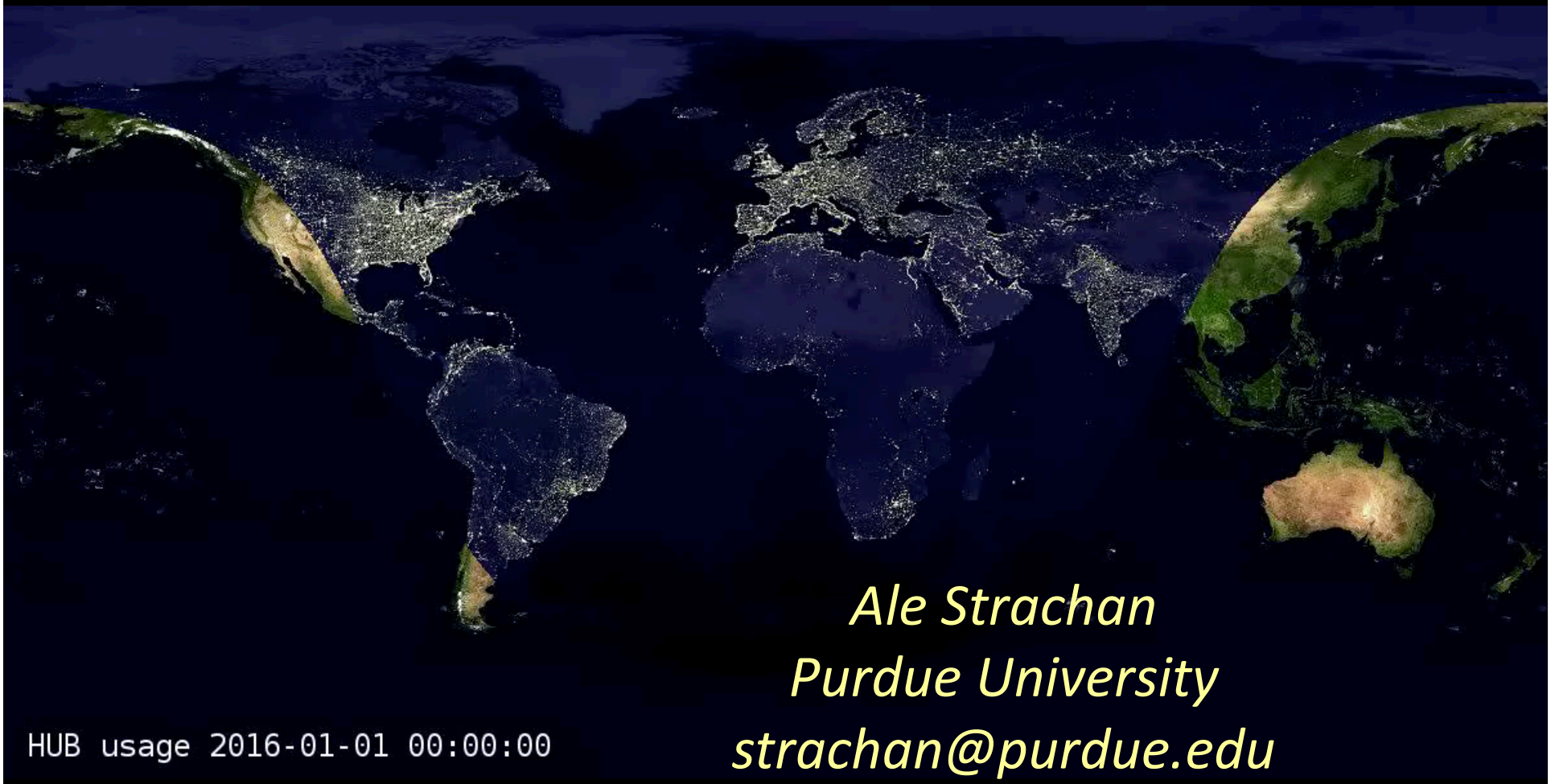
Predictive computational materials science

From nanoelectronics to explosives



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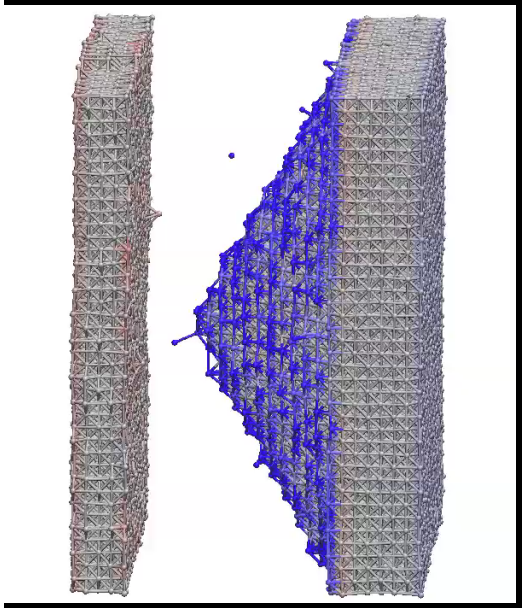
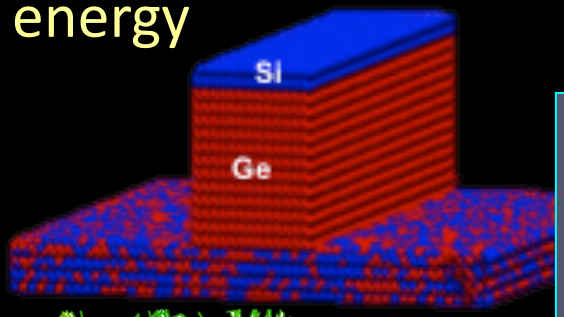
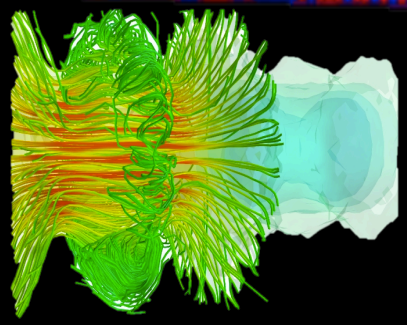
Strachan group application areas

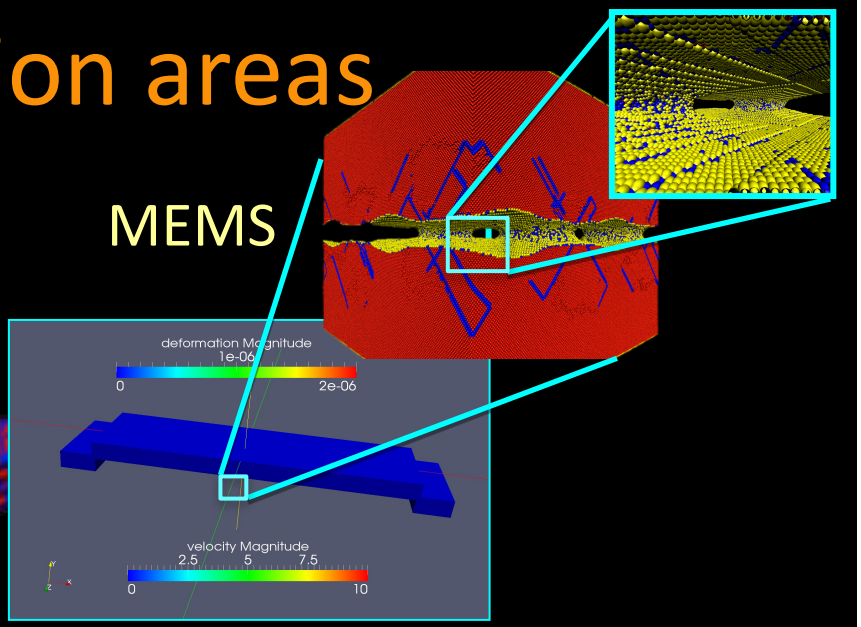
Nanoelectronics & energy



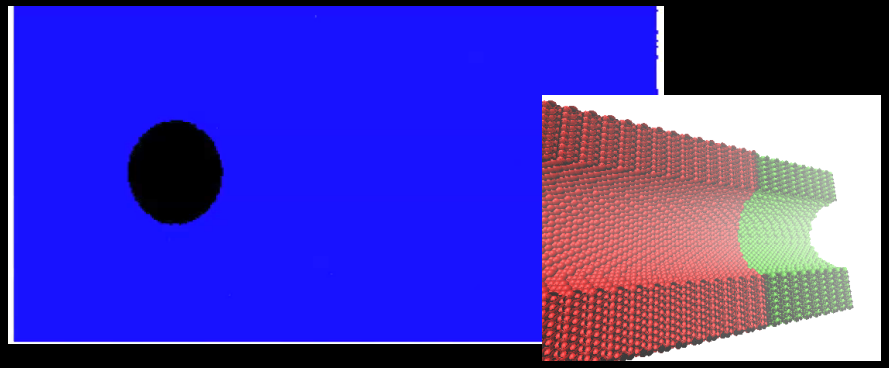




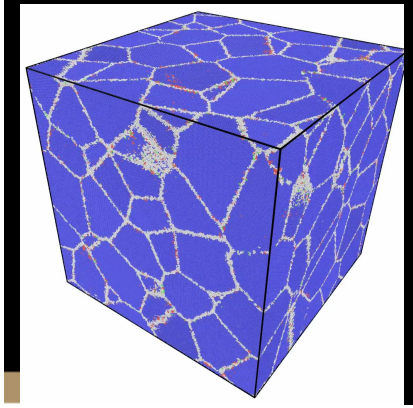
MEMS

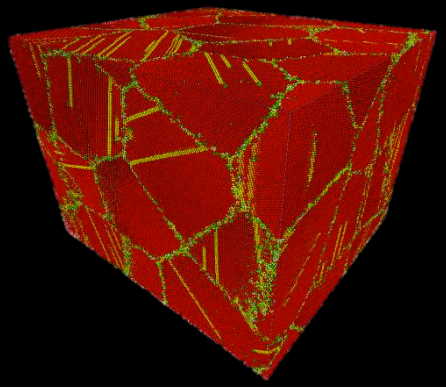


High-energy density materials

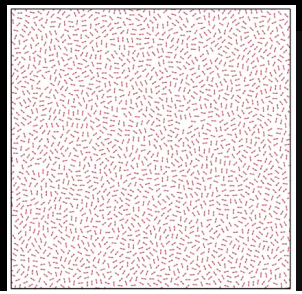


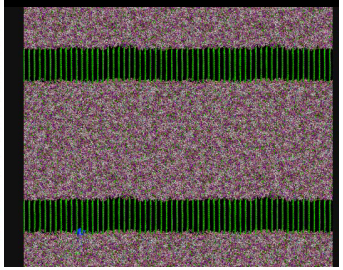
Thermo-mechanical response



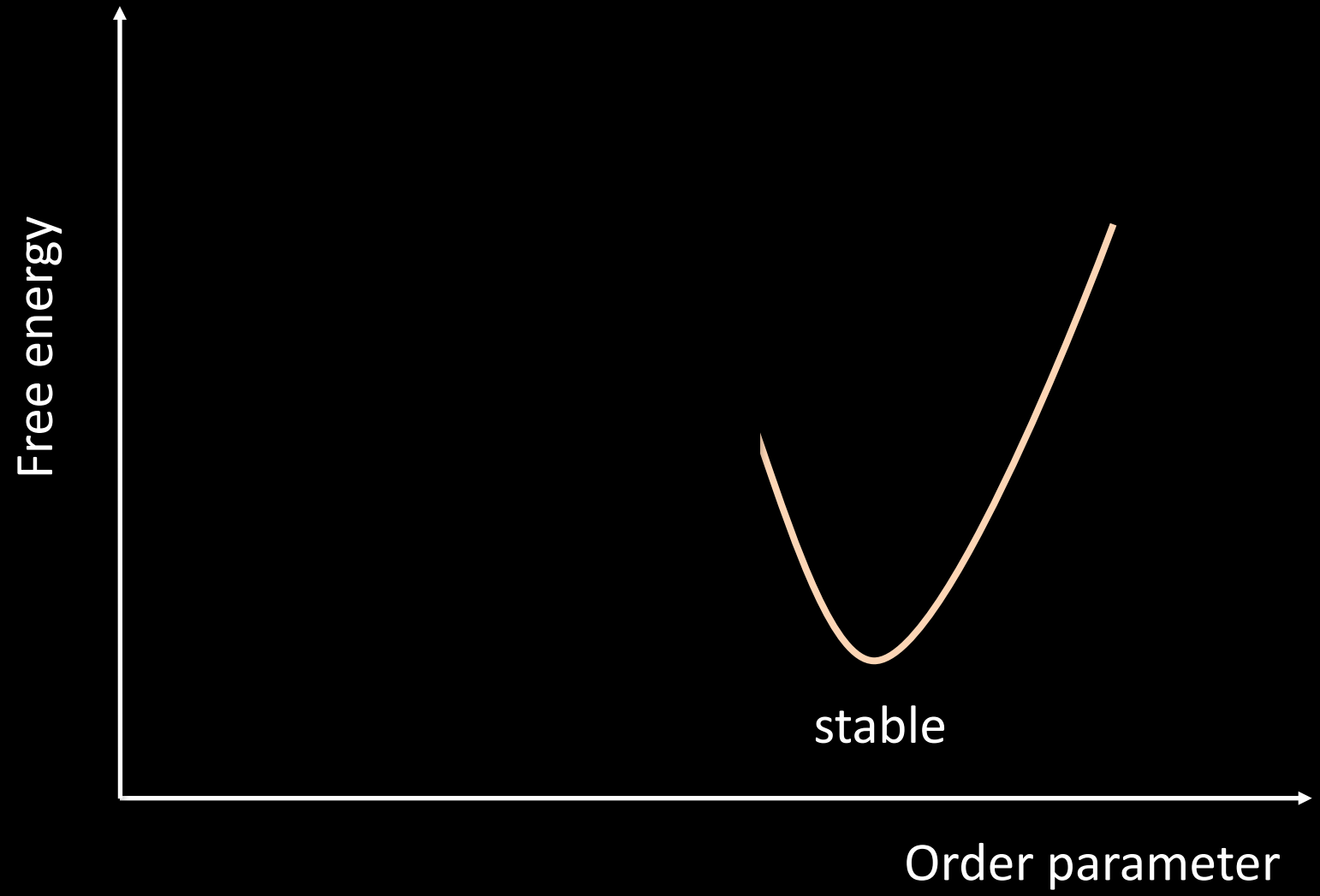


Polymers, fibers & composites





Materials with unprecedented properties



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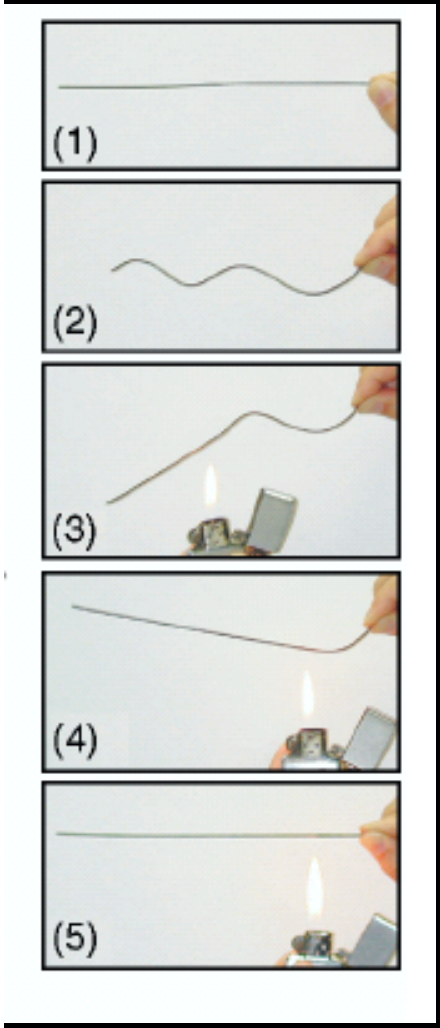
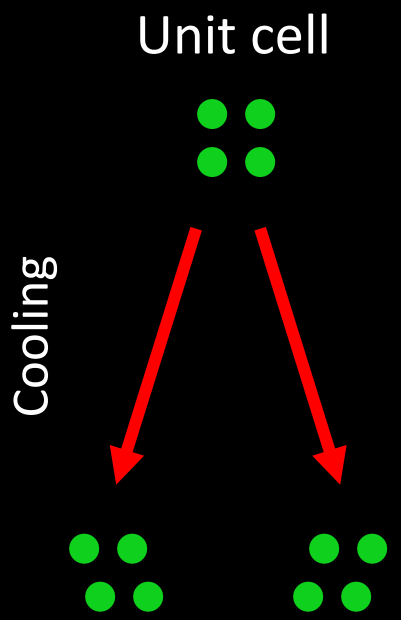
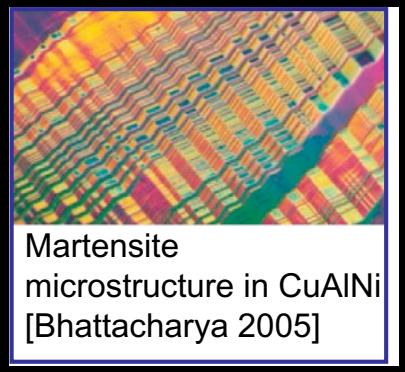
Shape memory & superelasticity

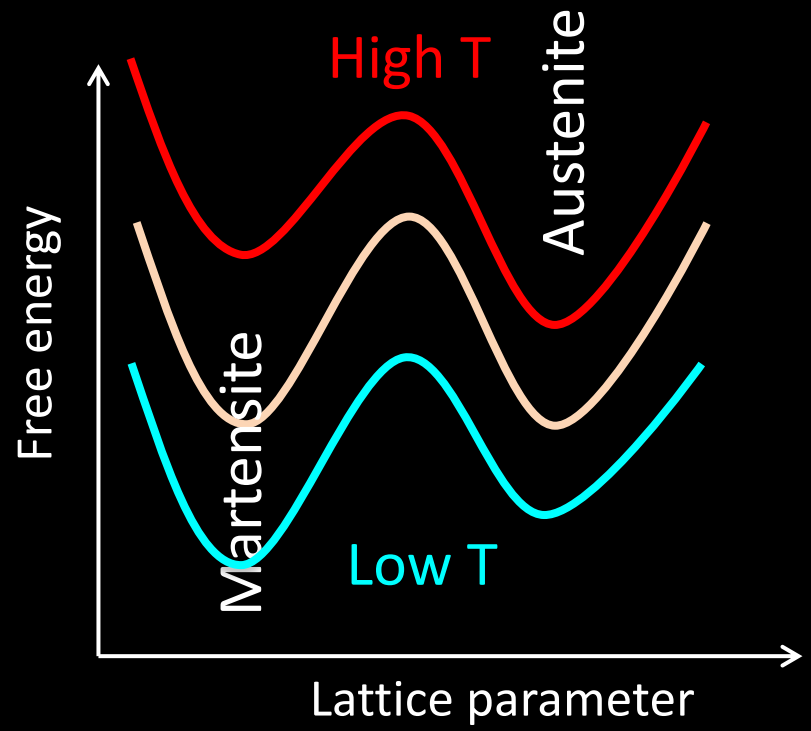


Otsuka et al. MRS Bulletin, February, 2002





Martensite microstructure in CuAlNi [Bhattacharya 2005]



Multiple domains to accommodate elastic strains

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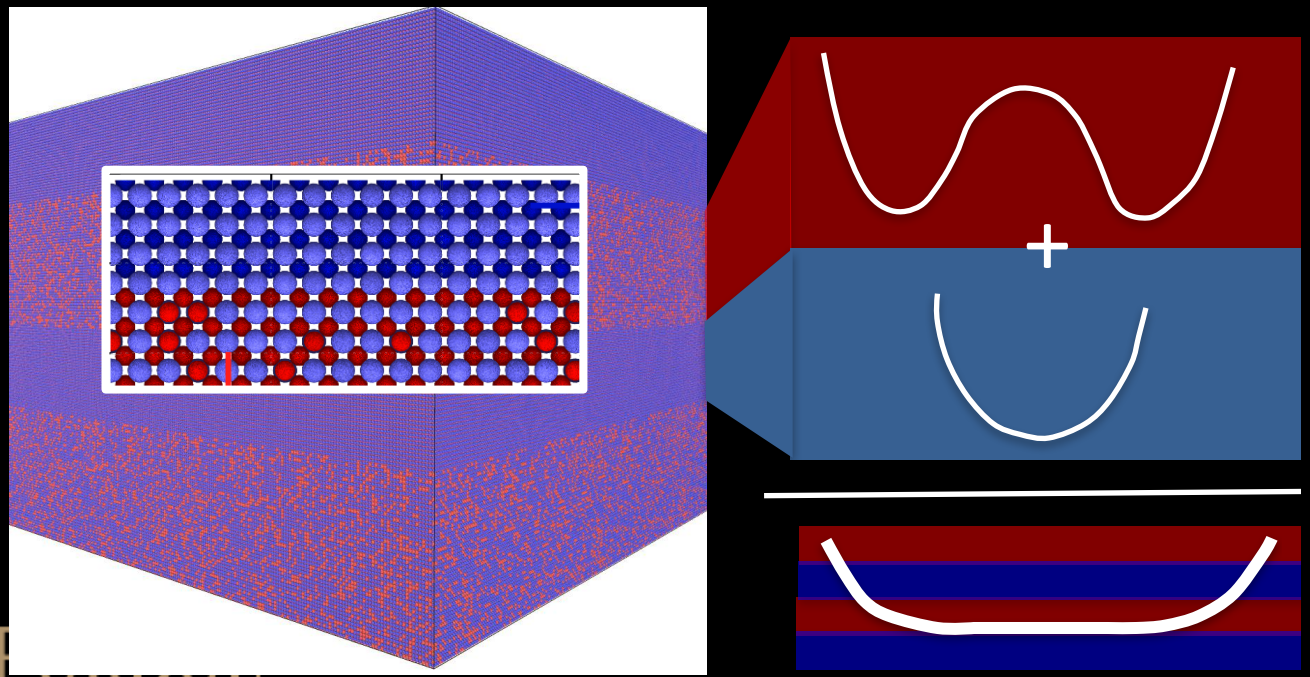
A new class of composite

- Modify the underlying energy landscape to achieve desired properties
- Epitaxial integration of dissimilar materials
  - Force them to have the same in-plane lattice parameter
  - Can one stabilize thermodynamically unstable states
- Can we break away from standard bounds of composite design?



NiAl alloys

- Disordered Ni_xAl_{1-x} (x>=0.61)
- Martensitic transition and shape memory

DEVELOPMENT OF NiAl(B2)-BASE SHAPE MEMORY ALLOYS

R. KAINUMA*, N. ONO** and K. ISHIDA*
*Department of Materials Science, and **Department of Machine Intelligence and Systems Engineering, Faculty of Engineering, Tohoku University, Sendai 980-77, Japan.

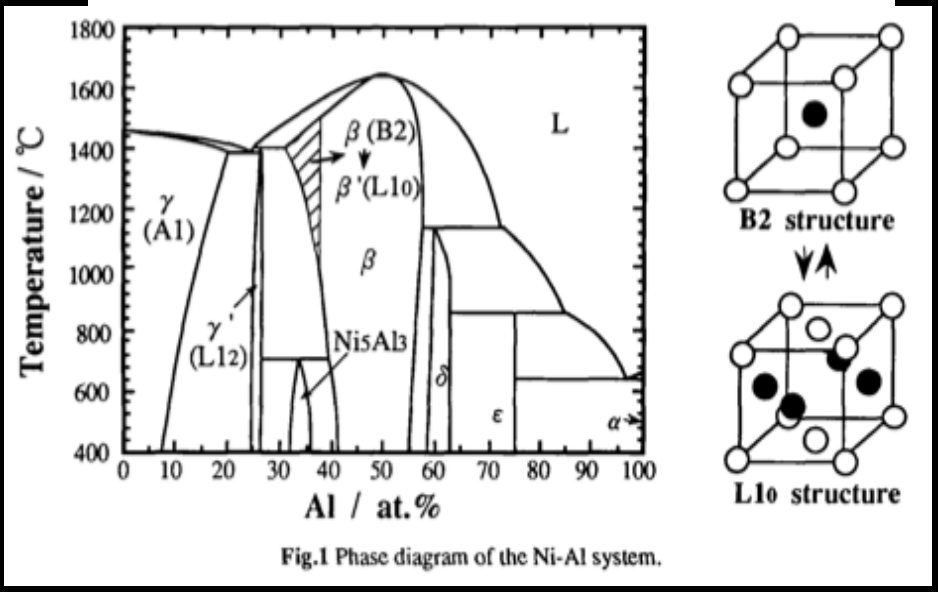
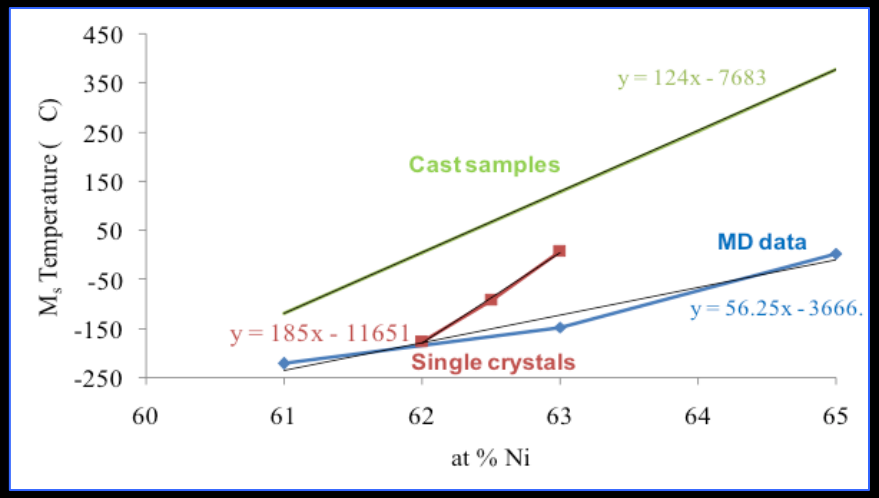
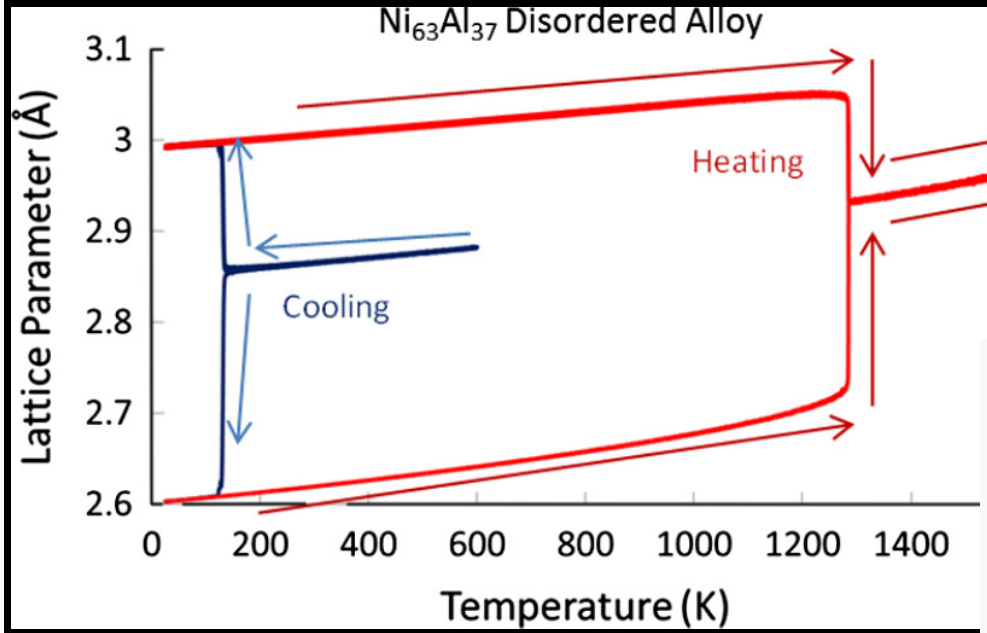


Fig.1 Phase diagram of the Ni-Al system.

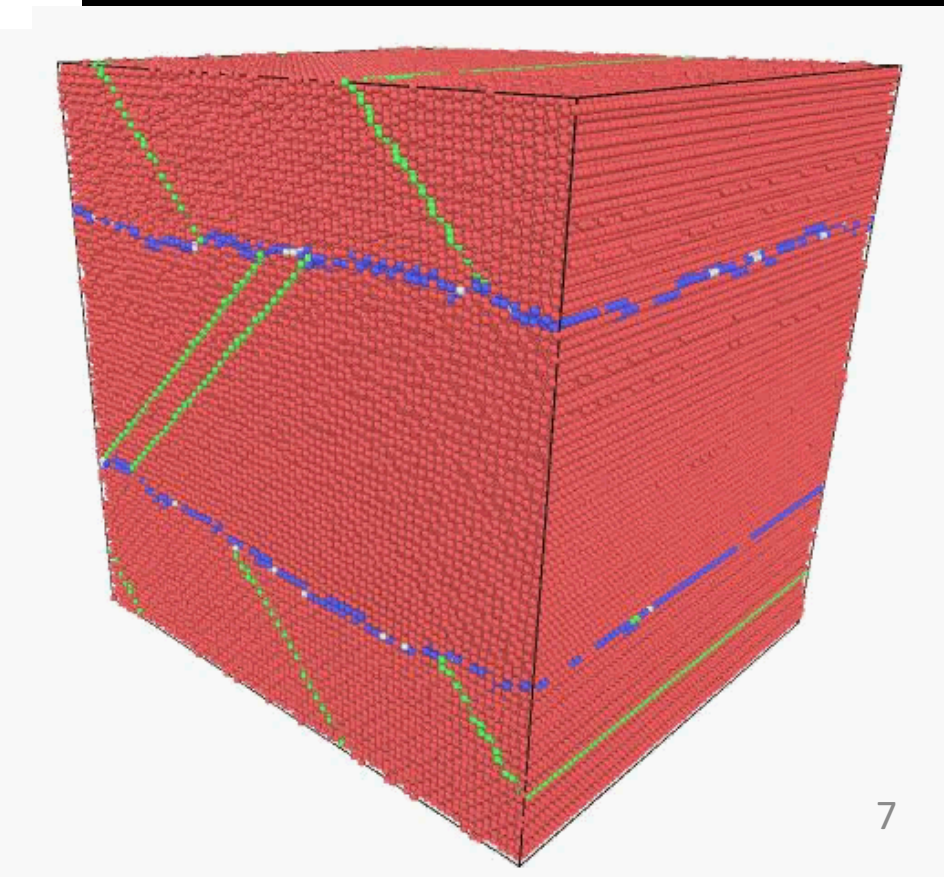
*EAM potential: Farkas et al. MSMSE, **3**, 201-214 (1995)*



Ni_xAl_{1-x} martensitic transformation



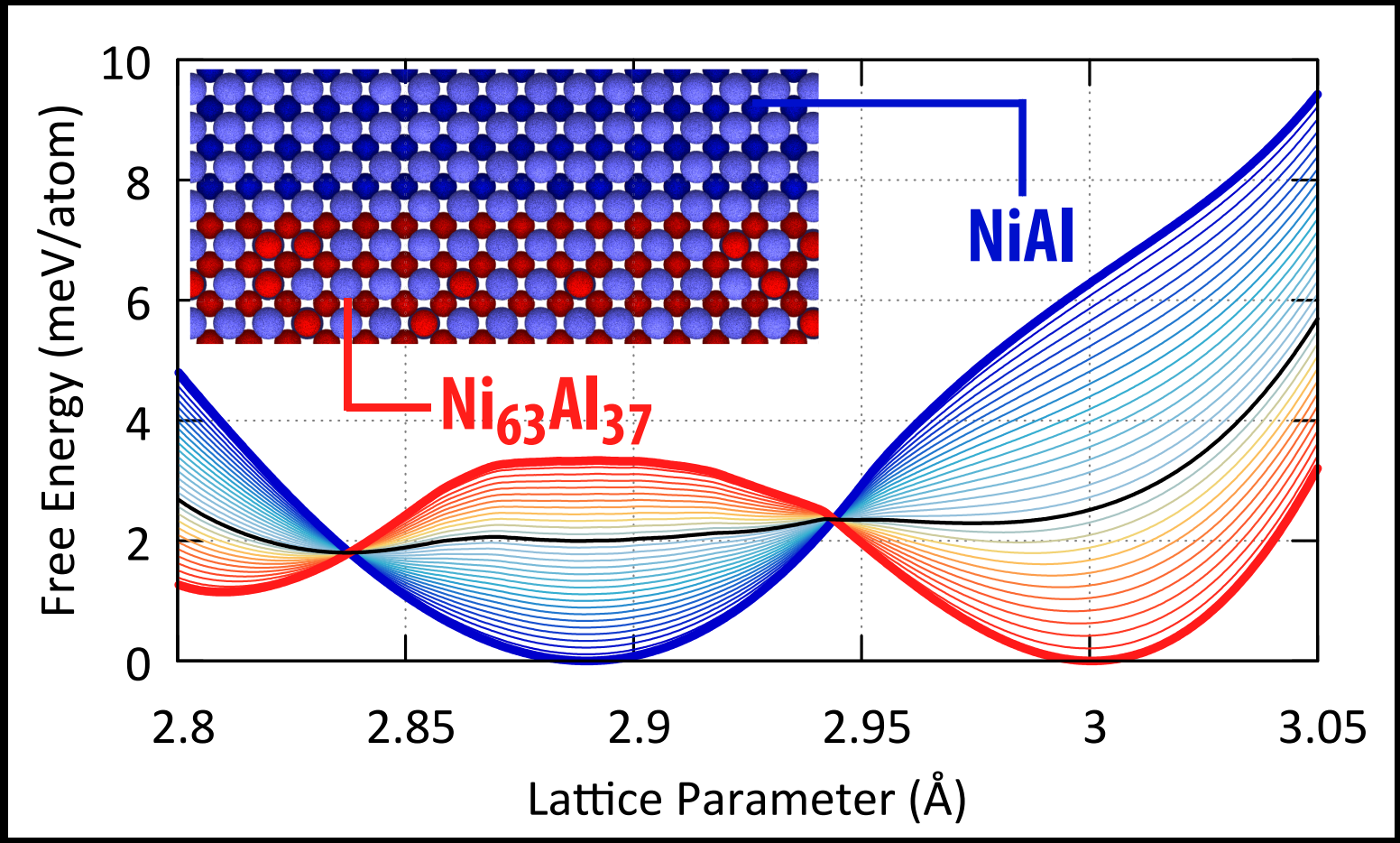
Austenite
Martensite
Stacking Fault



Austenite: cubic B2
Martensite: monoclinic structure (similar but not identical to the experimental 14M structure)

Morrison, Cherukara, and Strachan, Acta Materialia 69 30–36 (2014).

NiAl alloys and metamaterials



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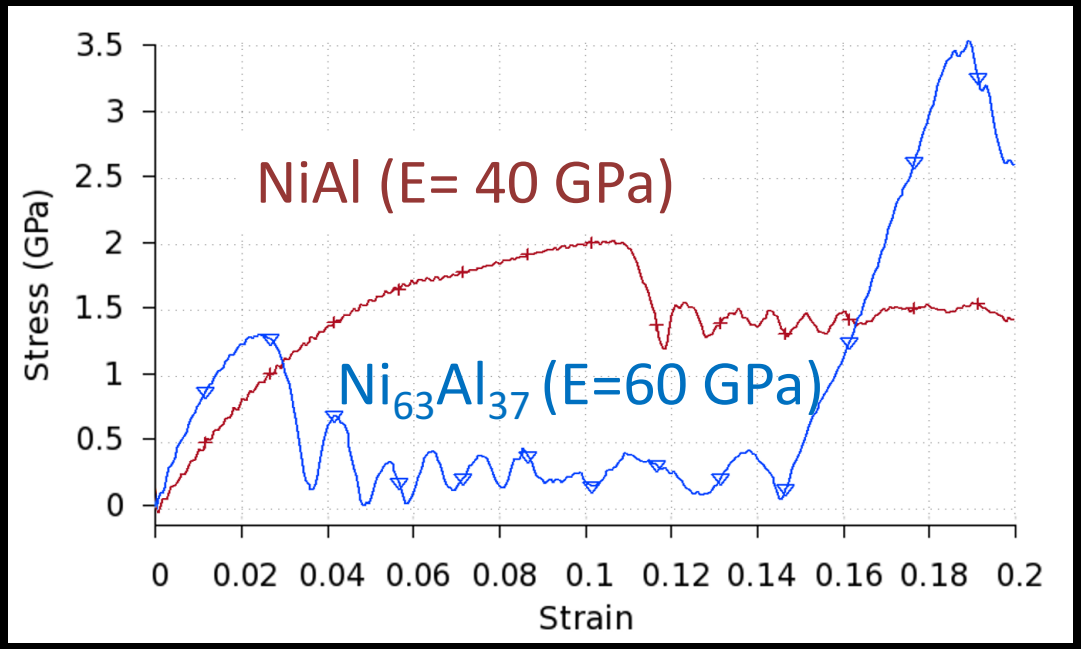
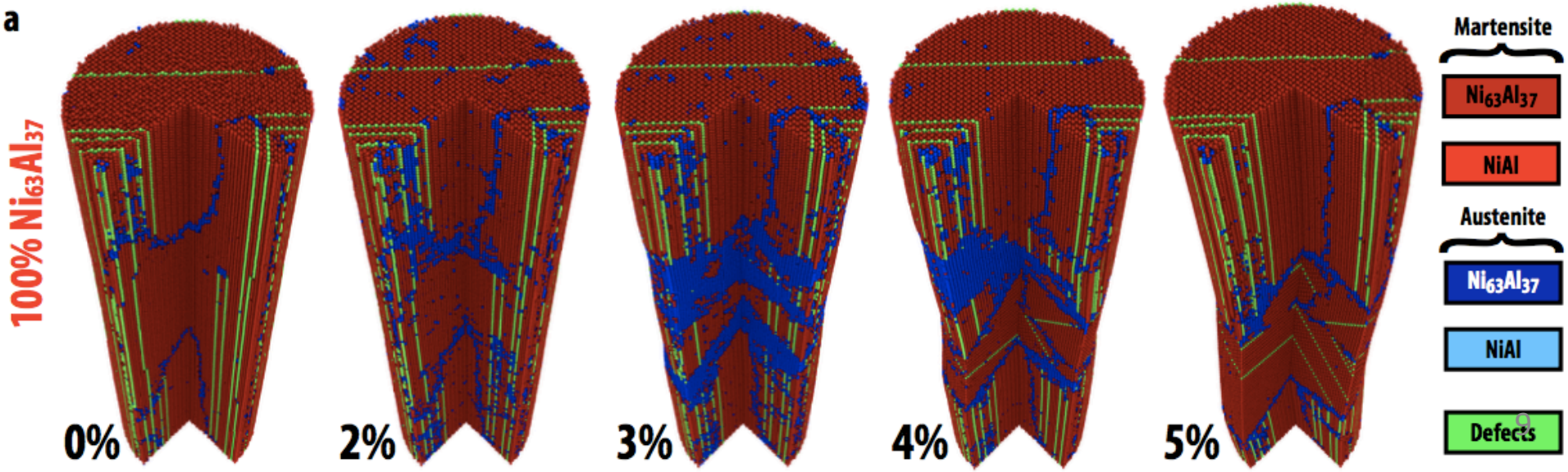
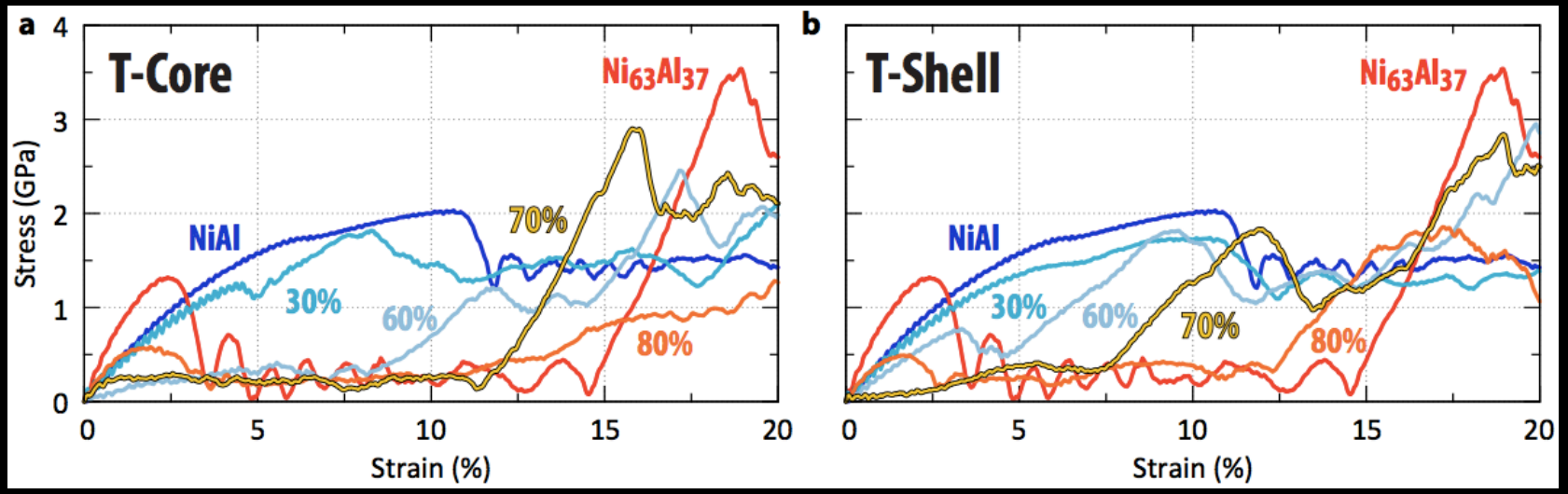
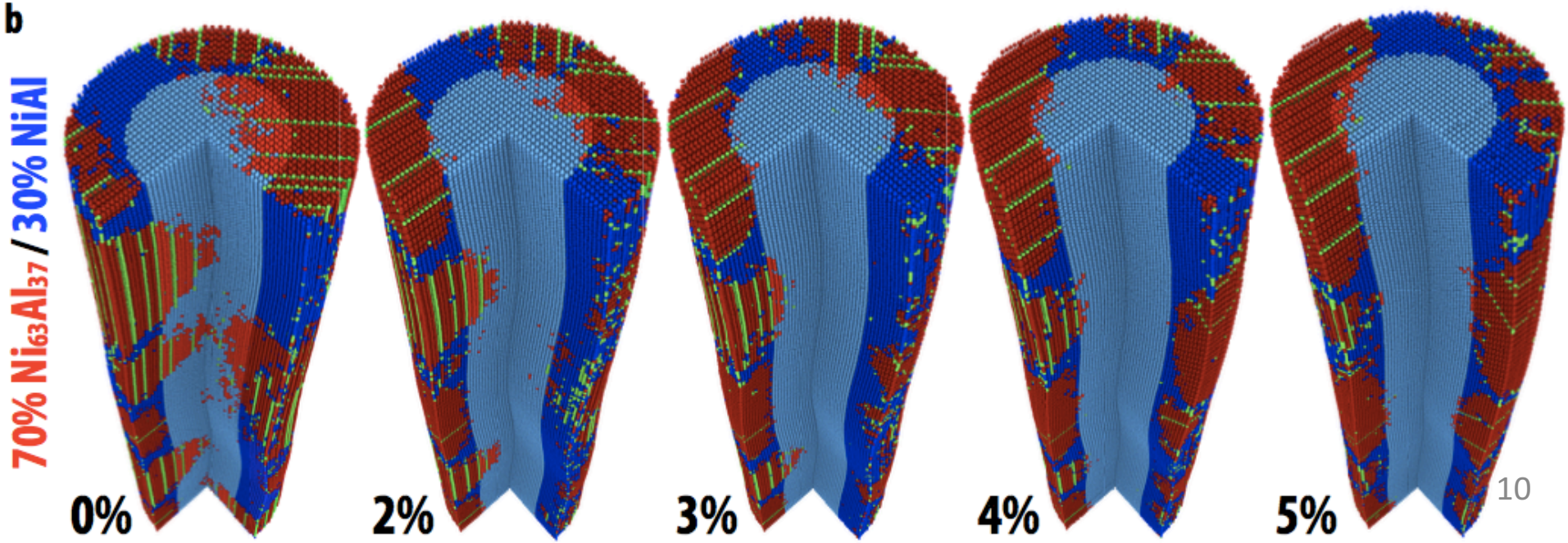
Mechanical properties of pure phases





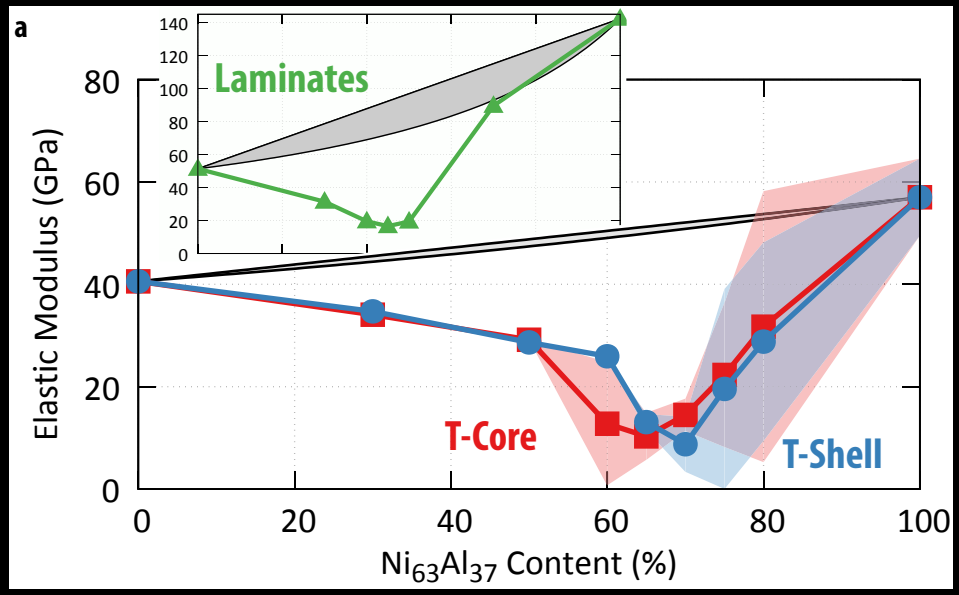
Ultralow stiffness materials





Defy composites design rules

- Epitaxial integration stabilizes negative stiffness states
- Defies traditional composite design bounds
- Fully dense metal with ultra-low stiffness (reaching ~2GPa)
- Works for different configurations and interatomic potentials



Reeve, Bellisiotis, Strachan, Nat. Comm. (accepted with minor changes)

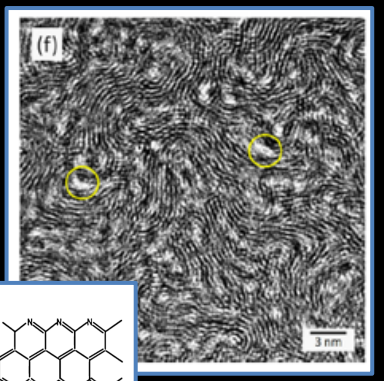
Beyond F=ma

- Length and timescales achievable
  - Rare events
  - Effect of microstructure

- Lack of explicit description of electrons
  - Thermal conduction in metals
  - Electrochemical reactions

Carbon fibers: processing-properties

Carbonization & graphitization



Kumar

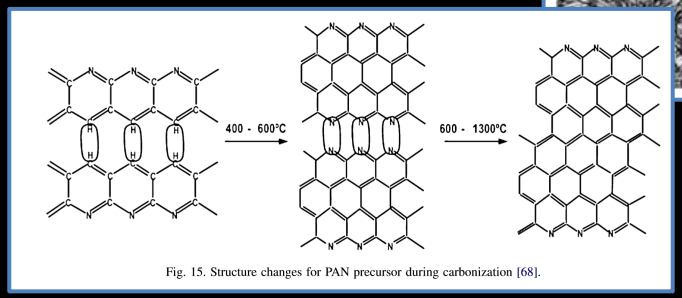
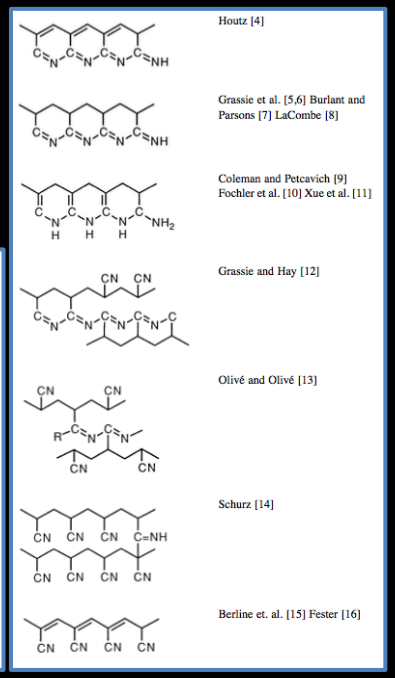


Fig. 15. Structure changes for PAN precursor during carbonization [68].

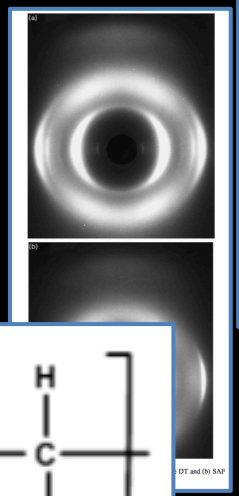
Rahaman et al 2007.

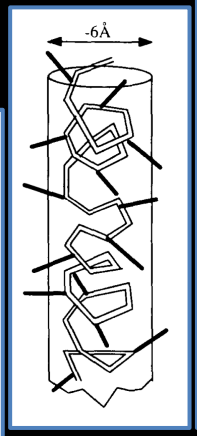
Oxidation & stabilization



Dalton et al. Polymer(1999)

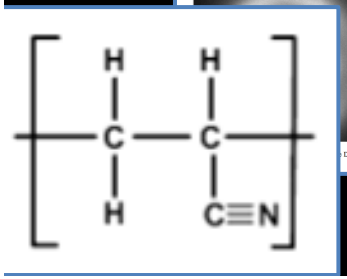
Spinning





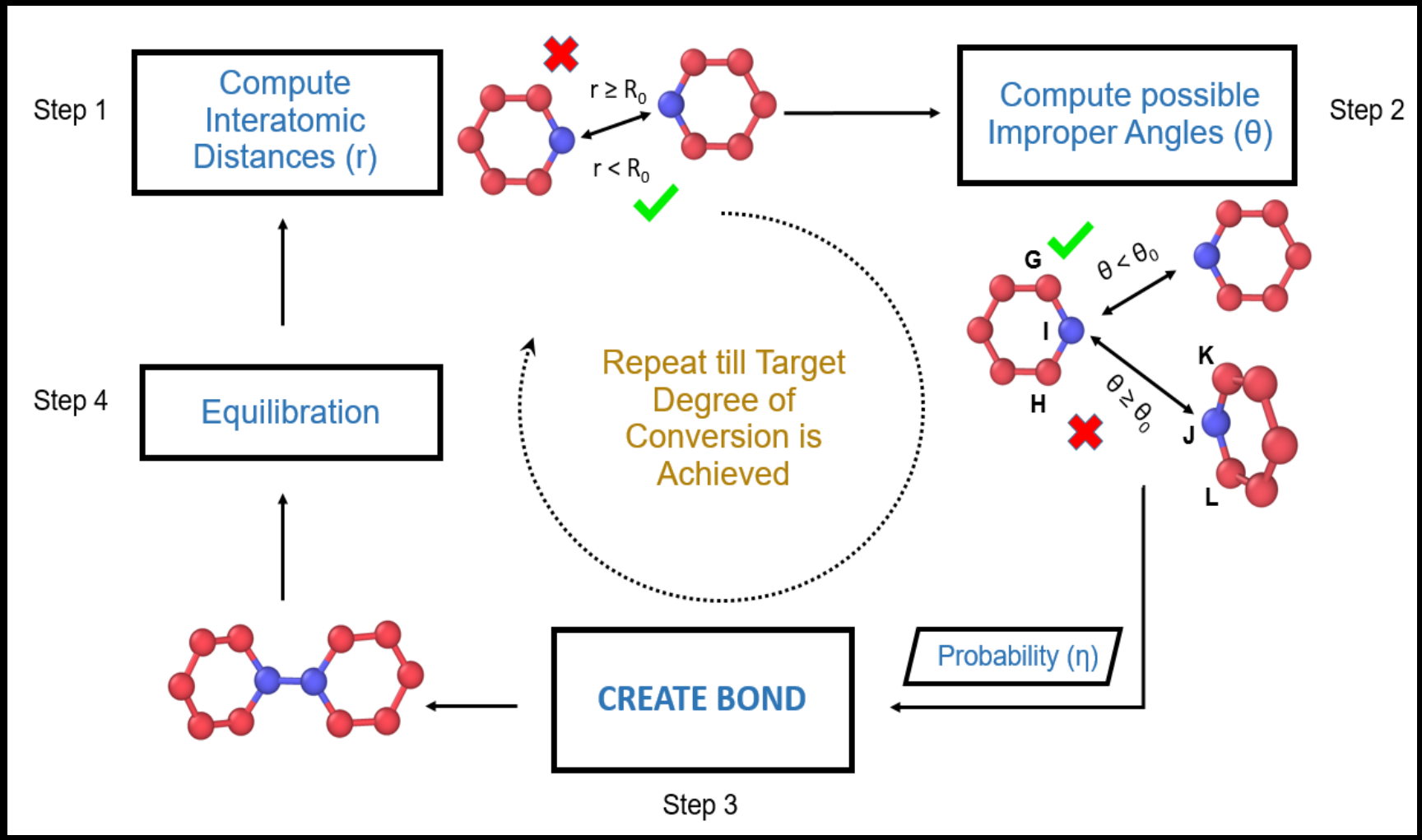
Gupta et al. Carbon (1996)

PAN



Dalton et al. Polymer(1999)

kMC + MD to mimic carbonization



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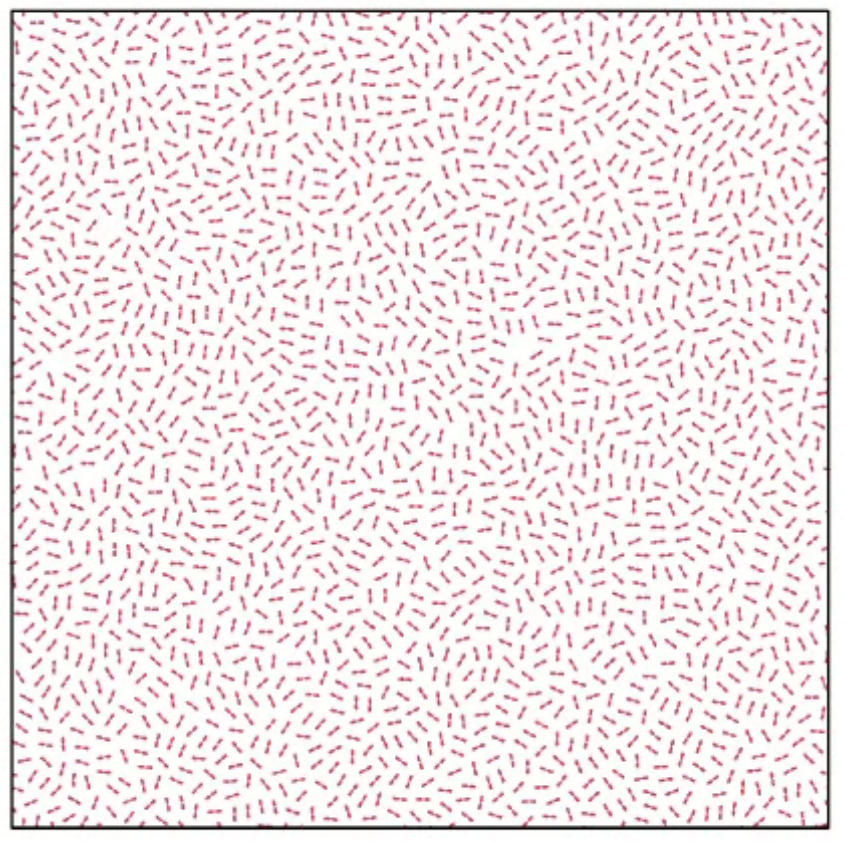
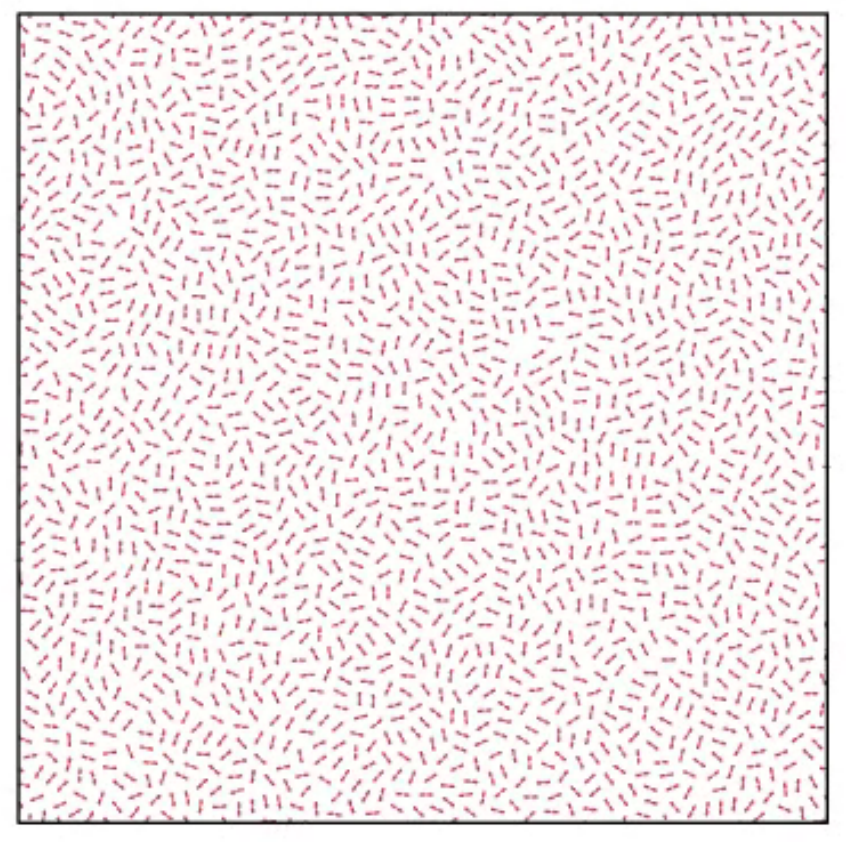
The birth of a carbon fiber



- Distance cutoff = 4.5 A°
- Angle cutoff < 20°
- Temp = 300K



- Distance cutoff = 5.0 A°
- Angle cutoff < 20°
- Temp = 300K

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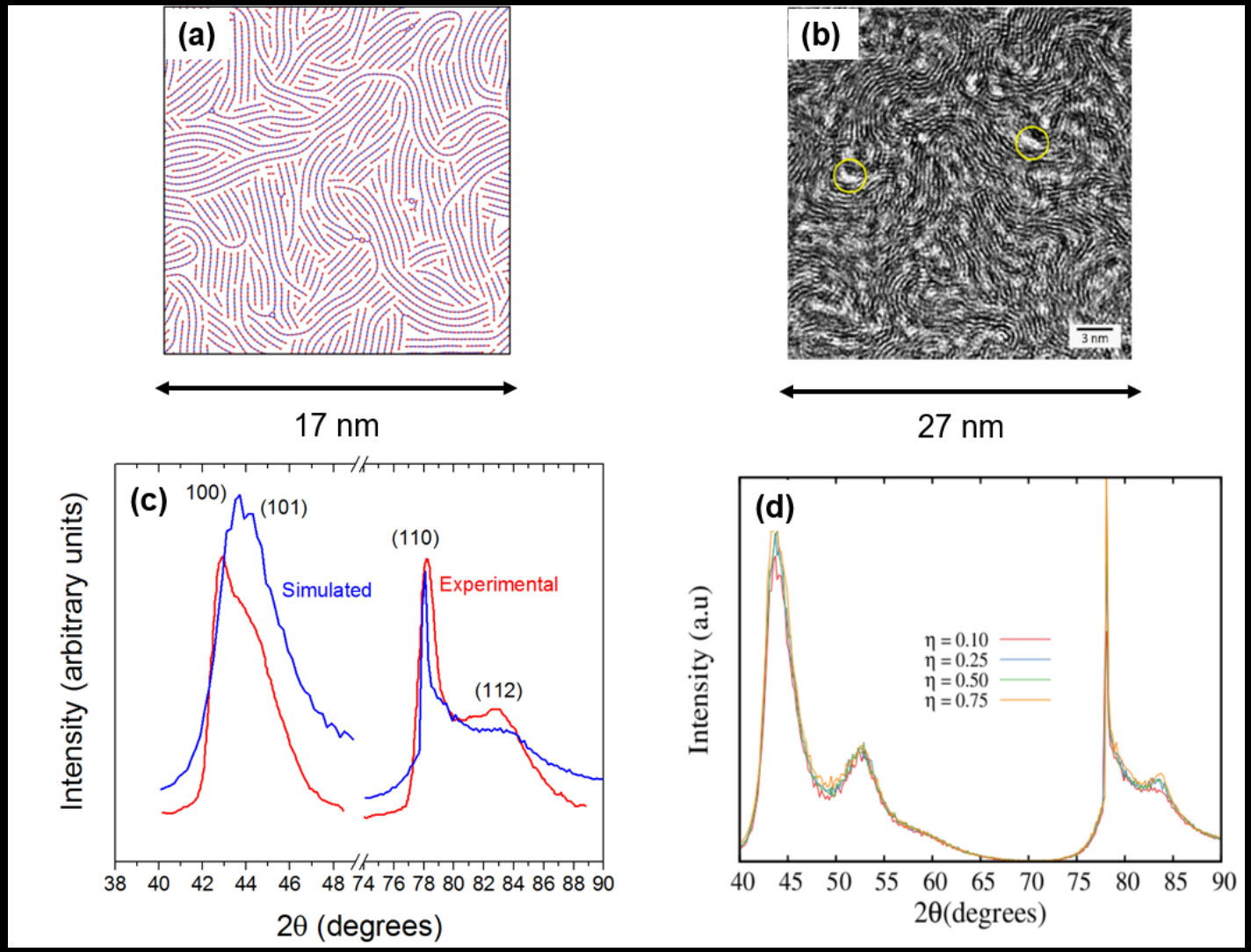
Good agreement with experiments

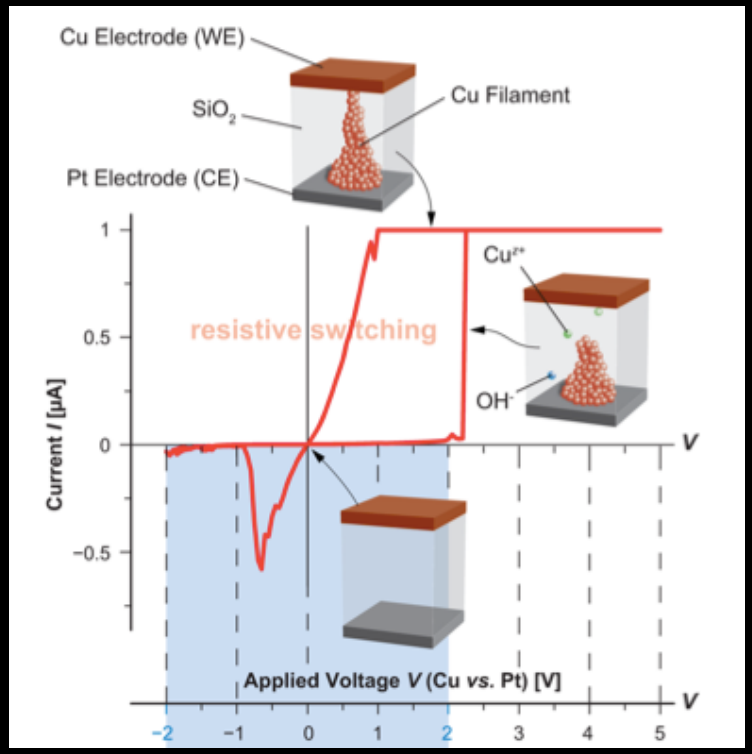


Desai et al. Carbon, under review.

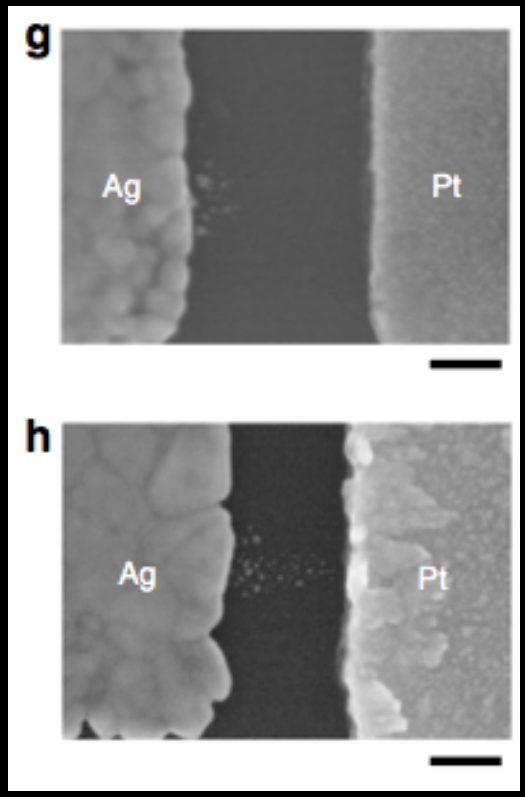
Resistive switching memory

Electrochemistry metallization cells

- Switching times in the nanoseconds
- Scalability down to the nanometer scale



Tappertzhofen et al. ACS Nano (2013)



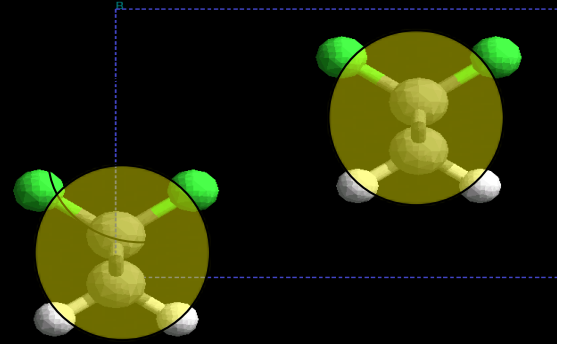
Lu group, Nat. Comm. (2012)

Dynamics with implicit degrees of freedom

$$\dot{R}_i = V_i$$

$$\dot{V}_i = F_i / M_i$$

$$\chi_i = \nu \frac{T_i^{part} - T_i^{int}}{T_0}$$



Other variables may play important roles:

- Internal degrees of freedom in coarse grain simulations
- Conduction electrons in simulations of metals
- Electrochemical potential in EMCs

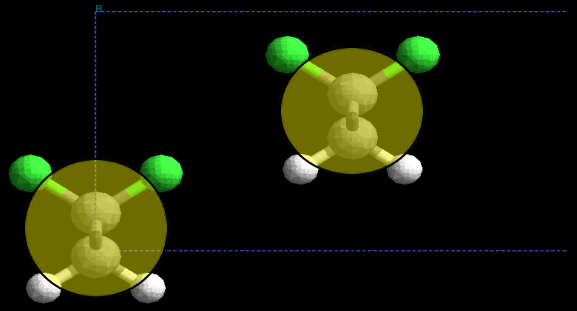
Key features of DID

- Total energy (meso + internal) is conserved
- c.m. velocity is conserved
- Galilean invariant
- Correct description of the ballistic regime

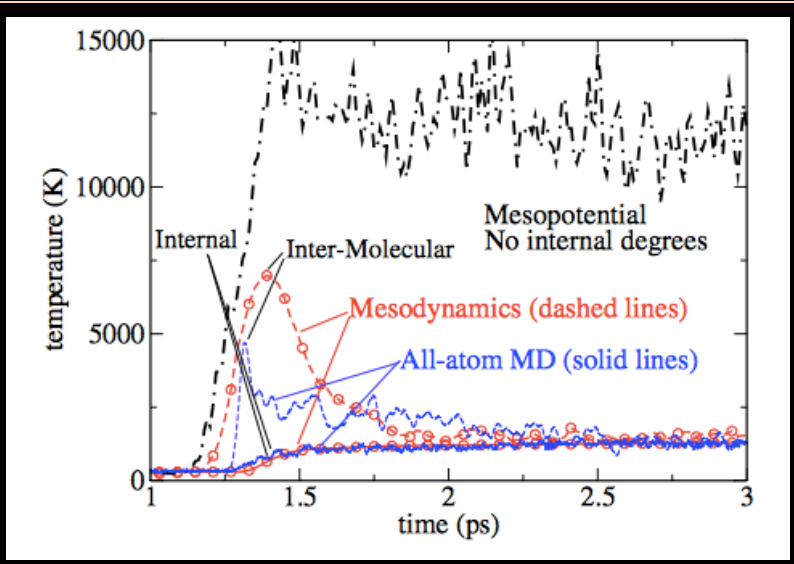
Strachan & Holian, Phys. Rev. Lett. (2005)
Lynch, Thompson, & Strachan, MSMSE, (2009)
Zhou, Anglin, Strachan, J. Chem. Phys. (2009)
Lin, Holian, Germann, Strachan, J Chem. Phys. (2014)

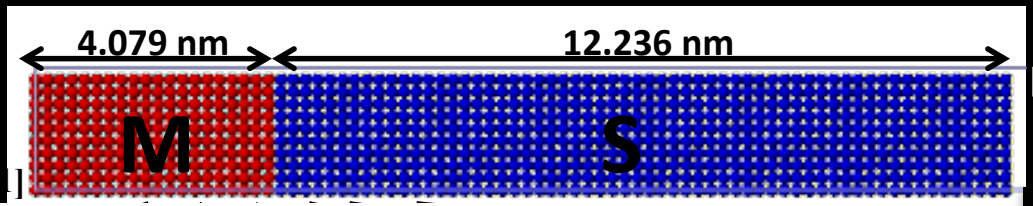
Sample DID applications

Shock wave propagation

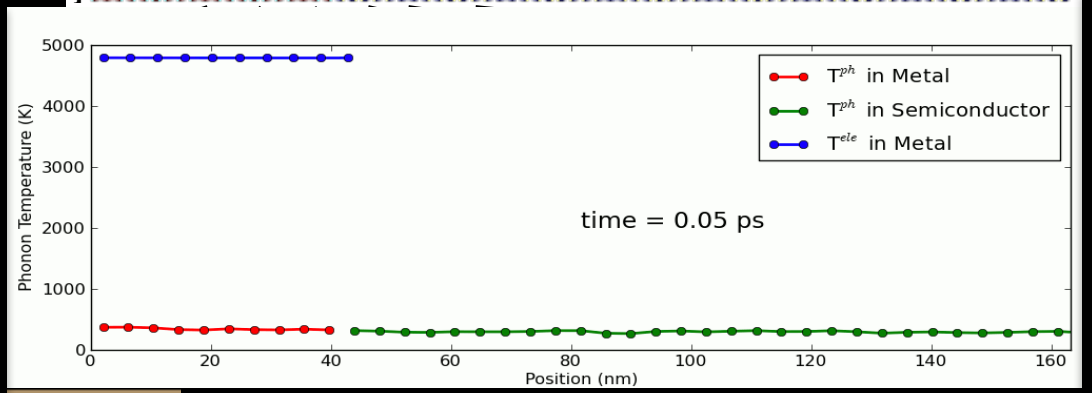


Strachan & Holian, Phys. Rev. Lett. (2005)



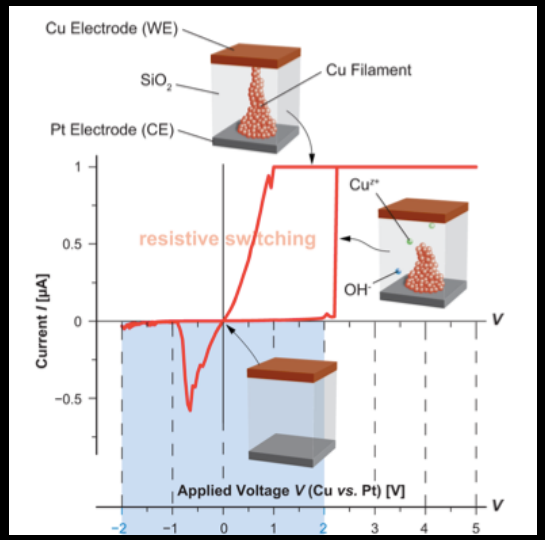


Laser heating experiments



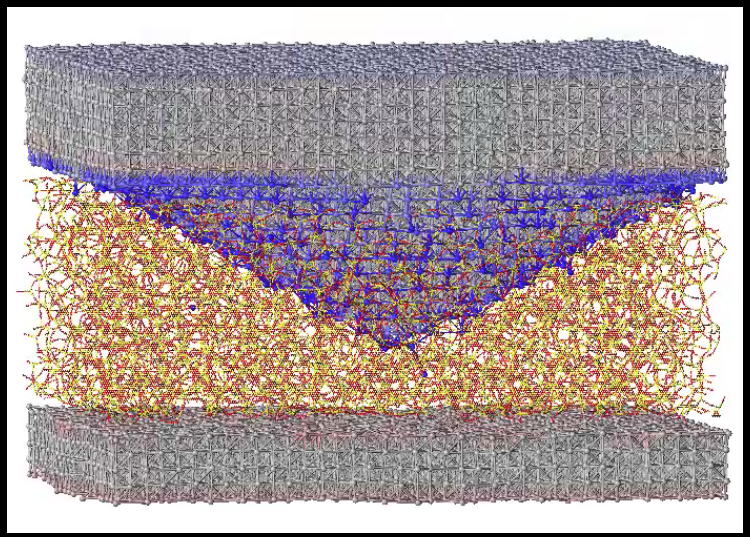
Lin et al. J. Chem. Phys. (2015)
Lin, Holian, Germann, Strachan, J Chem. Phys, (2014)

Modeling electrochemical reactions



Tappertzhofen et al. ACS Nano (2013)

Electro-metallization cells for nanoelectronics



Self-consistent atomic charges in reactive MD simulations

Total electronic energy:

$$E\left(\{q_i\};\{R_i\}\right)=\sum_i\left(\chi_i^0 q_i+\frac{1}{2}H_i q_i^2\right)+\sum_{i<j}q_i q_j J\left(\left|R_i-R_j\right|\right)$$

Electronegativity equilibration:

$$\chi_i=\chi_0=\frac{\partial E\left(\{q_i\};\{R_i\}\right)}{\partial q_i}=\chi_i^0+H_i q_i+\sum_{j\neq i}q_j J\left(\left|R_i-R_j\right|\right)$$

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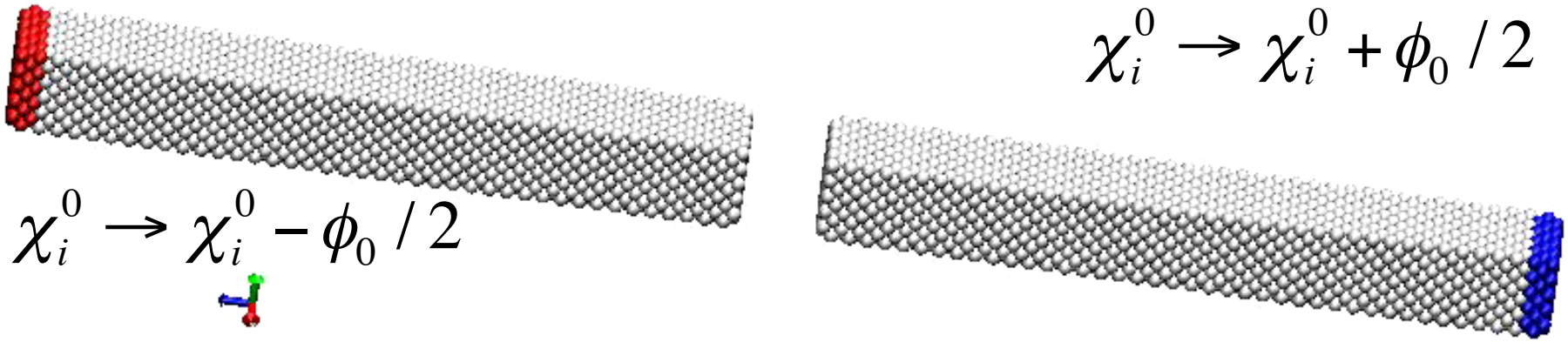
Electrochemical potential equalization

Total electronic energy: $$E\left(\{q_i\};\{R_i\}\right)=\sum_i\left(\chi_i^0 q_i+\frac{1}{2}H_i q_i^2\right)+\sum_{i<j}q_i q_j J\left(\left|R_i-R_j\right|\right)$$

Application of an external electrochemical potential by modifying the local atomic electronegativity



Voltage equilibration within metallic electrodes:

$$\dot{\phi}=k\nabla^2\phi$$

$$\dot{\phi}_i(t)=\sum_{j\neq i}\frac{\phi_i(t)-\phi_j(t)}{\left|R_{ij}\right|^2}w\left(R_{ij}\right)$$

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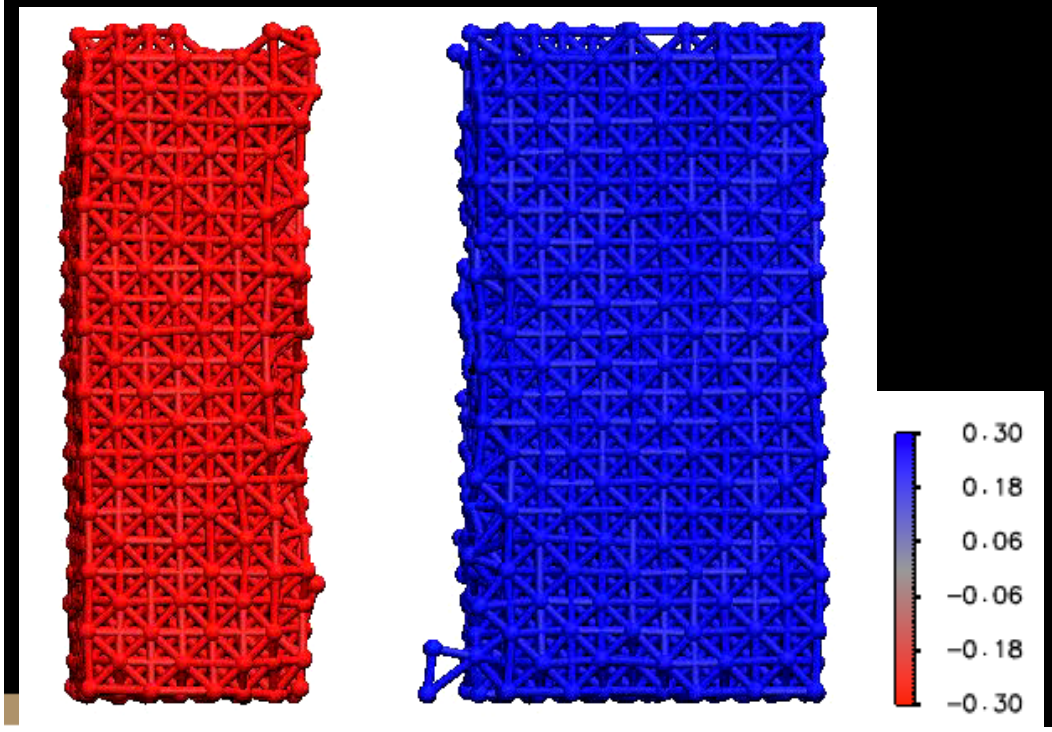
Onofrio and Strachan, J. Chem. Phys. (2015)

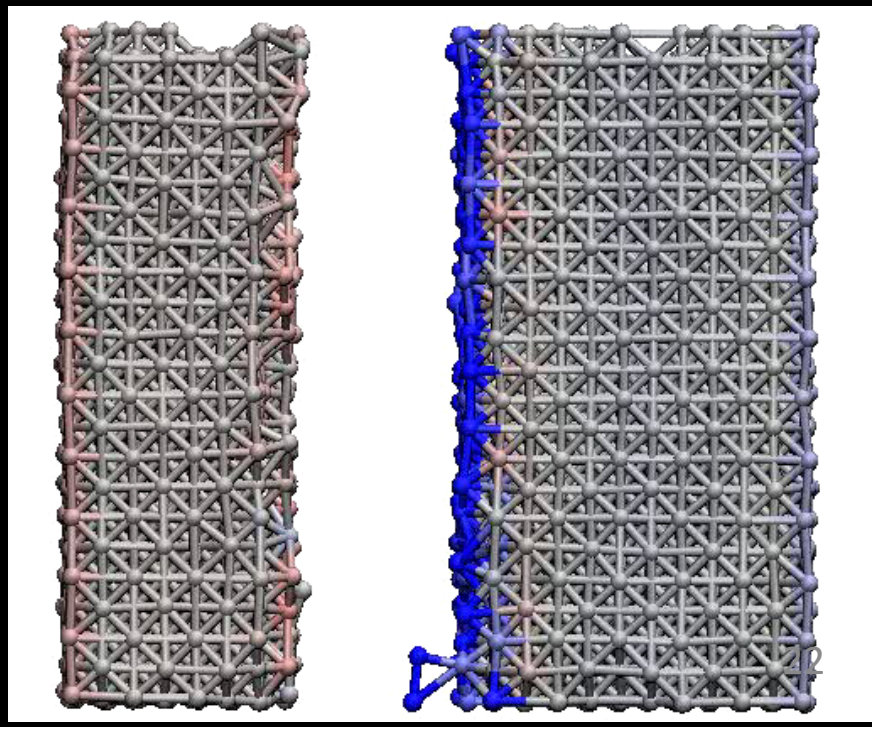
EChemDID at work

- Reactive interatomic potentials enable chemical reactions
- Charge transfer using charge equilibration (Qeq)
- **EChem-DID**: external voltage affects atomic electronegativity

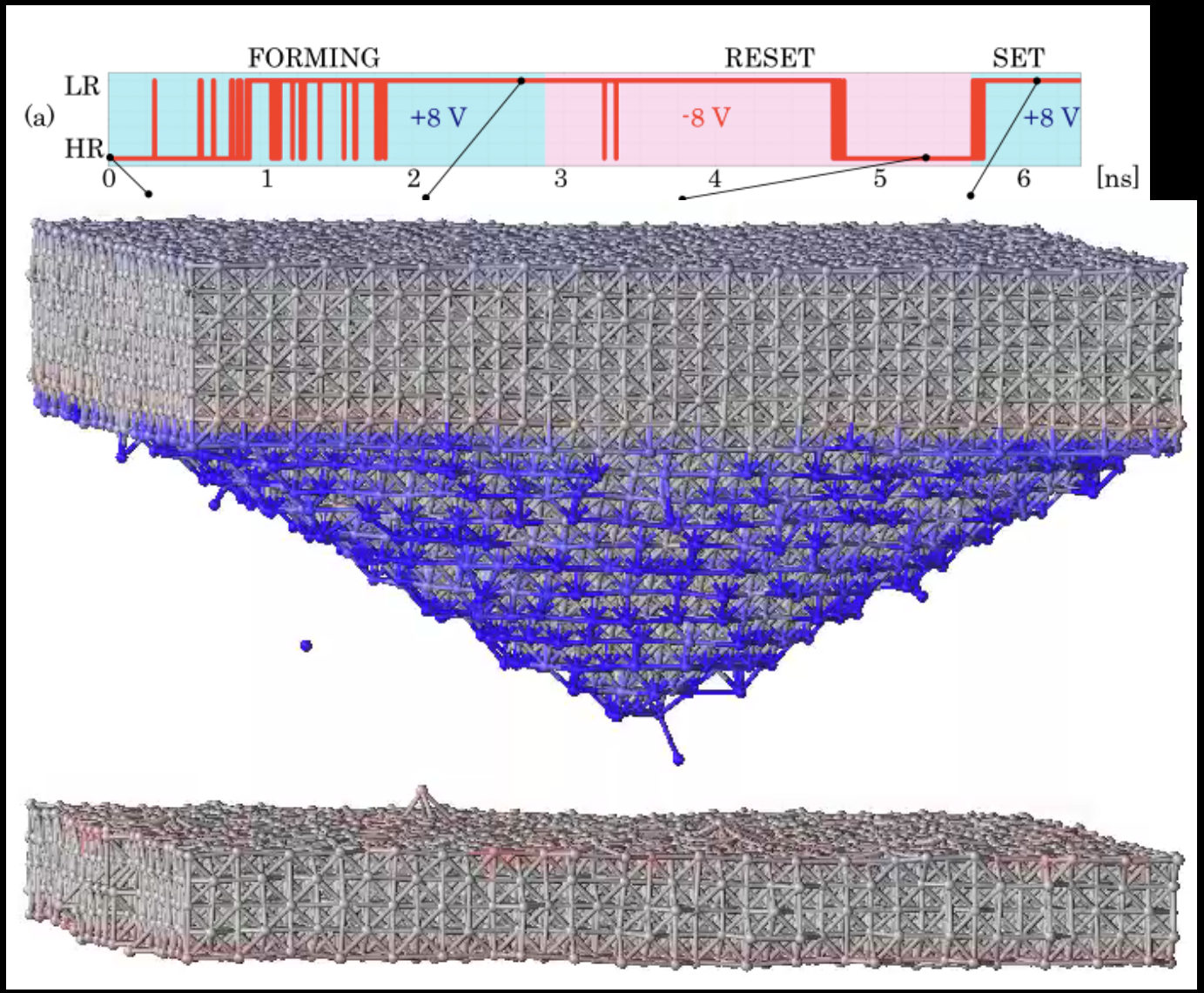
Local electrochemical potential



Partial charges



Atomistic simulations of switching

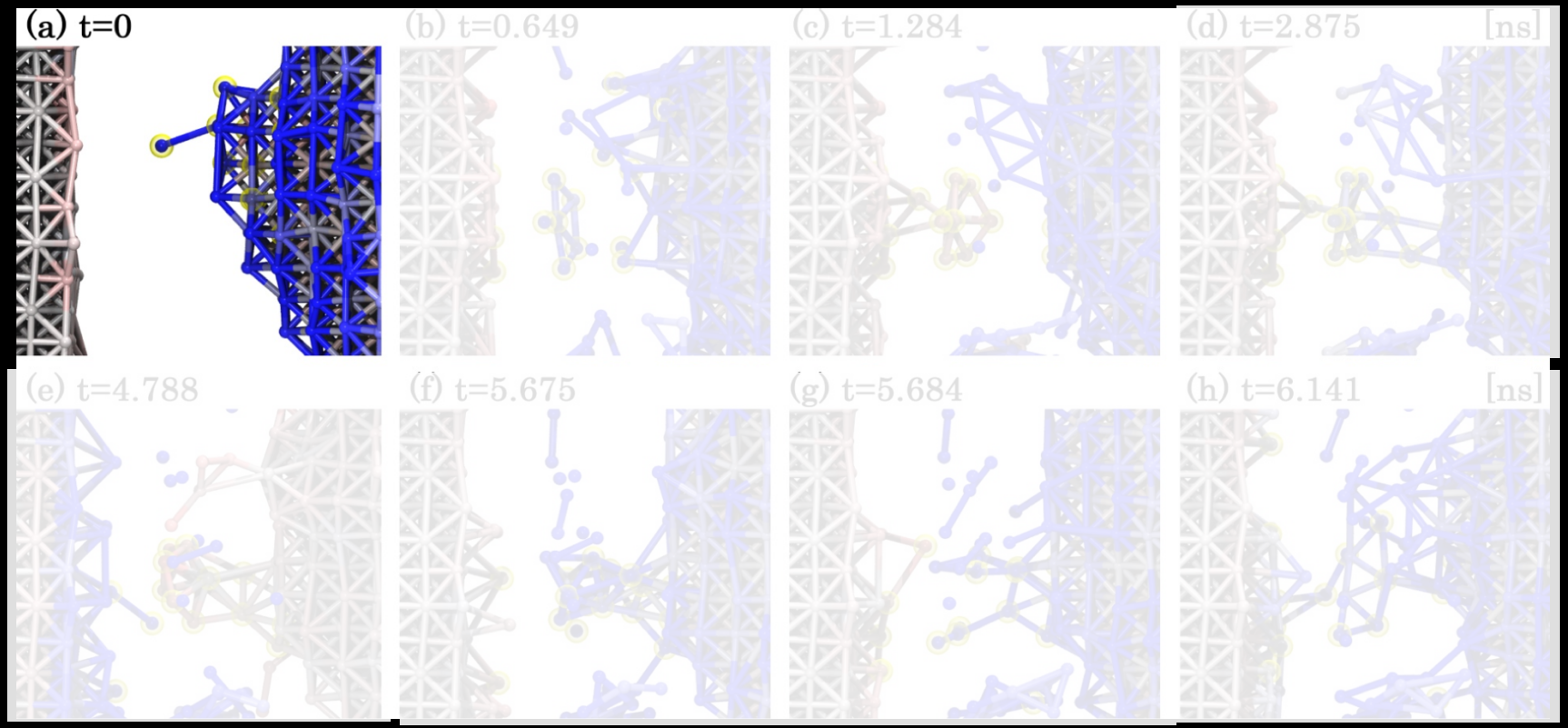


Onofrio, Guzman & Strachan, Nature Materials (2015)

Mechanism of switching

1. FORMING: Cluster formation

2. FORMING: Reduction stabilizes dissolved Cu



3. RESET: Filament breaks near inactive electrode

4. SET: Filament attached to active electrode dissolves

5 SET: cluster formation & reduction

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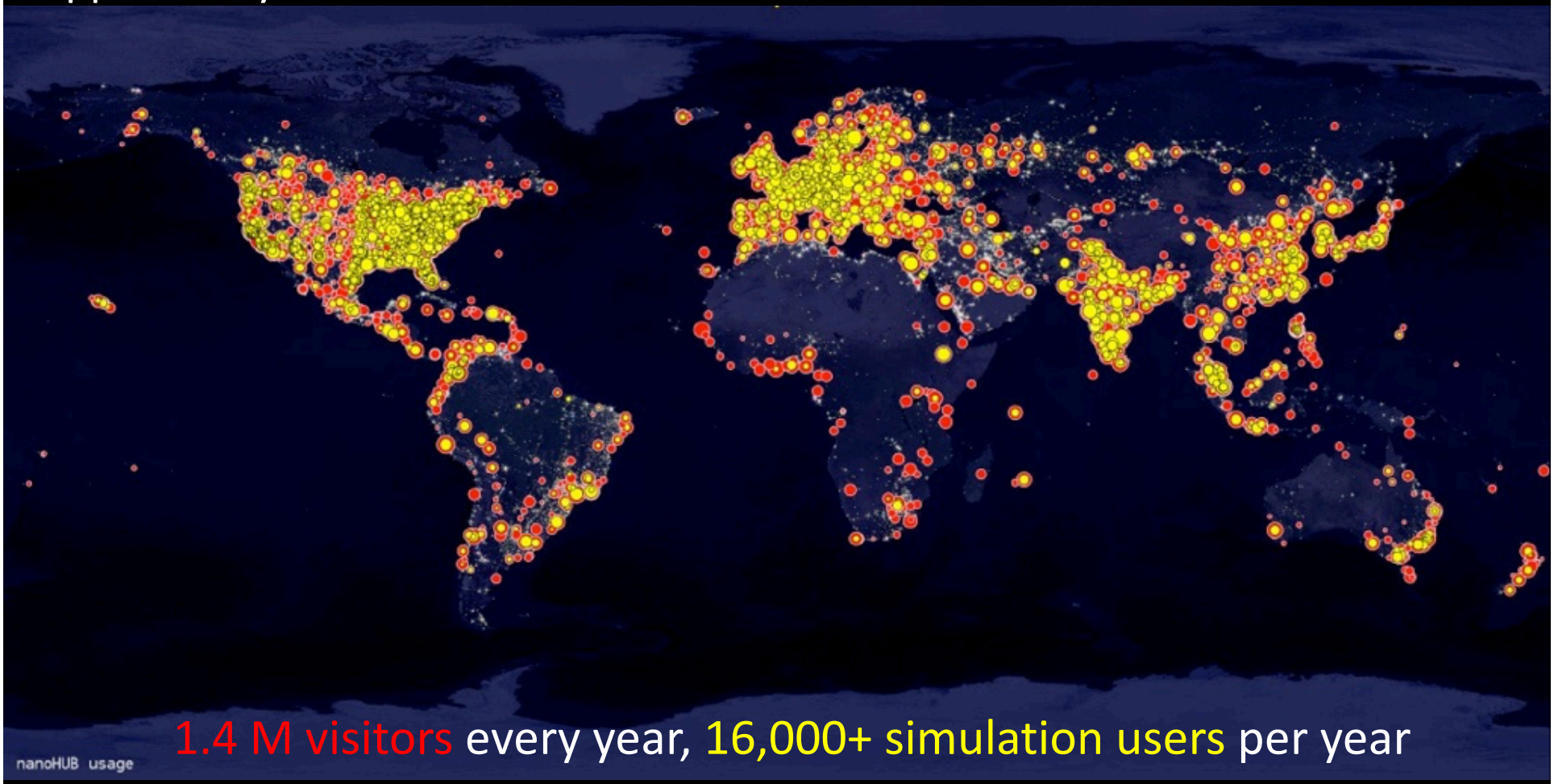
Online simulations using nanoHUB

Developed & operated by the Network for Computational Nanotechnology
Supported by the US National Science Foundation



1.4 M visitors every year, 16,000+ simulation users per year

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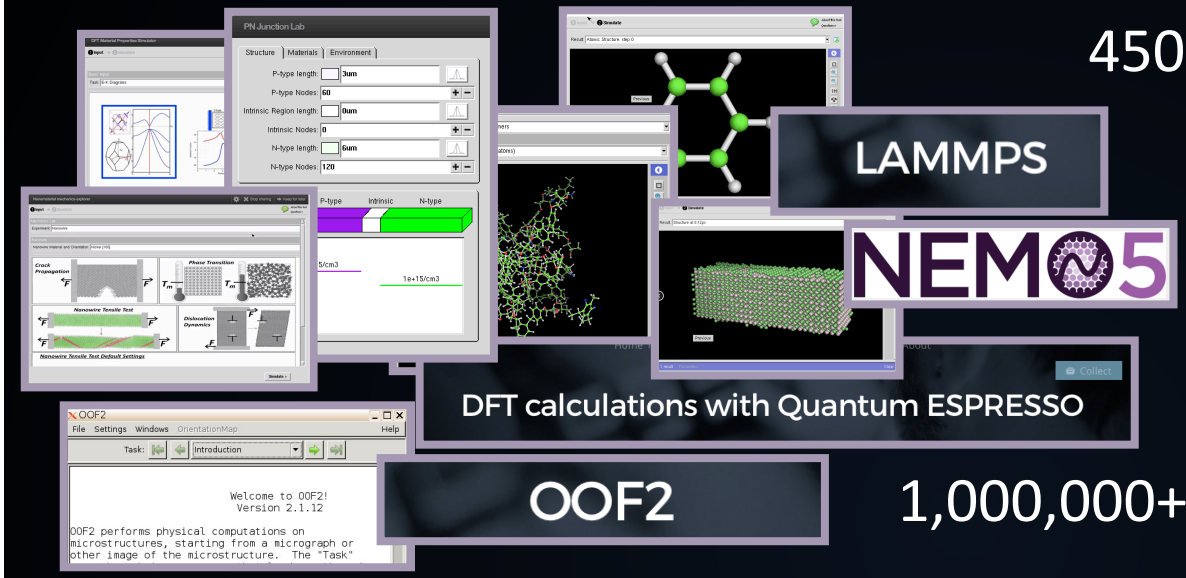
nanoHUB online simulations

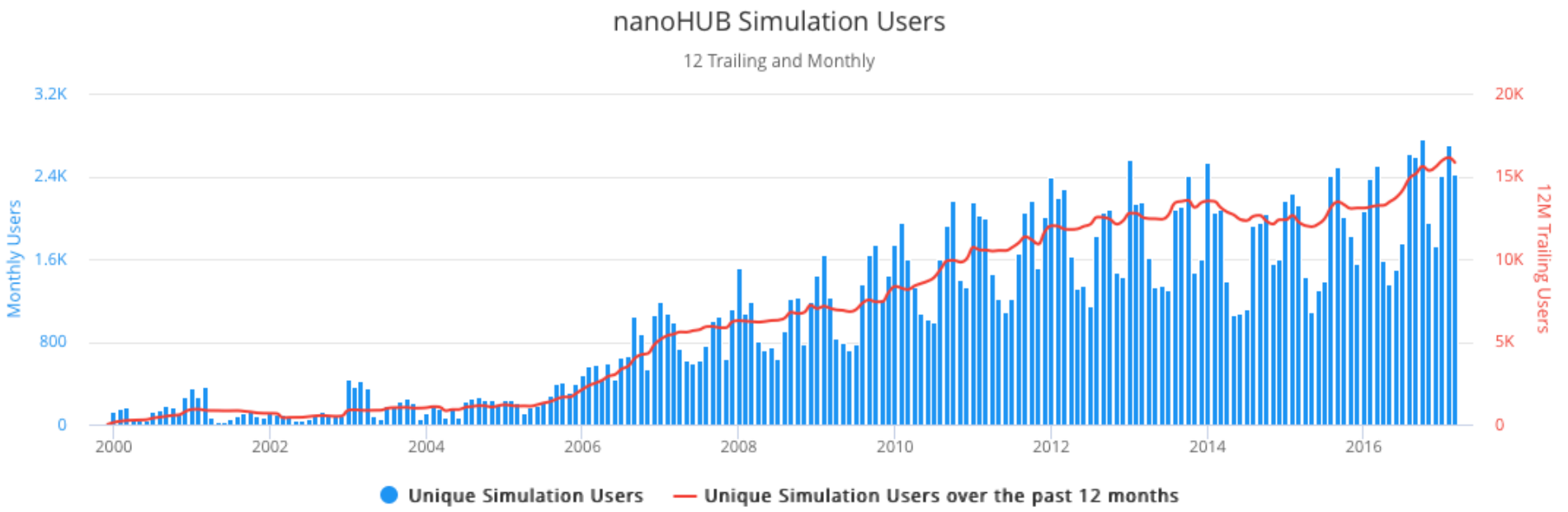


450+ simulation tools

1,800+ contributors

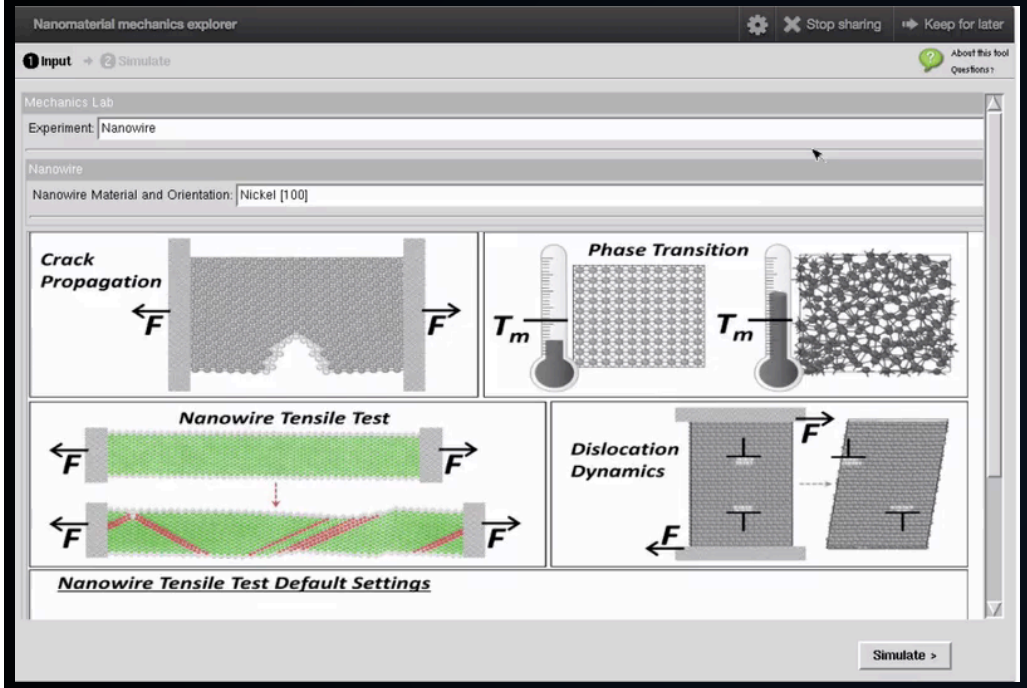
16,000+ annual simulation users

1,000,000+ simulations per year



Tools designed for end users

ttps://nanohub.org/tools/nanomatmech



Powered by LAMMPS

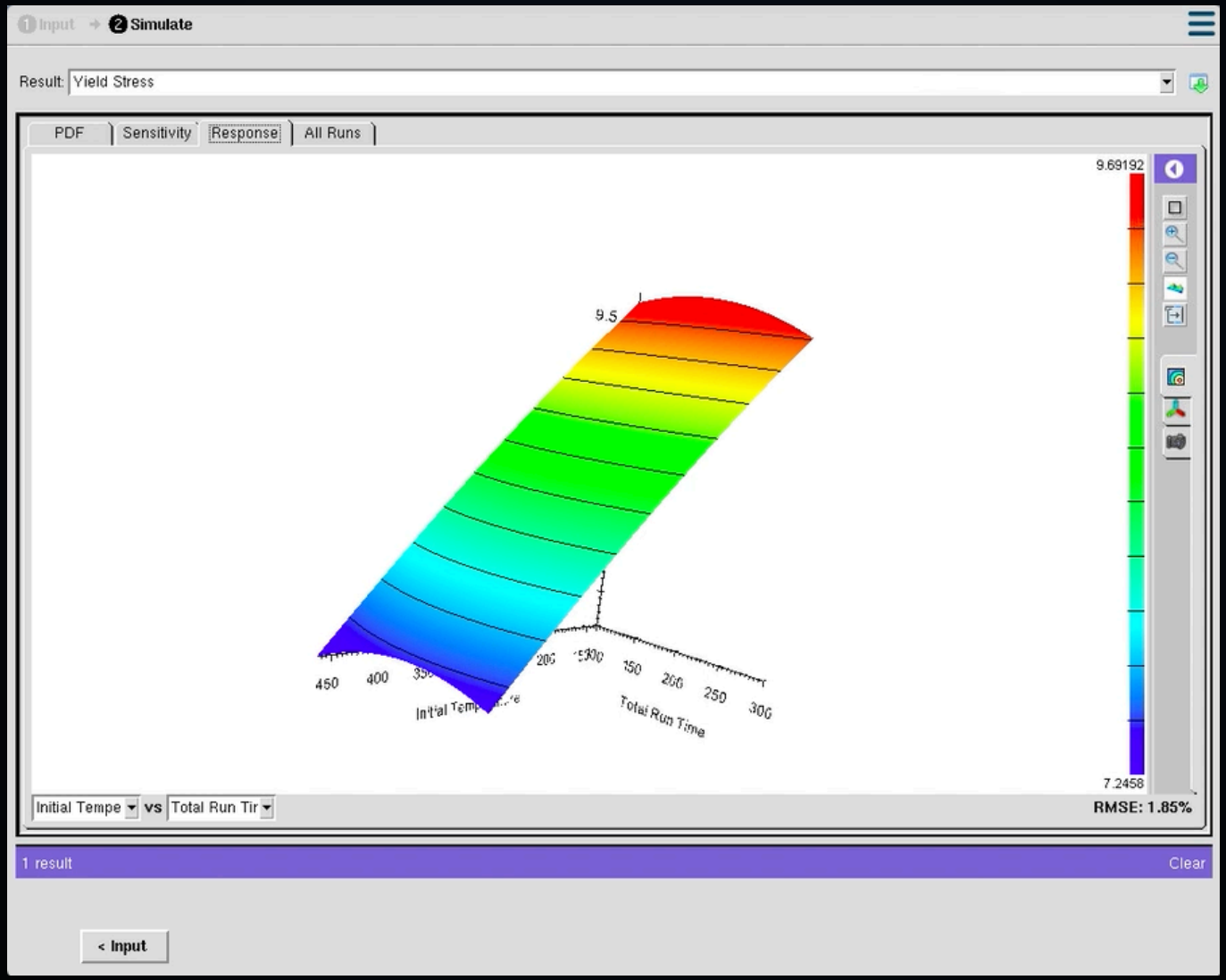
https://nanohub.org/tools/dftmatprop

Powered by Quantum Espresso

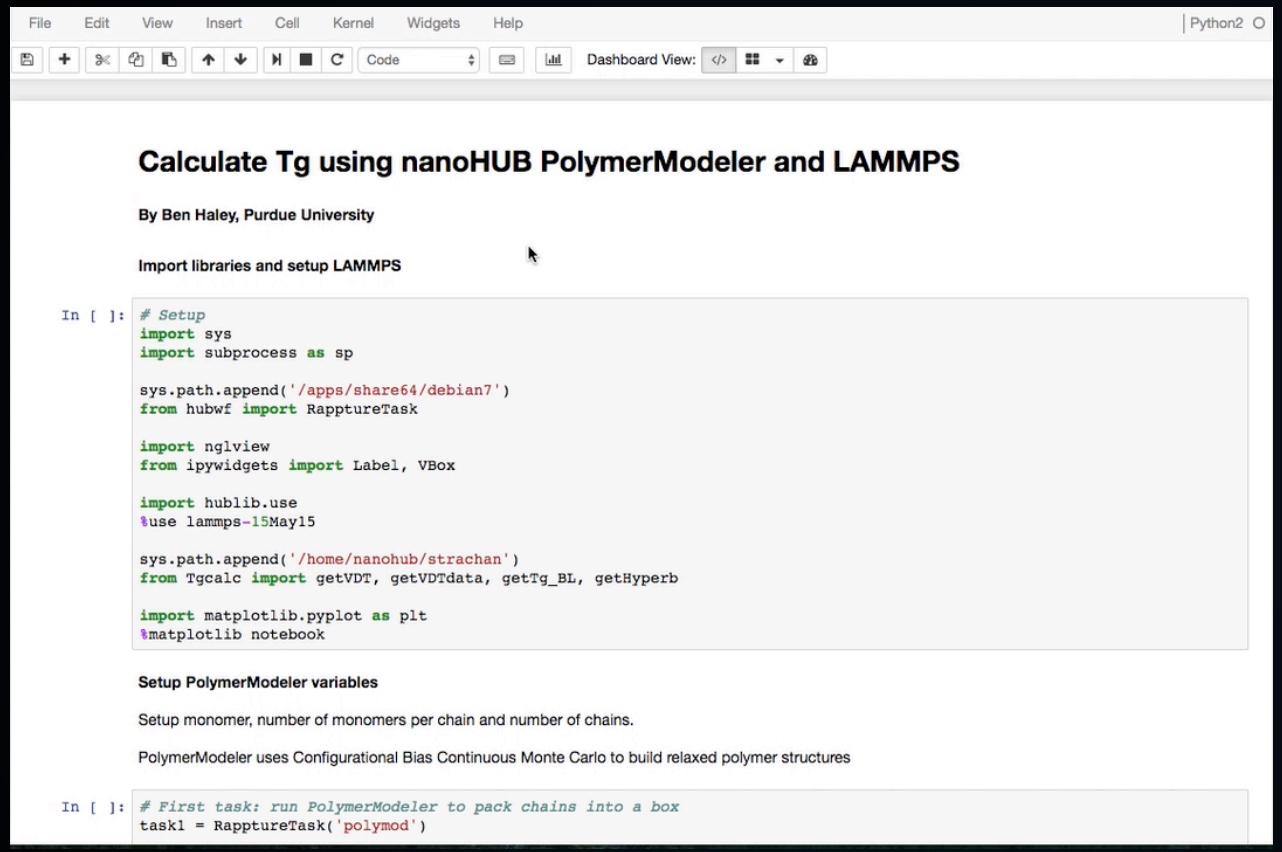
- Tool outputs stated at the outset
- Powerful visualization
- Experts can customize the simulation

Your tool … more powerful in nanoHUB

- Automatic UQ available for all Rappture tools



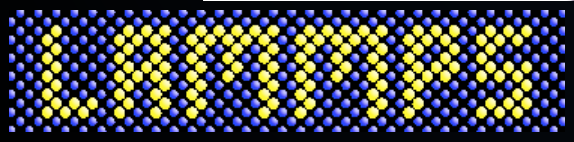
Jupyter notebooks in nanoHUB



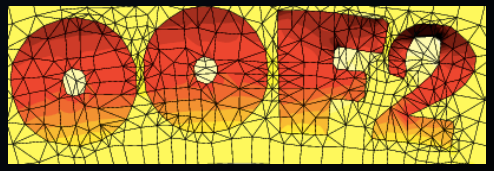
1. PolymerModeler (Rappture)
   - Amorphous builder
2. nglview
   - Visualizer
3. LAMMPS
   - Molecular dynamics

Ben Haley

NEMO5



siesta

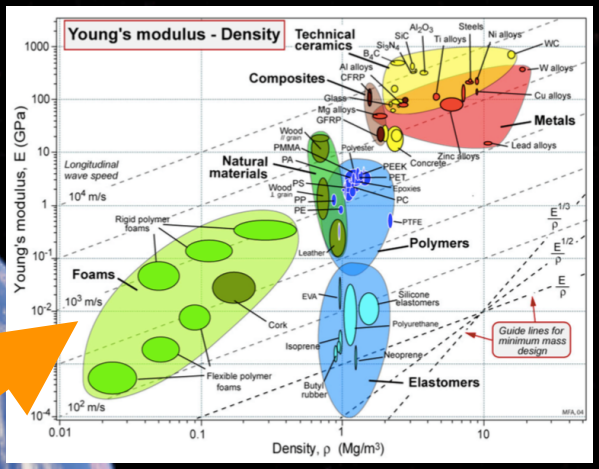


Connecting to other infrastructures

KIM

NSF Knowledge of Interatomic Models

nanoHUB



Granta MI, UK

The Materials Project

nanoHUB -KIM collaboration

Knowledge of Interatomic Models
NSF **Cyberenabled** Discovery & Innovation
Ellad Tadmor, Ryan Elliot, J. Sethna

KIM Models

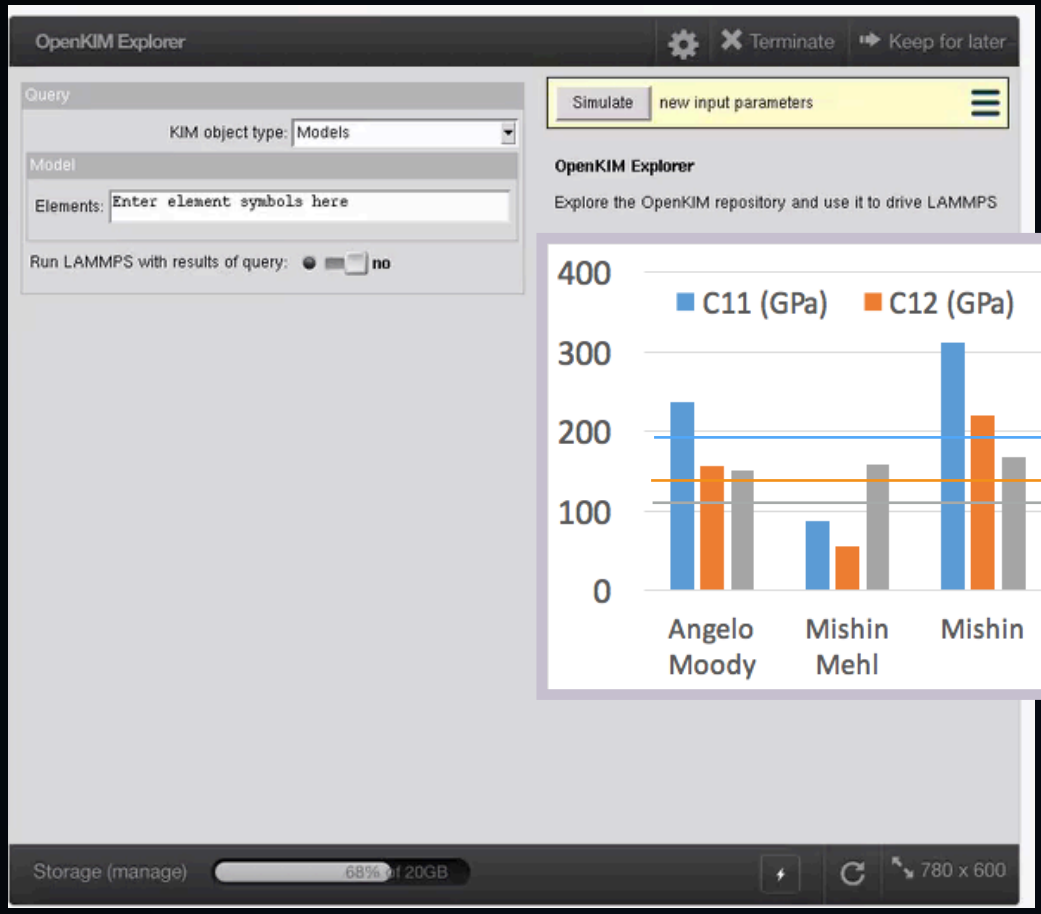
Click on an element in the periodic table for which you need an interatomic model.

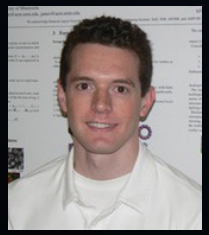
KIM Models (interatomic potentials and force fields) are software packages for describing atomic interactions that can be used with a variety of simulation codes, including LAMMPS, DL_POLY, IMD, ASE and GULP, that are compatible with the KIM API standard.

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

0 Models — 28 Models

Explore KIM potentials & run MD




Dan Karls


Ryan Elliott


Ellad Tadmor


Ben Haley


Steve Clark

KIM

Thanks

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an NCN project

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UNITED STATES AIR FORCE

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S&T

DEFENSE THREAT REDUCTION AGENCY
UNITED STATES OF AMERICA

BOEING