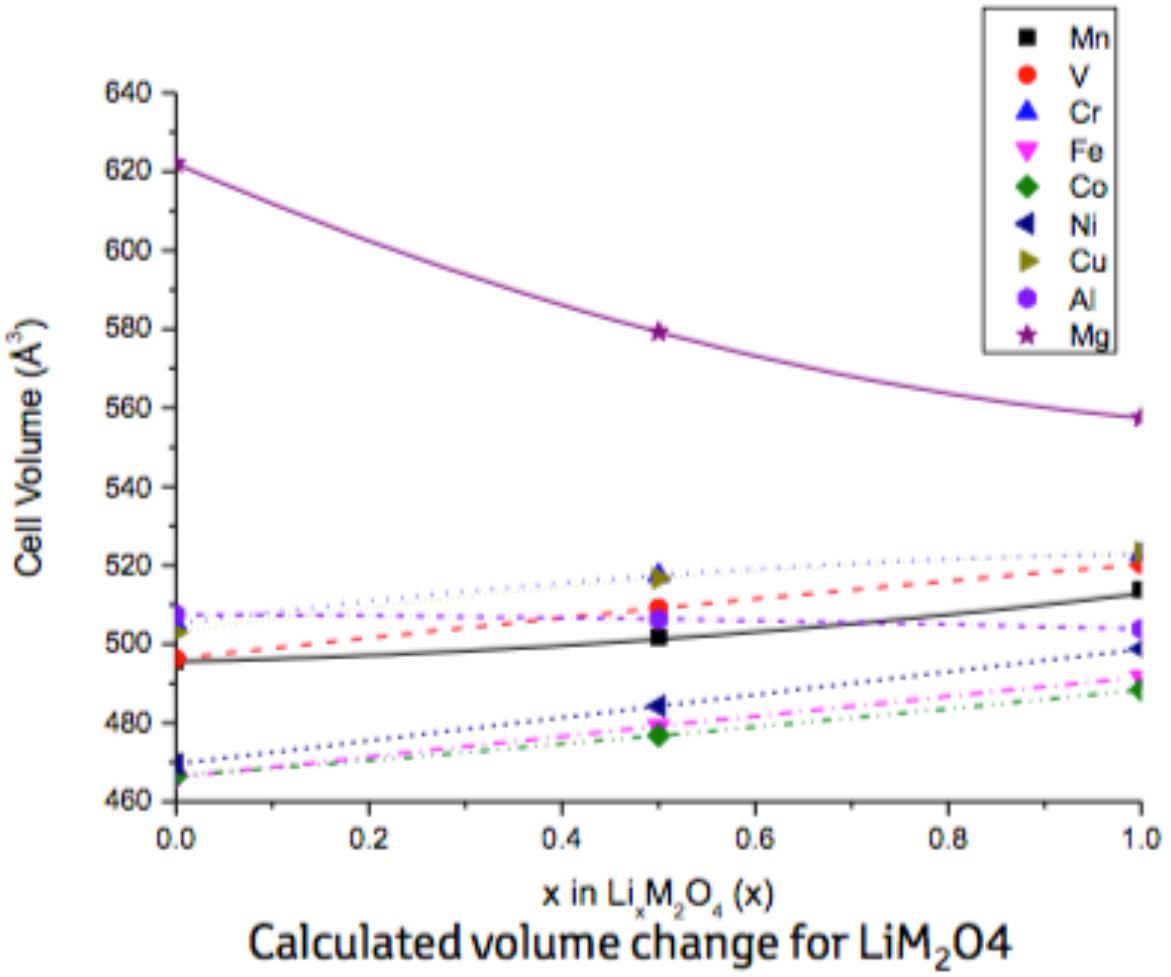
MedeA-VASP

- Start from pure compounds
  - calculate volume for $Li_xM_2O_4$ with x=0,0.5,1 (M=Mg, Al, V, Cr, Mn, Fe, Co, Ni, Cu)
- Only Mg would allow for efficient volume change compensation
- Minimize volume change in three-dimensional spaces spanned by three metals
- Choose three components:
  - **Mn** to provide structural stability
  - **Mg** to reduce volume change
  - **Cr** to compensate for electrochemical inactivity of Mg

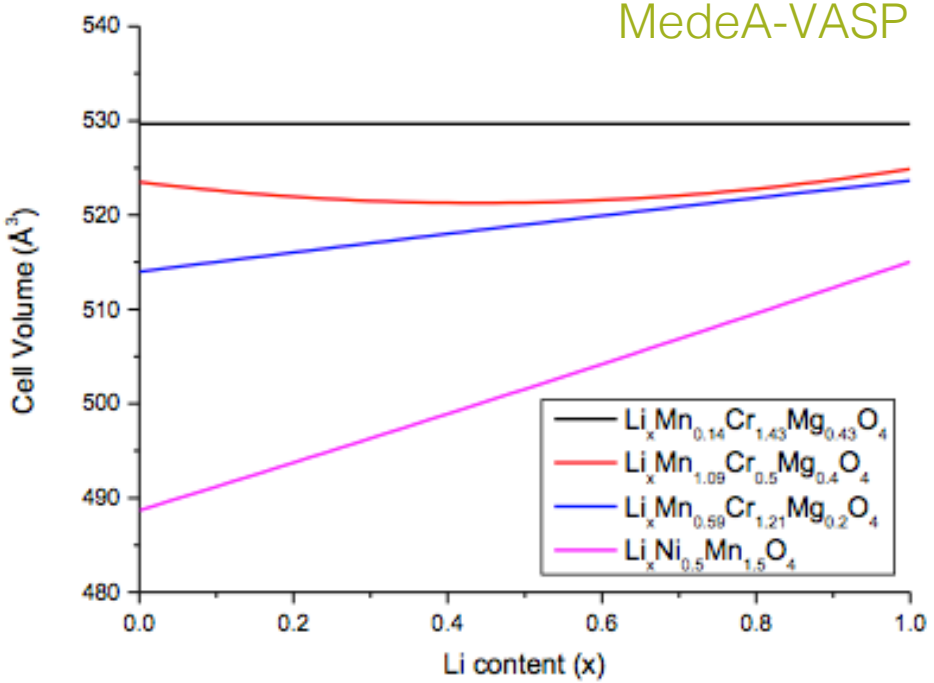


F. Rosciano et al., patent 2014

Minimization of Volume Change

- Choose Mn, Mg, and Cr
- Mix according to three different principles
  - free optimization to obtain true zero-strain material
  - optimization constraining Mn content ≥ 0.1
  - optimization constraining Mg content ≤ 0.4

MedeA-VASP



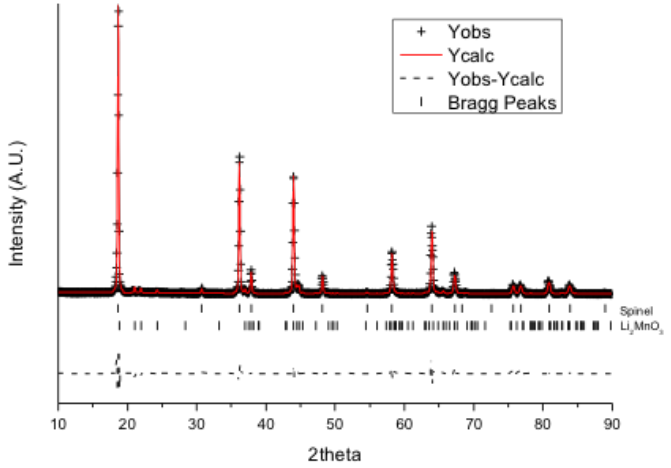
Calculated volume change for the optimized compositions

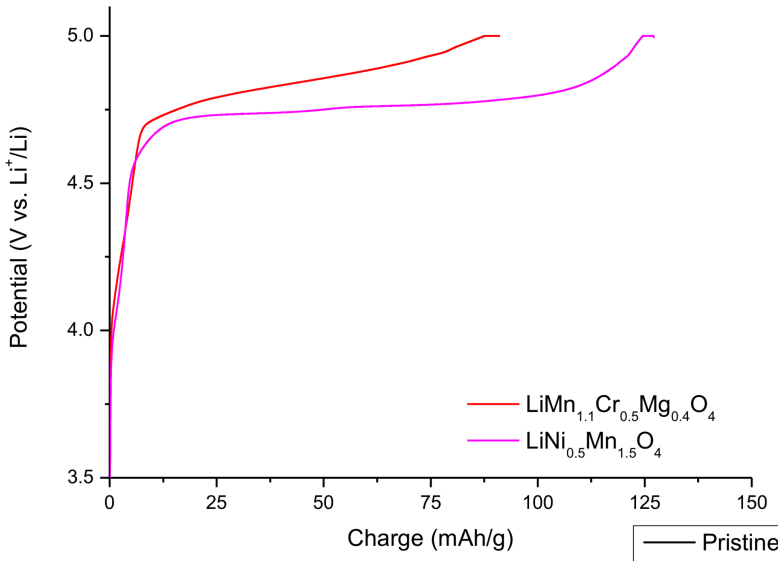
- Result
  - $LiMn_{0.14}Cr_{1.43}Mg_{0.43}O_4$ → ΔV = 0 Å³
  - $LiMn_{1.1}Cr_{0.5}Mg_{0.4}O_4$ → ΔV = 3 Å³
  - $LiMn_{0.59}Cr_{1.21}Mg_{0.2}O_4$ → ΔV = 8 Å³
  - $LiMn_{1.5}Ni_{0.5}O_4$ (benchmark) → ΔV = 30 Å³

Passed on to Toyota Motors

F. Rosciano et al., Patent 2014

Synthesis and Characterization





$LiMn_{1.1}Cr_{0.5}Mg_{0.4}O_4$

- synthesized in mostly pure form (3% Li_2MnO_3 impurity phase)
- used to build electrochemical cells to study volume change on lithiation/delithiation
- measured volume change ≈ 4Å^3
- first-charge curve shows reduced capacity as compared to benchmark $LiNi_{0.5}Mn_{1.5}O_4$

Patent

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MedeA-VASP

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(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

Published:

— *with international search report (Art. 21(3))*

Microscopic Origin

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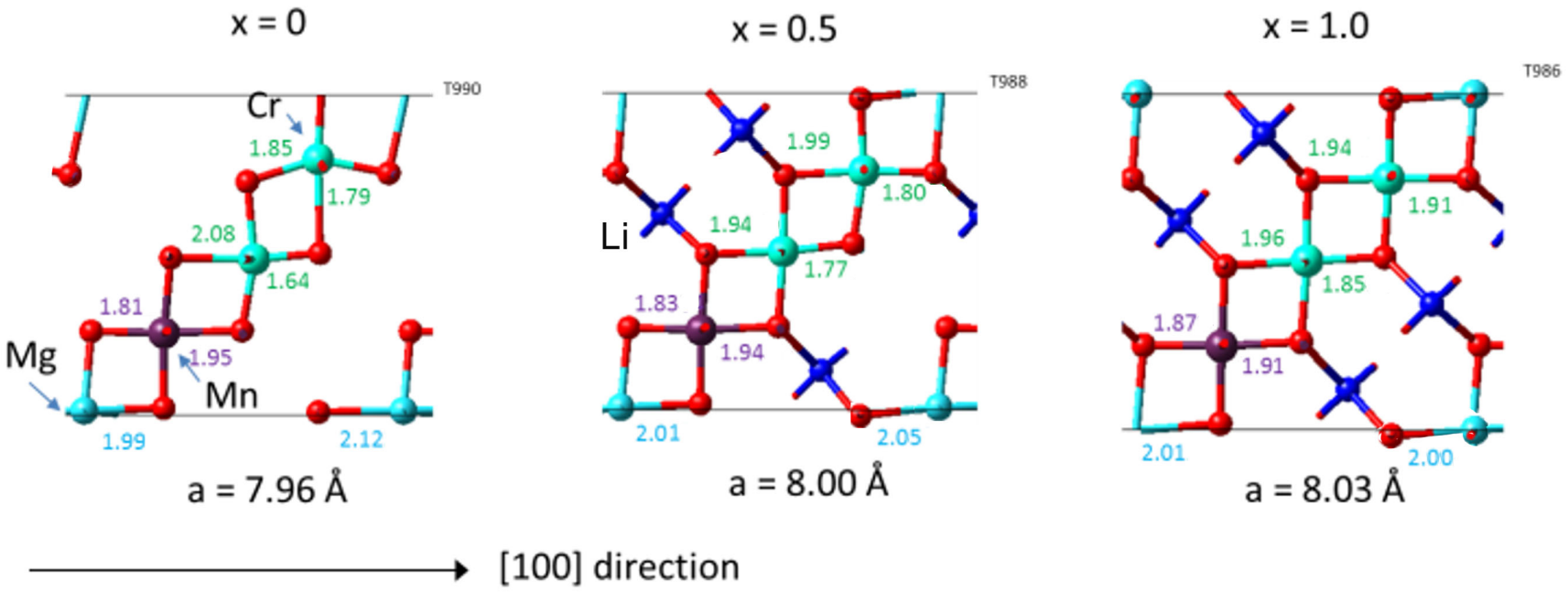
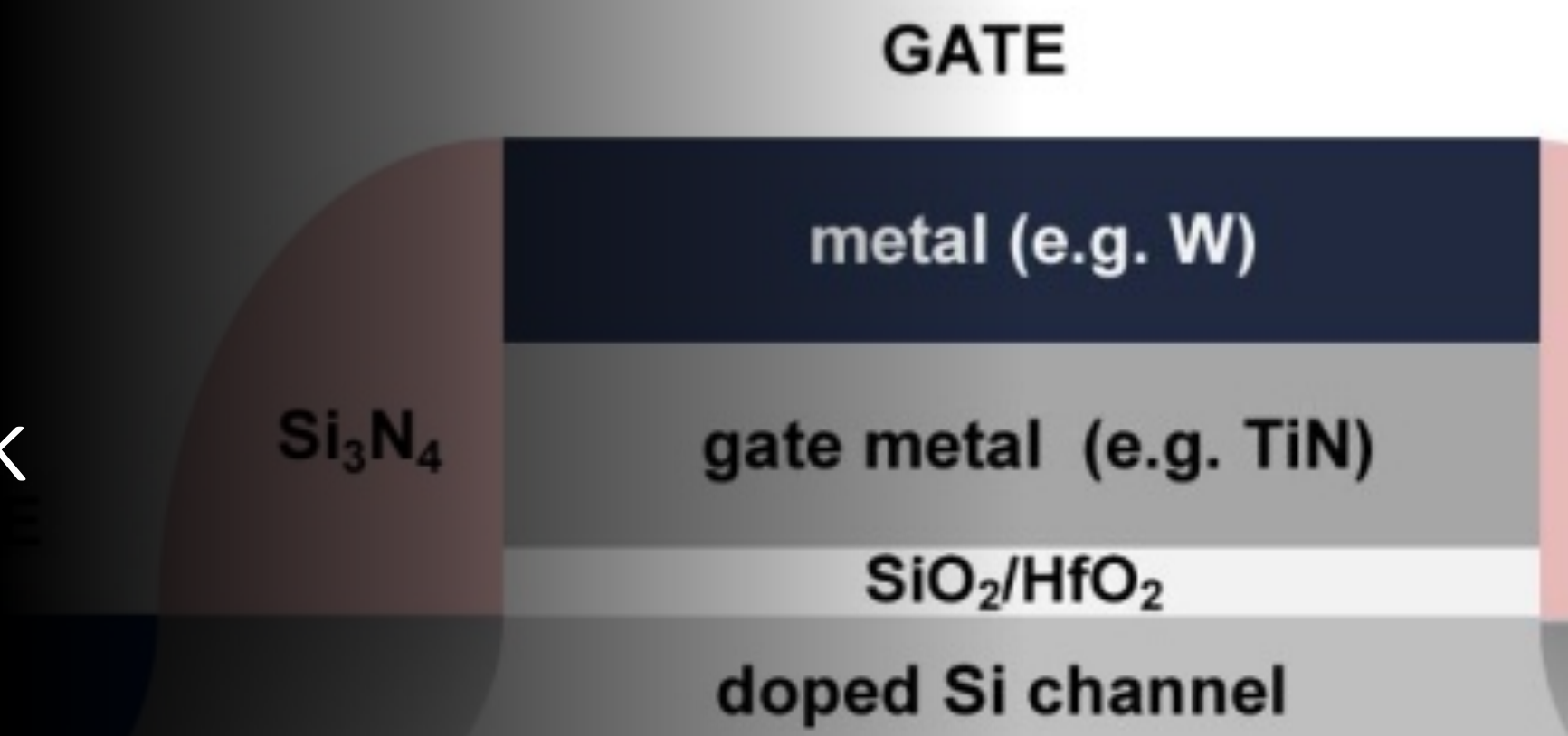
MedeA-VASP



- With increasing Li concentration
  - Mg-O bond lengths decrease, Mn-O bond lengths remain similar, Cr-O bond lengths increase
- Zero-strain behavior of $Li_4Ti_5O_{12}$ anode likewise based on balance of different local distortions

Effective Work Function in Gate Stacks



Technology Issue

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Metal Gate Electrode Impurity Engineering for Control of Effective Work Function

Jim Chambers, Hiro Niimi, Andrei Li-Fatou and Judy Shaw
Texas Instruments, Incorporated, Advanced CMOS

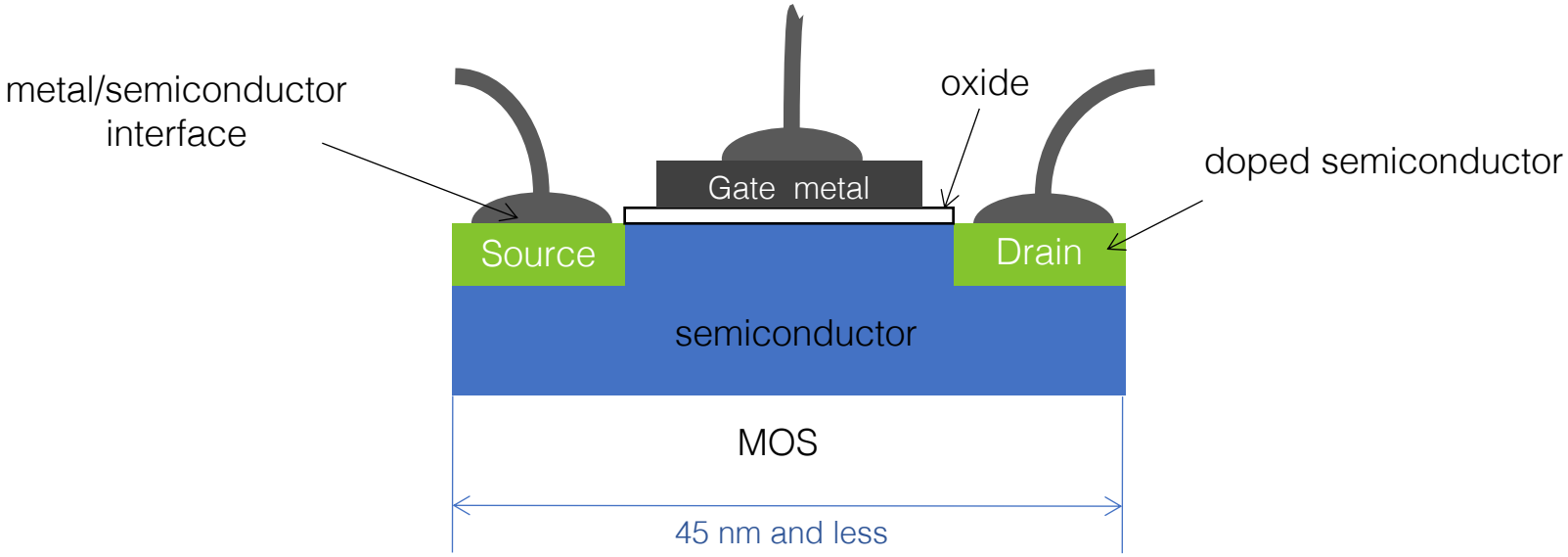
Chris Hinkle, Jim Burris, Husam Alshareef, Richard Chapman, Rohit Galatage and Eric Vogel
University of Texas at Dallas, Department of Materials Science and Engineering

Mikael Christensen, Clive Freeman and Erich Wimmer
Materials Design, Incorporated

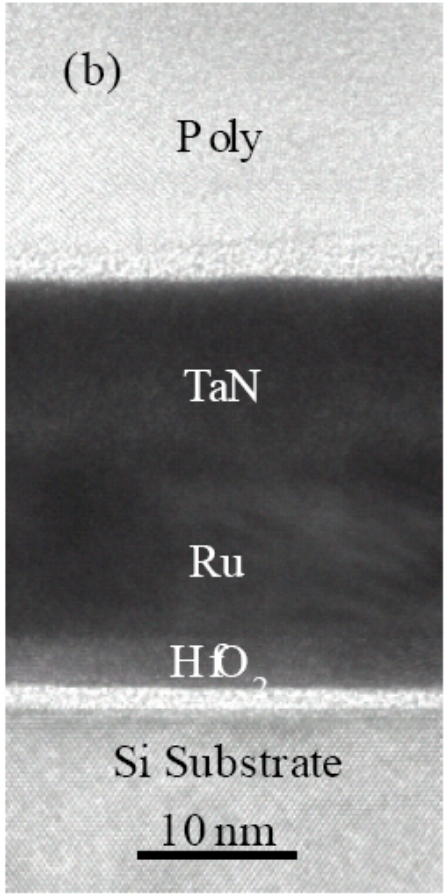
Problem

- Green electronics
  - How can one reduce the power consumption?

Complementary Metal Oxide Semiconductor



Next-Generation CMOS Devices

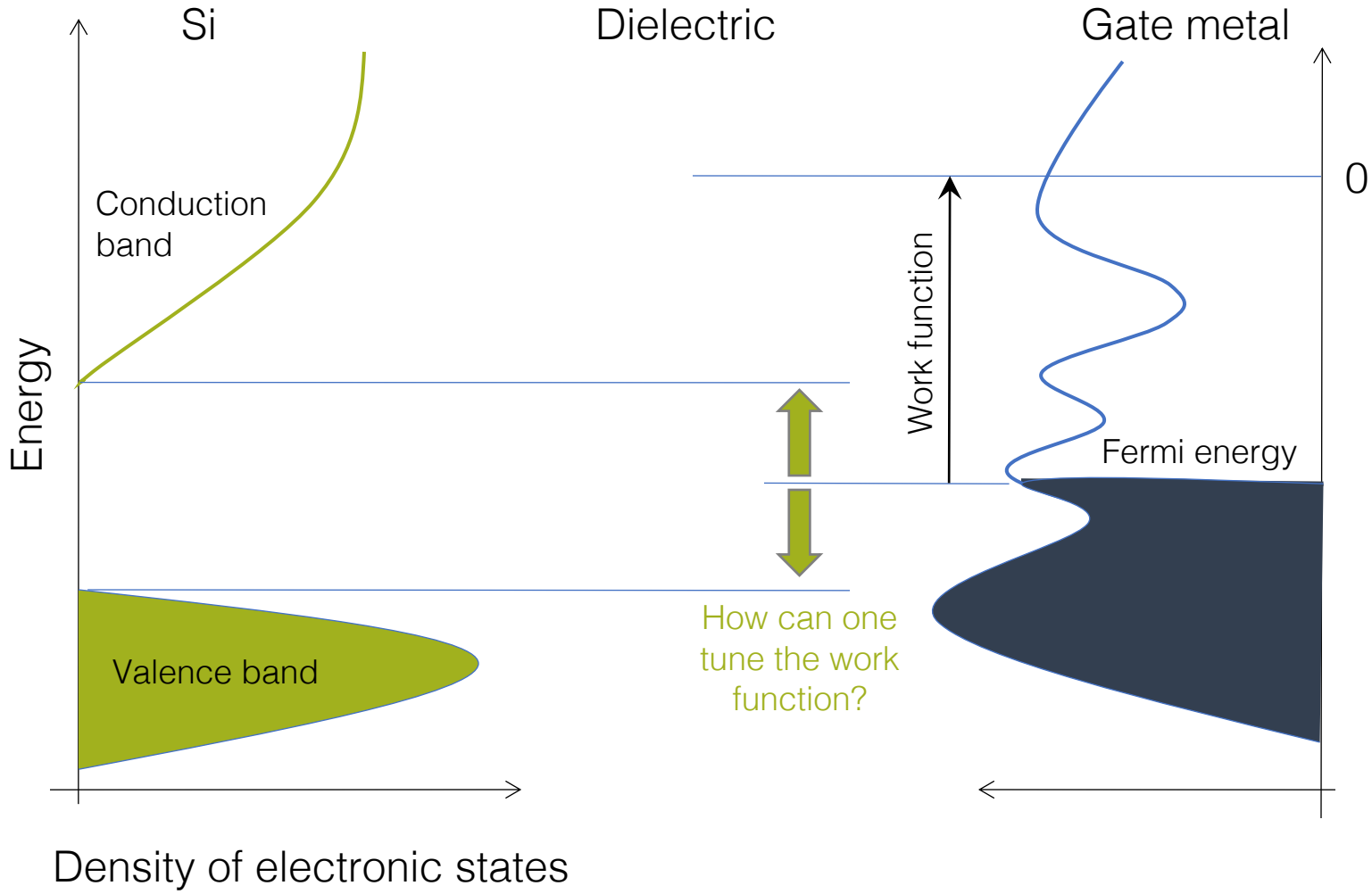


HfO_2/Ru/TaN gate stack

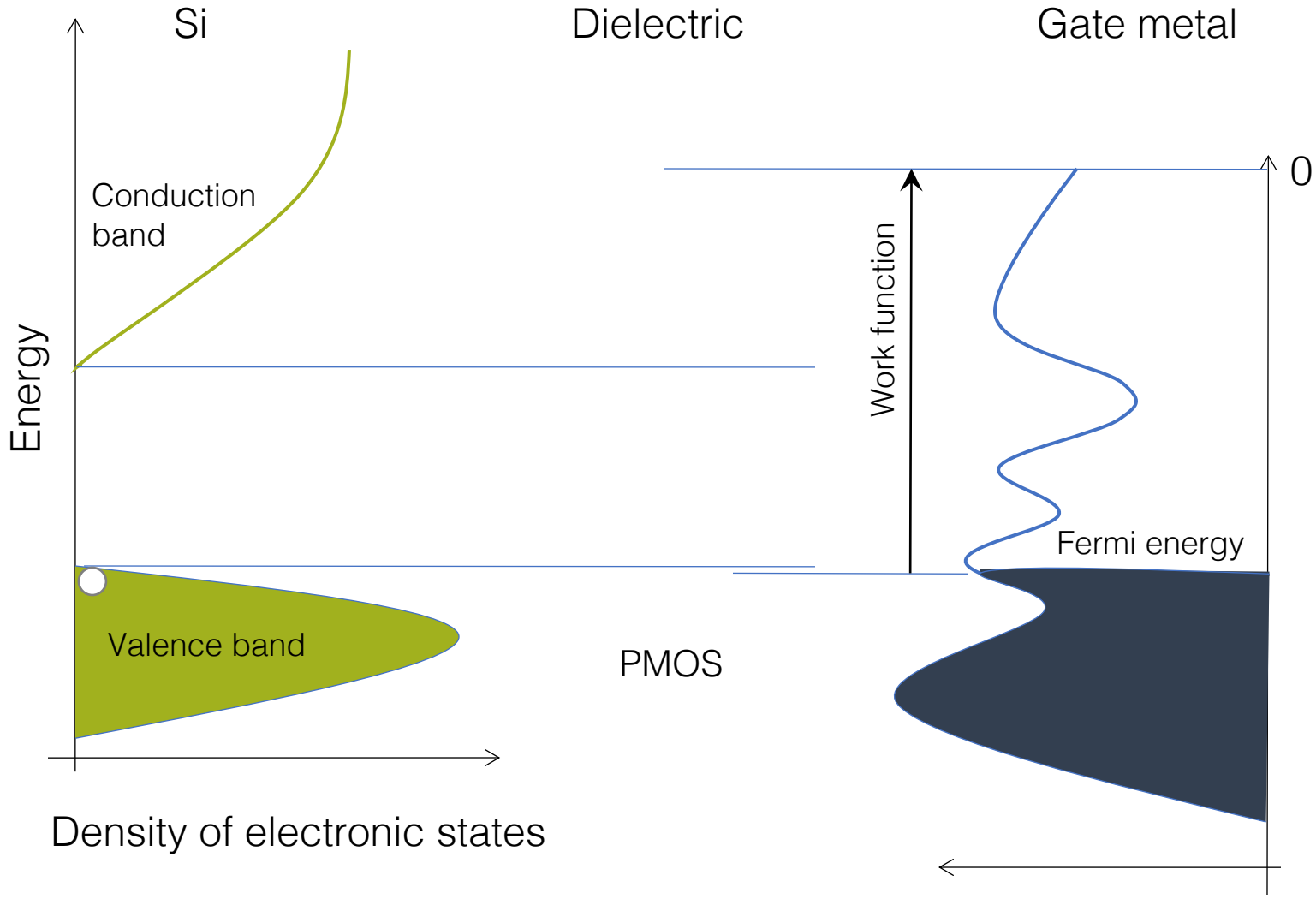
- SiO_2 cannot be used at thicknesses less than 15 Å (leakage current is too high)
- HfO_2 replaces for SiO_2 as a dielectric
- A critical design parameter is the work function of the metal. Which metallic material should be used so that it can be tuned for PMOS and NMOS devices?

Muhammad Mustafa Hussain
ADVANCED FABRICATION PROCESSES FOR SUB-50 nm CMOS
PhD thesis, University of Texas at Austin
https://repositories.lib.utexas.edu/bitstream/handle/2152/2449/hussainm51214.pdf

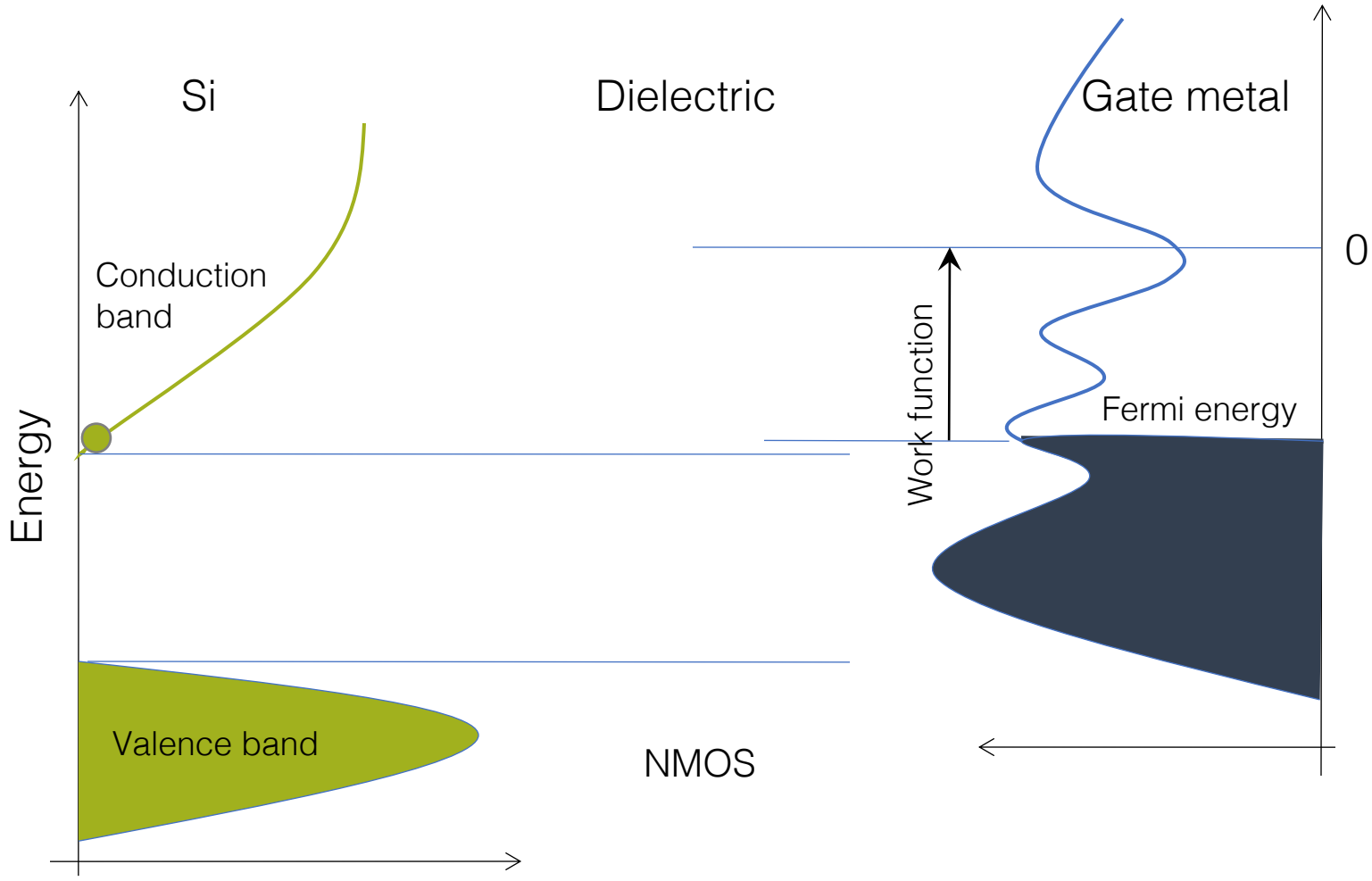
Work Function in Device Stack



Work Function in Device Stack



Work Function in Device Stack



Structure of the Interface

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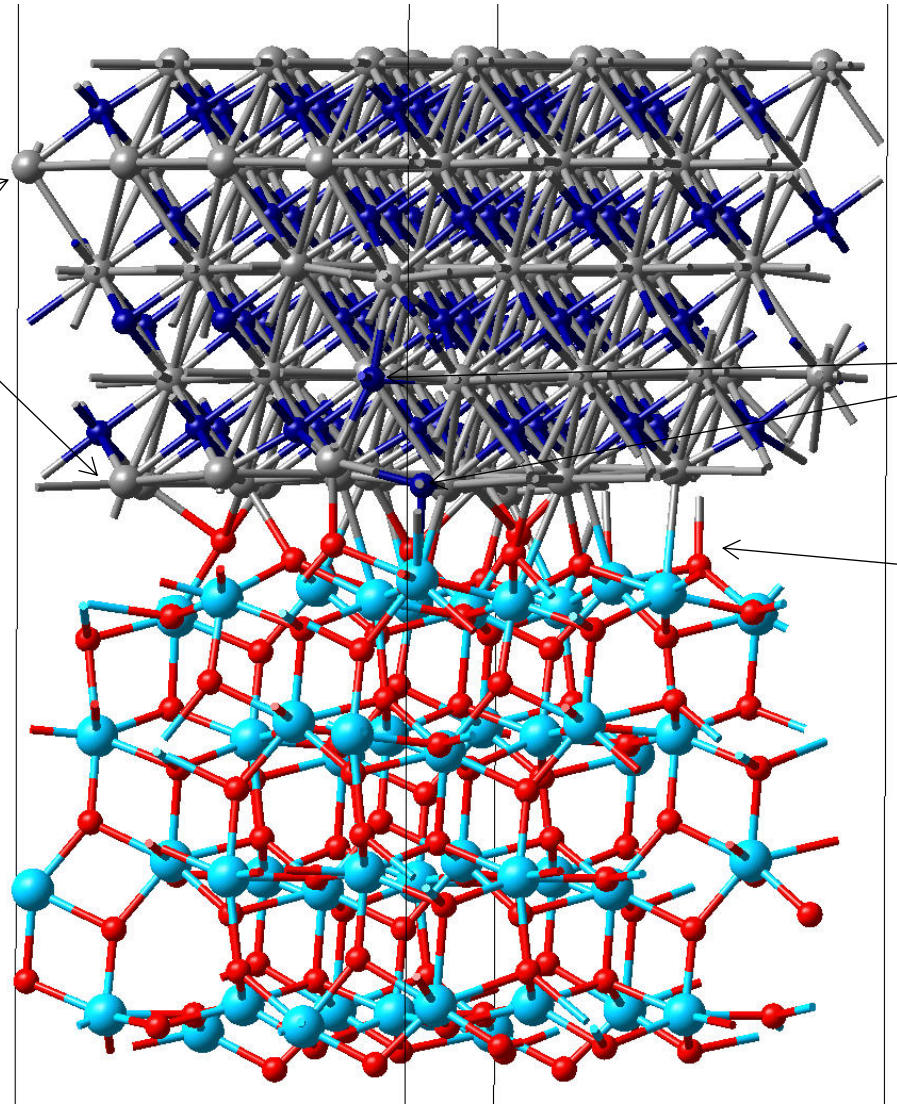
MedeA-Interface Builder
MedeA-VASP



TiN Thin Film on HfO_2 Substrate

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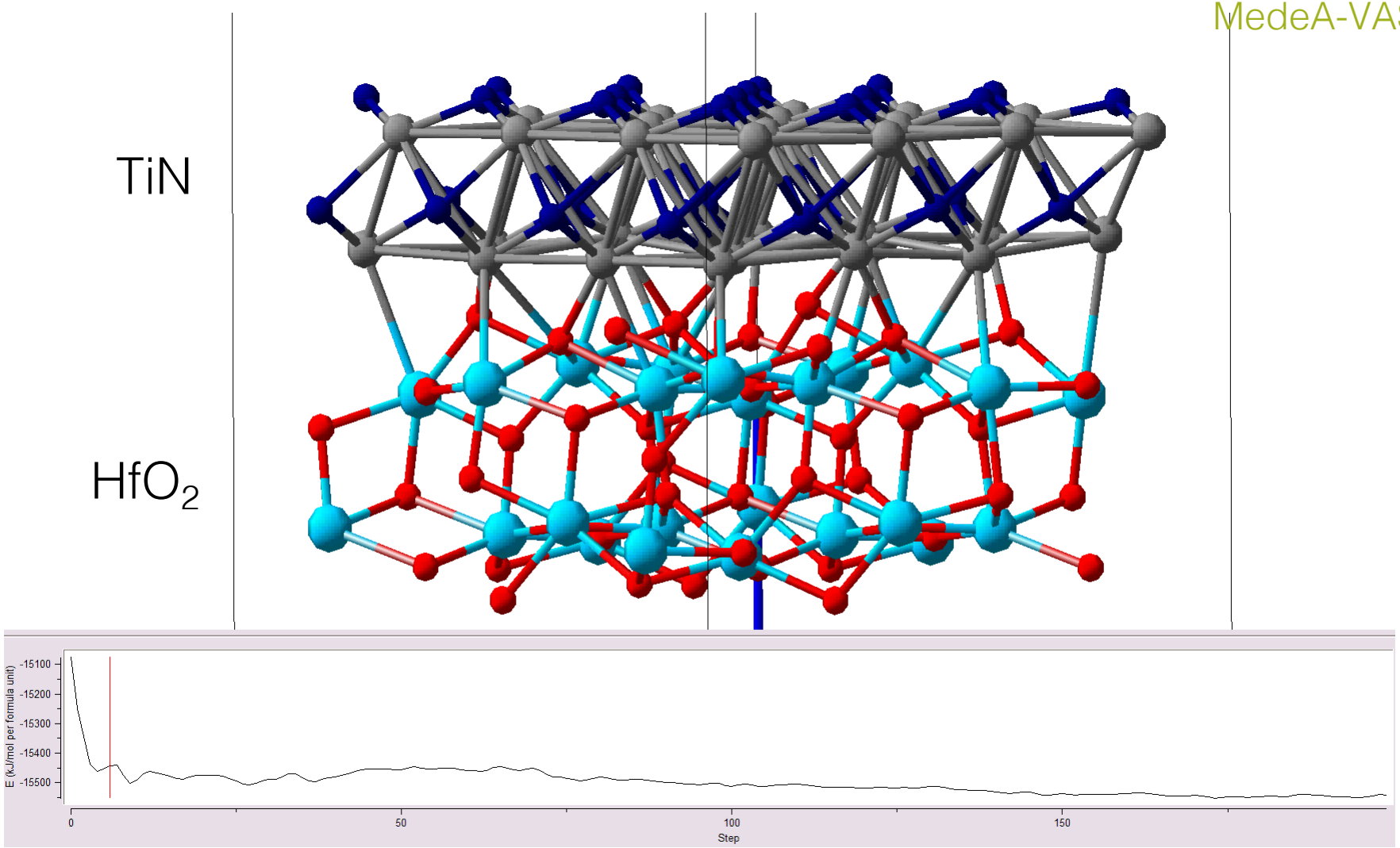
MedeA-VASP



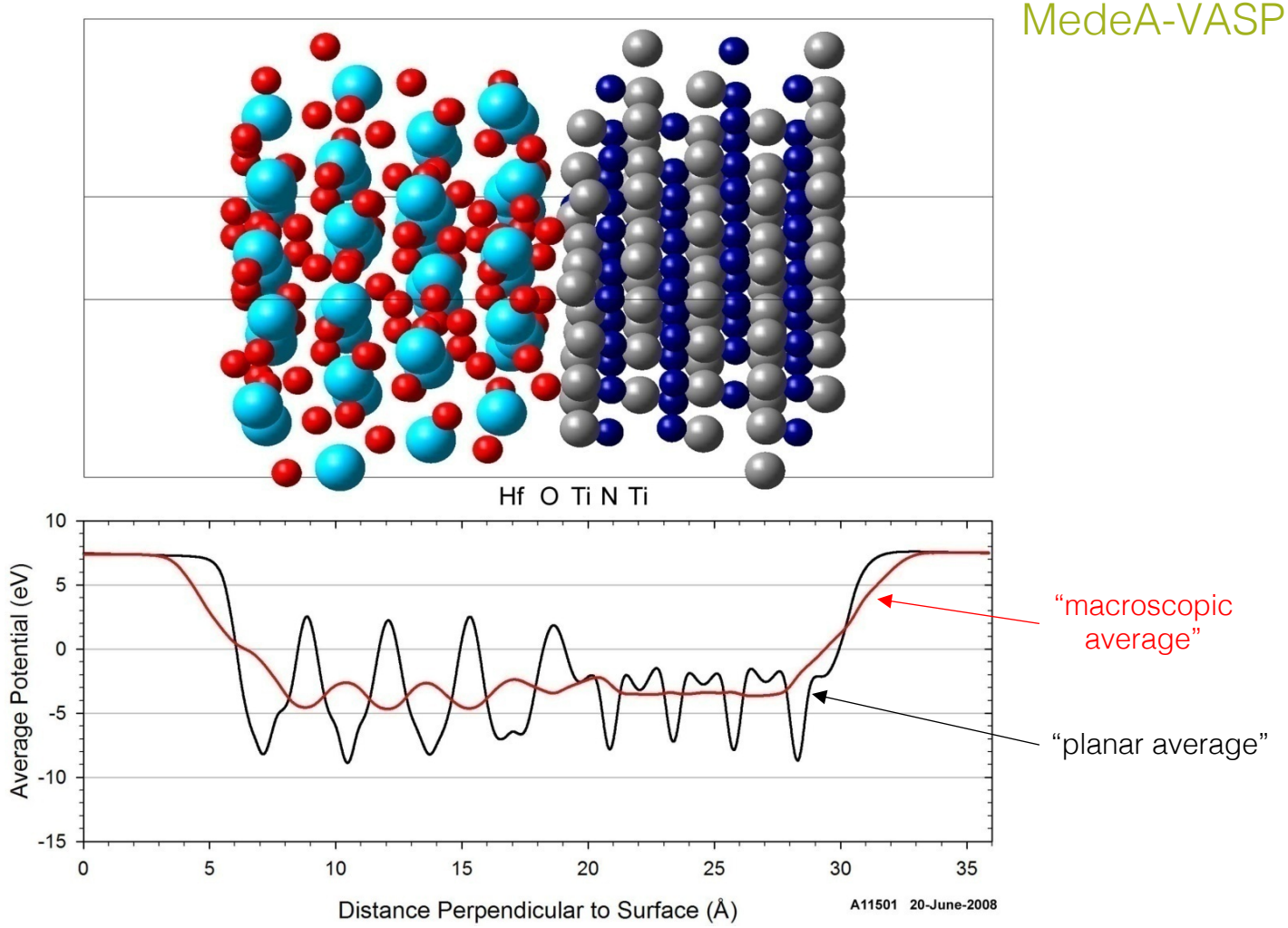
Animation: see pptx slide

Electrostatic Potential at Interface

- Planar average exhibits ripples associated with each atomic layer
- Macroscopic average taken as the moving average across several layers
- Macroscopic average used as basis for comparison between test cases

$(Hf_{12}O_{24})_4$-$(Ti_{16}N_{16})_4$-Ti_{16}

MedeA-Interface Builder
MedeA-VASP



HfO_2/TiN Effective Work Function

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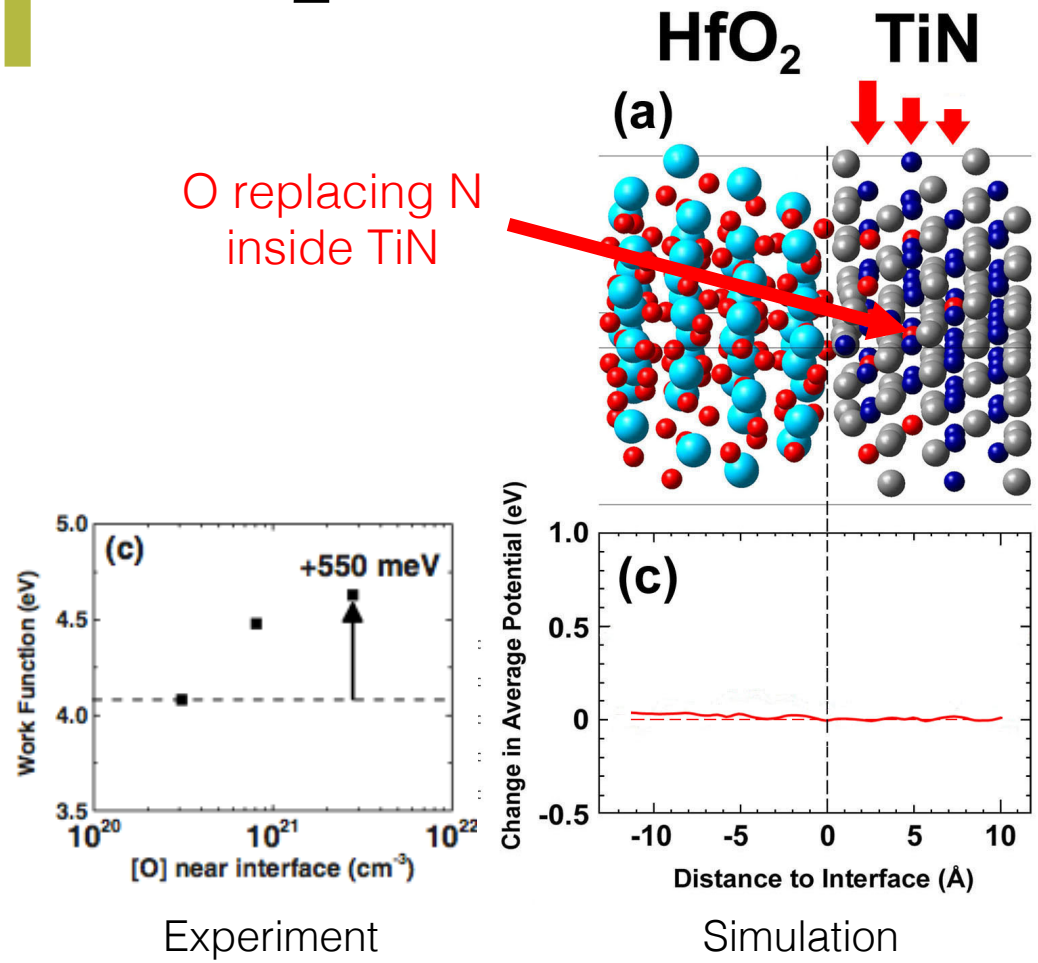
MedeA-Interface Builder
MedeA-VASP

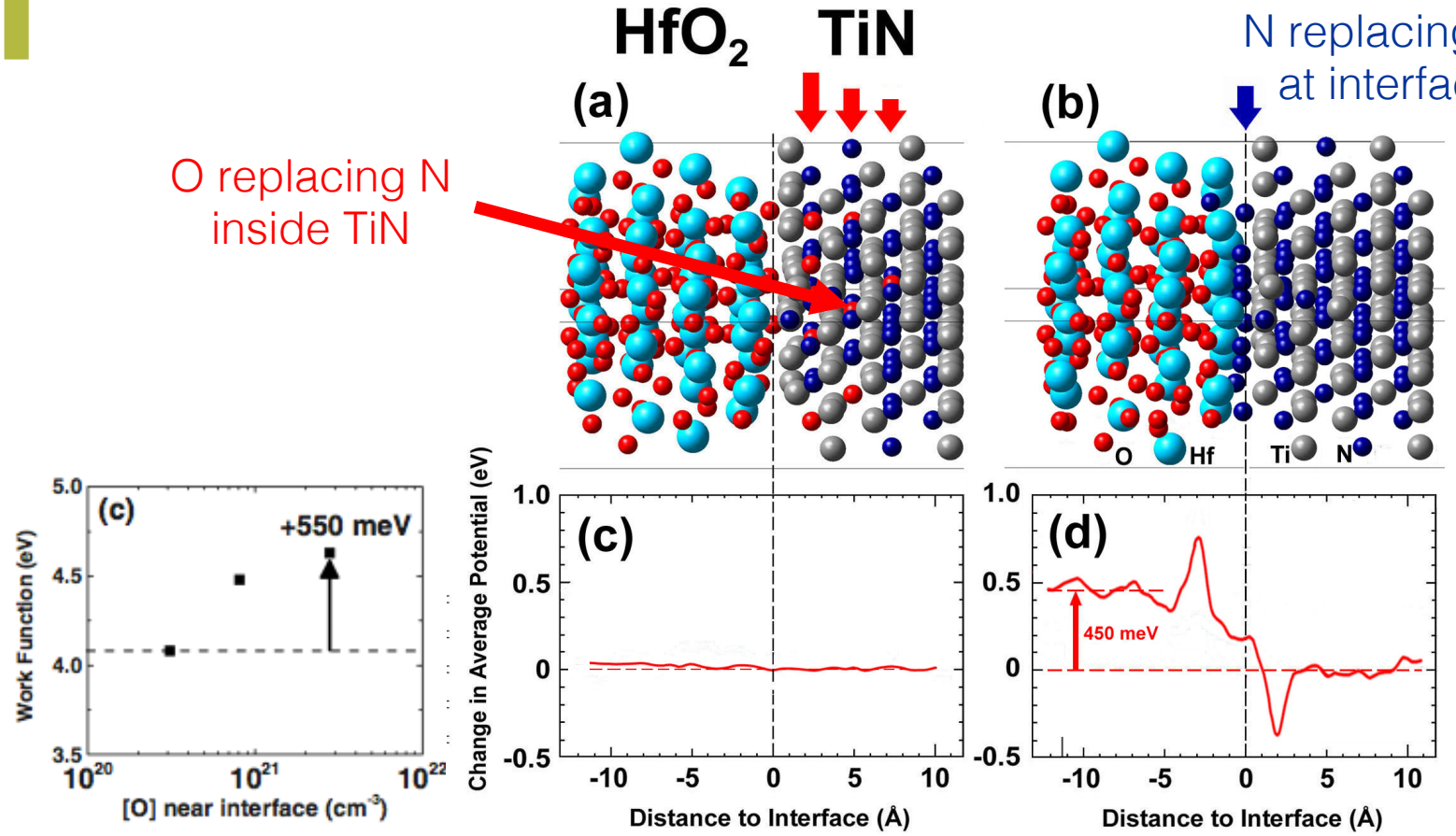


Experiment Simulation

- Experiments showed increase of EWF after annealing of stack under oxygen atmosphere
- Interpretation: oxygen inside TiN increases the work function

- O replacing N in TiN cannot explain measured increase of EWF

HfO_2/TiN Effective Work Function



Experiment

Simulation

- Interfacial O moves to HfO_2 to fill vacancies
- N builds up at interface
- O refills vacancies in TiN

- Dipole due to O replacing N screened in metallic TiN
- Dipole due to N replacing O at interface unscreened in dielectric HfO_2

HfO_2/TiN Effective Work Function

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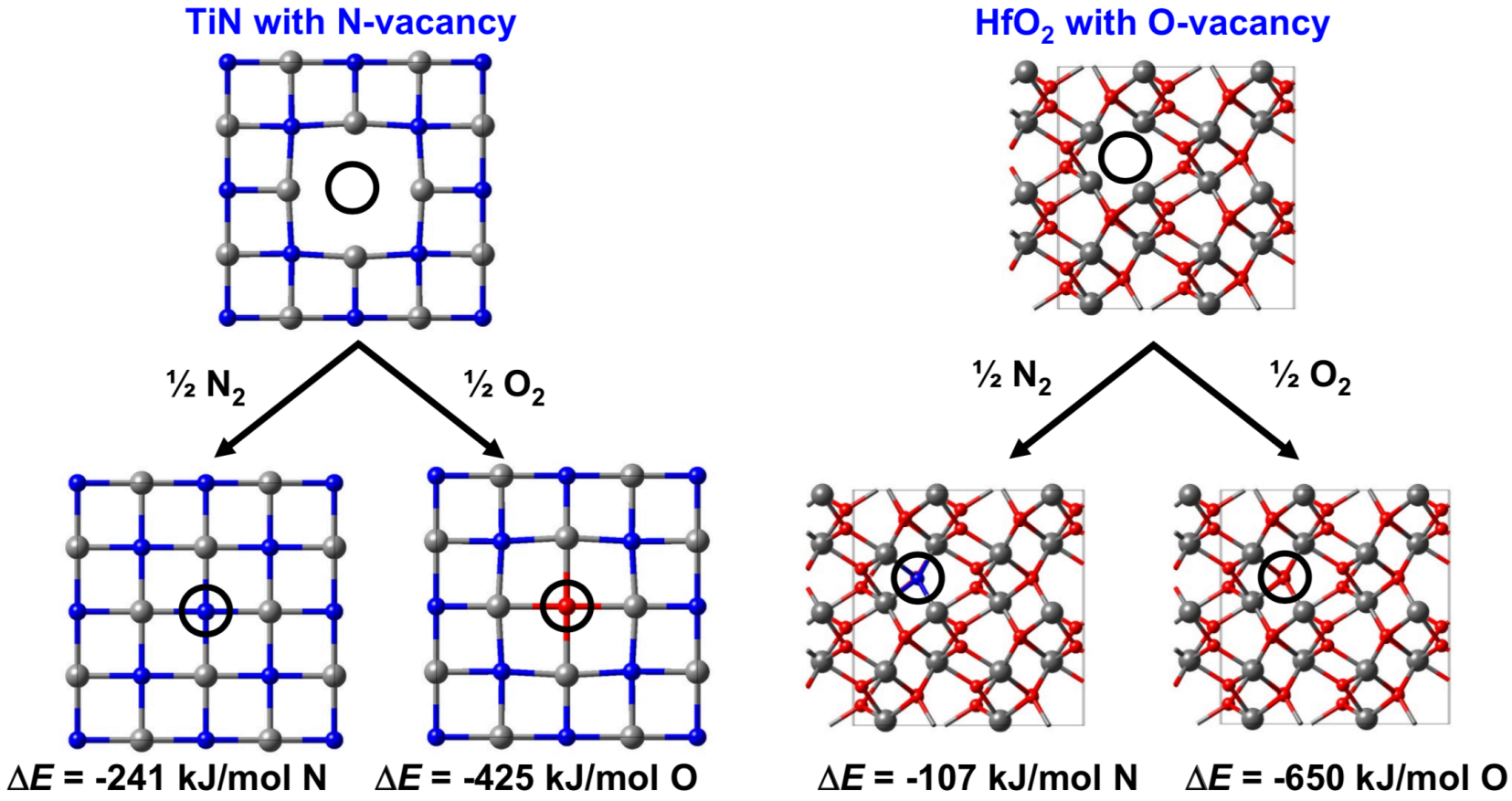
MedeA-VASP

Thermodynamics of Vacancy Filling in TiN and HfO_2



- Vacancy filling by O highly favorable in both TiN and HfO_2

HfO_2/TiN Effective Work Function

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APPLIED PHYSICS LETTERS **96**, 103502 (2010)

Interfacial oxygen and nitrogen induced dipole formation and vacancy passivation for increased effective work functions in TiN/HfO_2 gate stacks

C. L. Hinkle,[1,2,a)] R. V. Galatage,[2] R. A. Chapman,[2] E. M. Vogel,[1,2] H. N. Alshareef,[3] C. Freeman,[4] E. Wimmer,[4] H. Niimi,[5] A. Li-Fatou,[5] J. B. Shaw,[5] and J. J. Chambers[5]
[1]*Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA*
[2]*Department of Electrical Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA*
[3]*King Abdullah University of Science & Technology, Thuwal 23955-6900, Saudi Arabia*
[4]*Materials Design, Incorporated, Angel Fire, New Mexico 87710, USA*
[5]*Advanced CMOS, Texas Instruments Incorporated, Dallas, Texas 75243, USA*

(Received 20 November 2009; accepted 14 February 2010; published online 9 March 2010)

Effective work function (EWF) changes of TiN/HfO_2 annealed at low temperatures in different ambient environments are correlated with the atomic concentration of oxygen in the TiN near the metal/dielectric interface. EWF increases of 550 meV are achieved with anneals that incorporate oxygen throughout the TiN with $[O]=2.8\times10^{21}$ cm^{-3} near the TiN/HfO_2 interface. However, further increasing the oxygen concentration via more aggressive anneals results in a relative decrease of the EWF and increase in electrical thickness. First-principles calculations indicate the exchange of O and N atoms near the TiN/HfO_2 interface cause the formation of dipoles that increase the EWF. © *2010 American Institute of Physics*. [doi:10.1063/1.3353993]

MedeA-Interface Builder
MedeA-VASP

Complete Gate Stack Model

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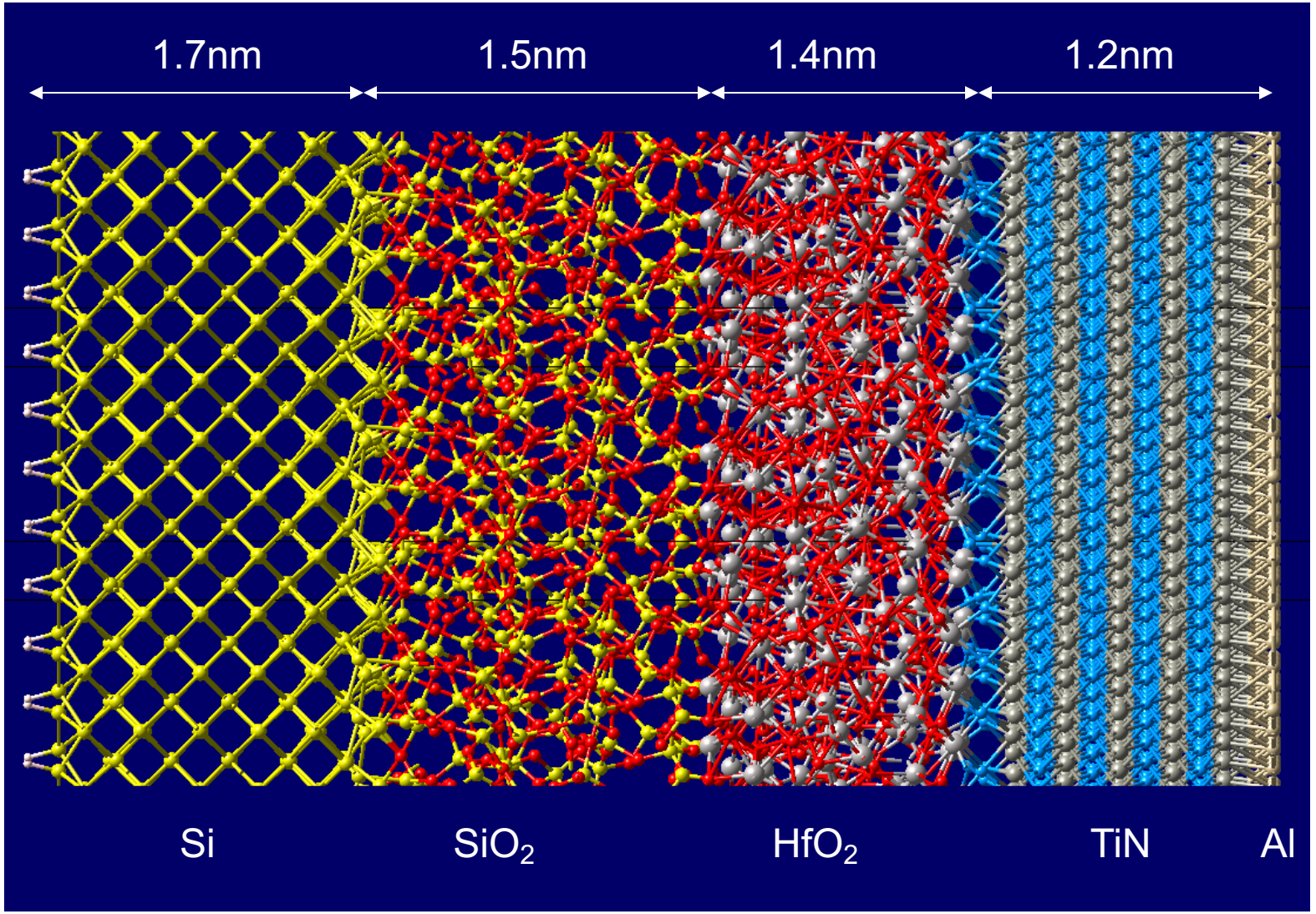
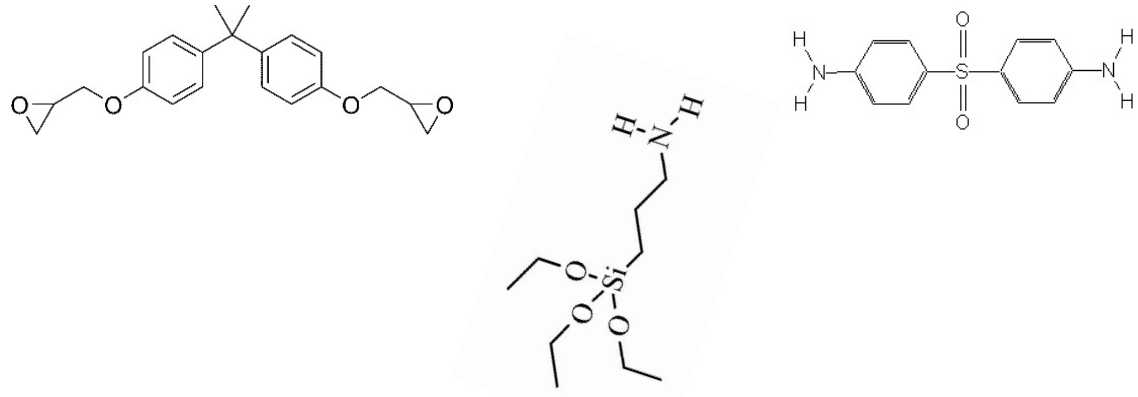
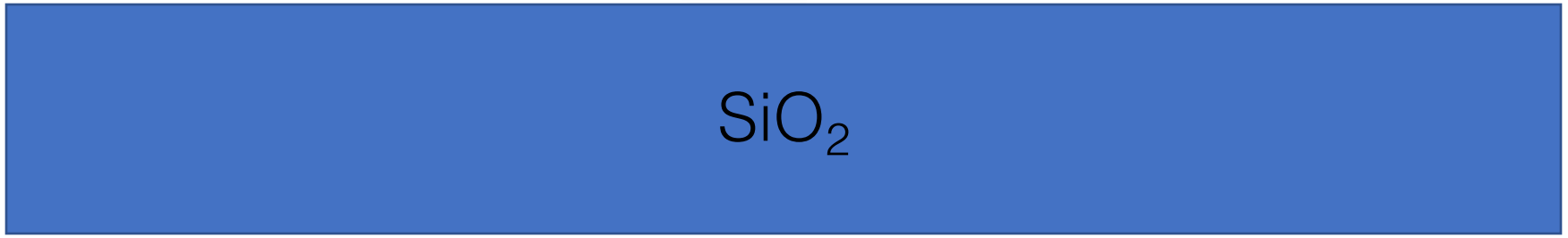


Composite Materials

Epoxy Thermosets

- Composites contain multiple components – e.g. cured resins, coupling agents (primers), reinforcing particles or fibers. Properties of complex multiphase materials need to be studied.
- Example: Effect of primer concentration on mechanical properties
  - How much primer (coupling between SiO_2 surface and polymer) is optimal?





Epoxy-SiO_2: Model Building

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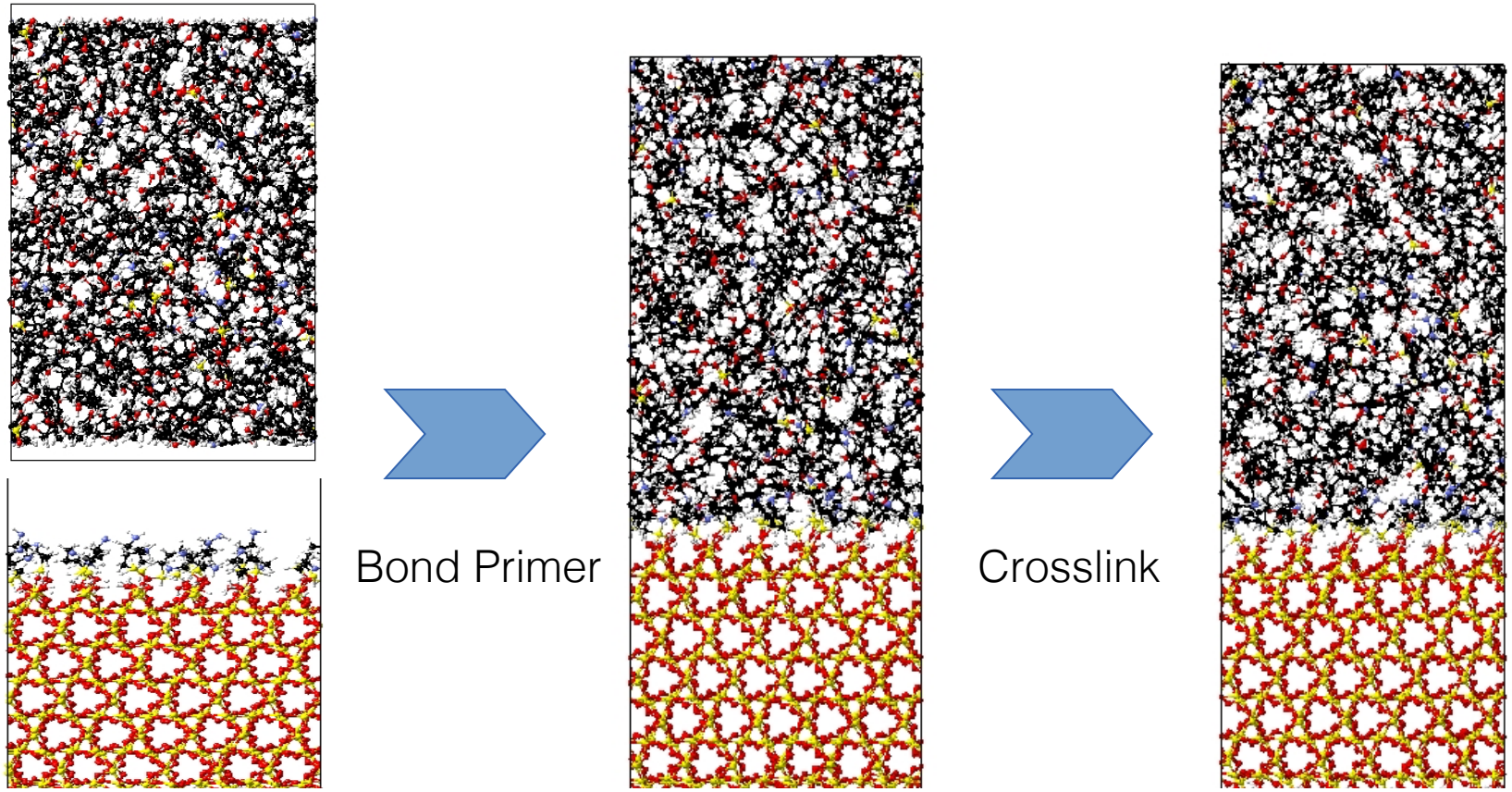
MedeA-Amorphous Builder
MedeA-Thermoset
MedeA-LAMMPS

Primed SiO_2+ unreacted epoxy, crosslinking and equilibration



Epoxy-SiO_2: Mechanical Properties

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Stiffness coefficient C_{33} for SiO_2 - epoxy composite layer systems with various levels of primer coverage:

MedeA-MT

Primed surface sites (%)	C_{33} (GPa)
0	7.2
12.5	7.8
25	8.8
50	5.0
Reference: Bulk Cured Resin	5.97 +/-0.29

Primer coverage at intermediate concentration produces optimal enhancement in small strain mechanical behavior

Fluids

Normal Boiling Point Temperature

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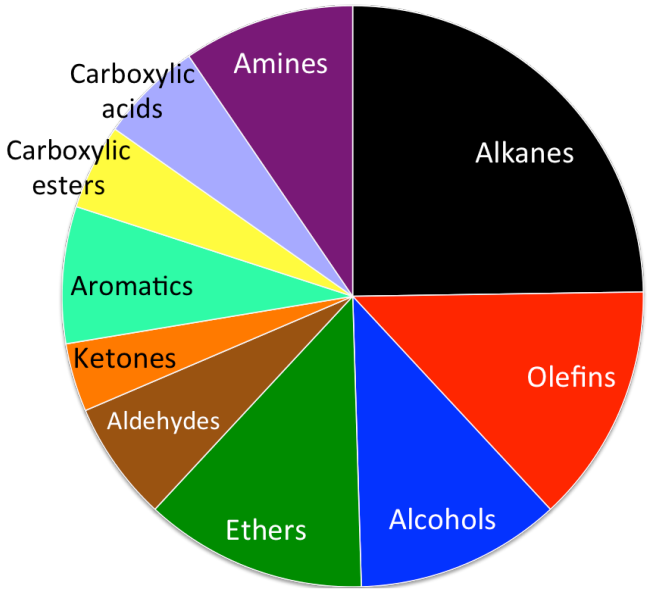
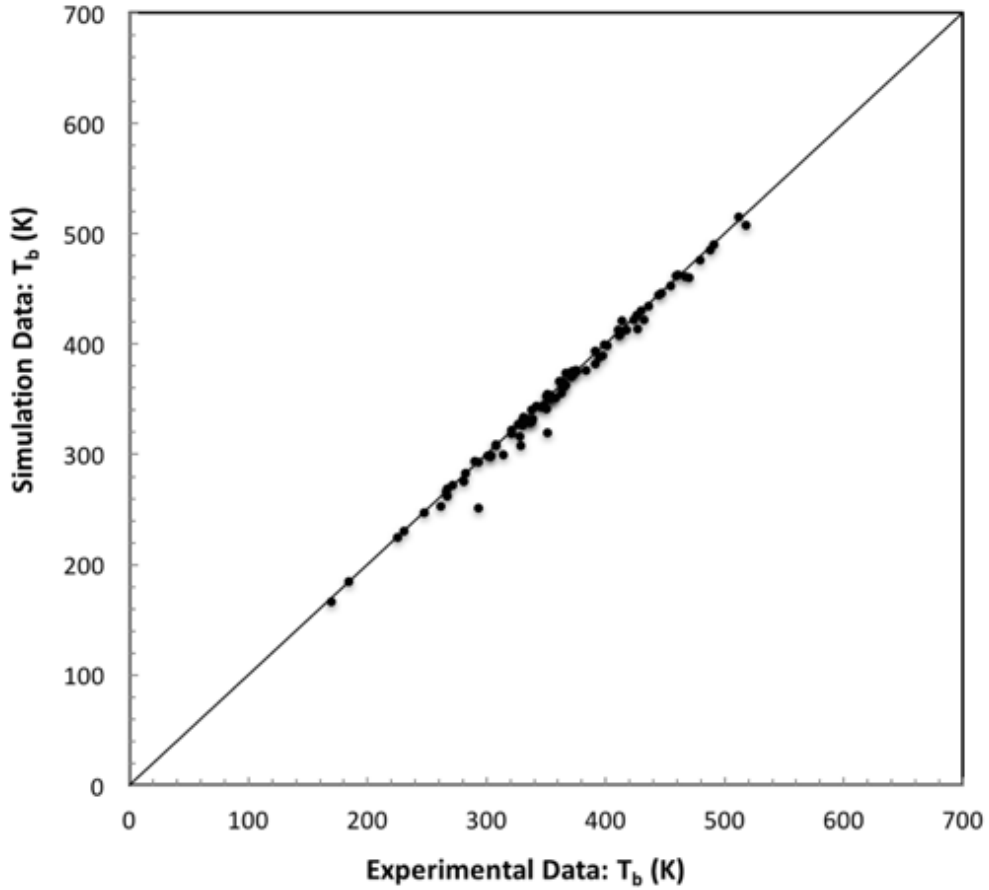
MedeA-Gibbs

- Sample shown in the plot: 100 compounds
- Absolute average deviation of T_b calculated by GEMC simulation from the DIPPR* data is 1.4%.
- More than half of the compounds have an absolute deviation of T_b below 1.0%.



MedeA-GIBBS simulations (AUA & TraPPE-UA FF)



* Source experimental data: DIADEM: The DIPPR Information and Data Evaluation Manager for the Design Institute for Physical Properties, Version 6.0.0, Database 2011

Conclusion

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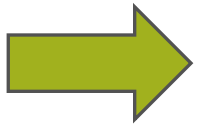
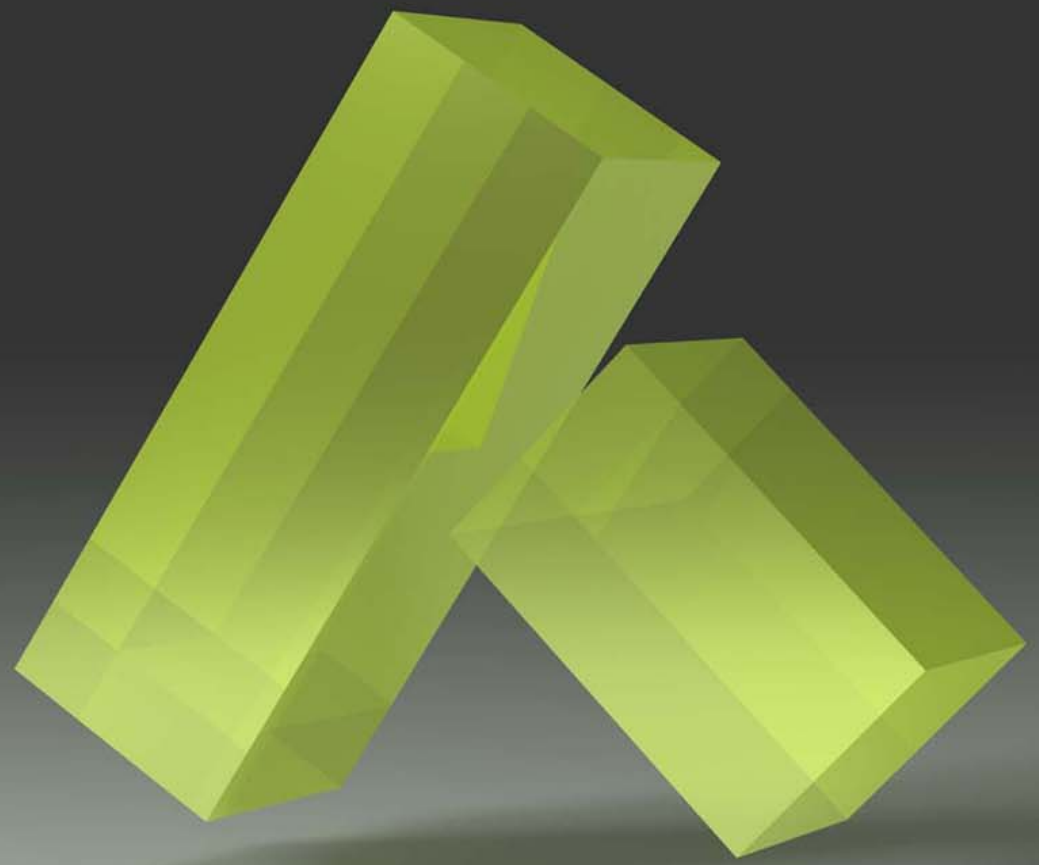
- Atomic-scale modeling and simulations are becoming an integral part of industrial R&D
- Value
  - Predicting properties
  - Understanding mechanisms



  - Driving innovation
  - Creating valuable products
  - Protecting the environment
- Examples
  - Stability of microstructures
  - Optimization of cathode materials
  - Control of effective work functions
  - Composites and Fluids
- Future trends: better coupling in multi-scale models: theoretical approaches, algorithms, software



MedeA

Innovation by Simulation