Purdue MSE597G
Modeling and Simulations of Materials

R. Edwin Garcia and Alejandro Strachan

Lectures on Molecular Dynamics simulations of materials

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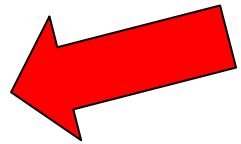
Molecular Dynamics simulations



Introduction

- What is molecular dynamics (MD)? Examples of current research
- Why molecular dynamics?

Part 1: the theory behind molecular dynamics

- Basic ideas & algorithms
- Brief introduction to the physics necessary to run & understand MD

Part 2: total energy and force calculations

- Quantum mechanical origin of atomic interactions
- Inter-atomic potentials: "averaging electrons out"

Part 3: advanced techniques, mesodynamics, verification and validation

- MD in under isothermal and isobaric conditions
- Coarse grain approaches and dynamics with implicit degrees of freedom
- Before you perform production runs

- **Tutorial to perform MD simulations using the nanoMATERIALS simulation tool at the nanoHUB**
- **Homework exercises**

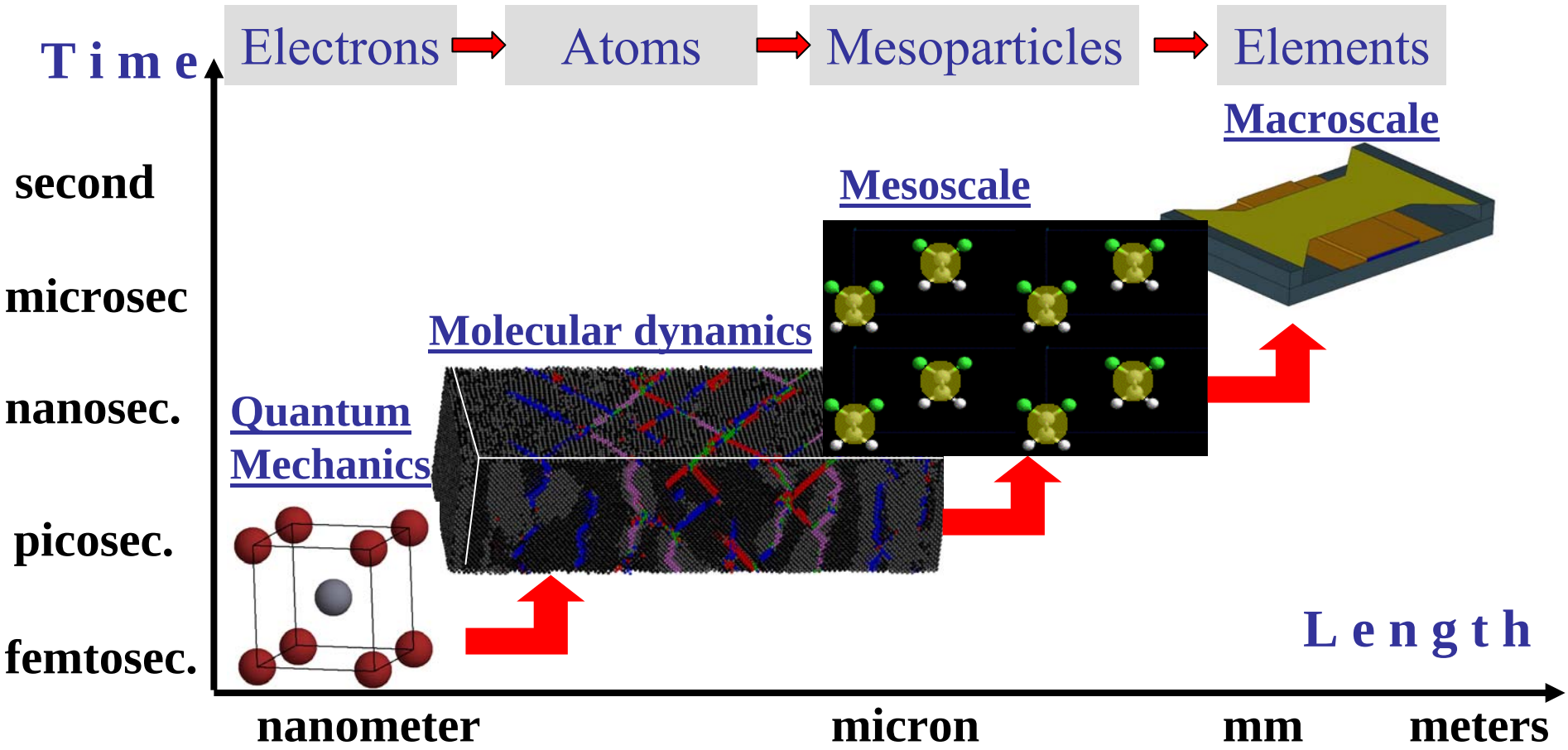
What is molecular dynamics?

Follow the dynamics (motion) of all the atoms in your material

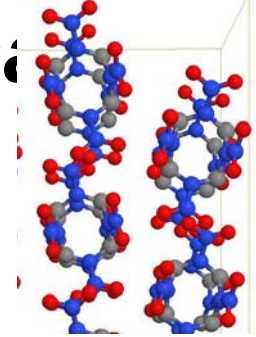
Numerically solve classical equations of motion (Newton's):

Forces on atoms come from the total potential energy:

Materials modeling and MD

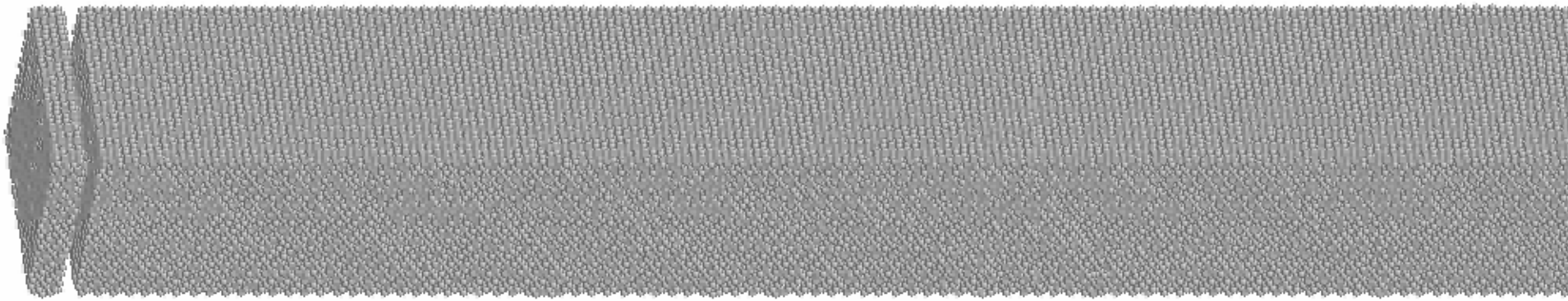


MD examples: molecular mechanisms tha govern mechanical response

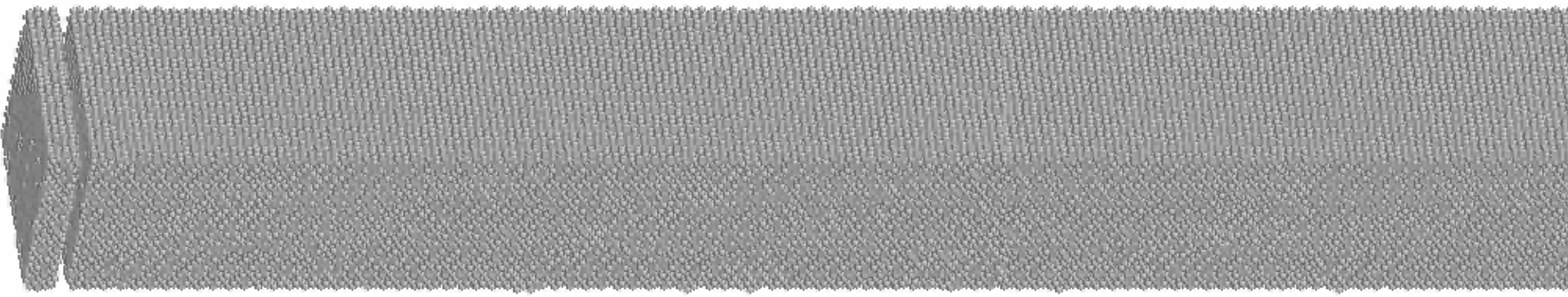


Response of HMX [cyclic $(CH_2\text{-}N\text{-}NO_2)_4$] to dynamical loading

Shock along [001] with piston velocity 0.5 km/s



Shock along [001] with piston velocity 0.75 km/s



Jaramillo, Sewell, and Strachan, Phys. Rev. B (2007)

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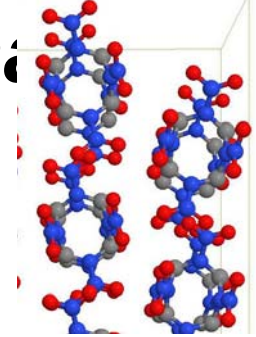

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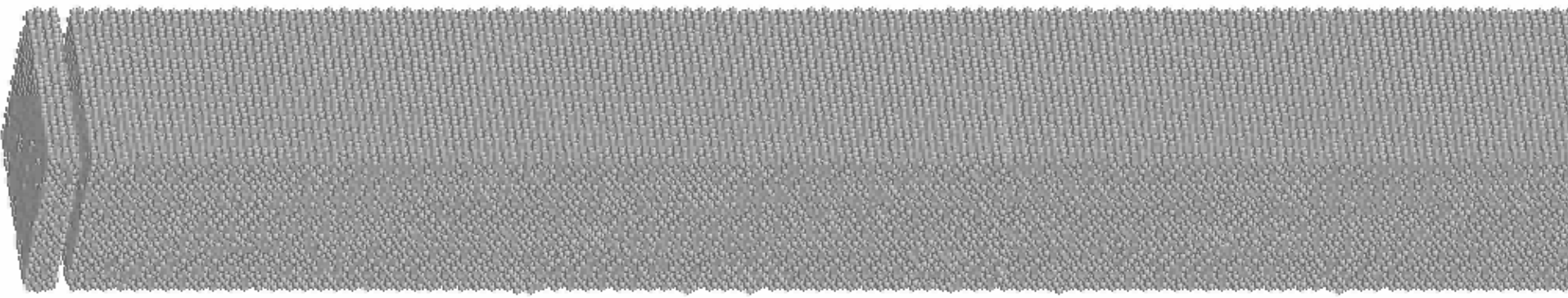

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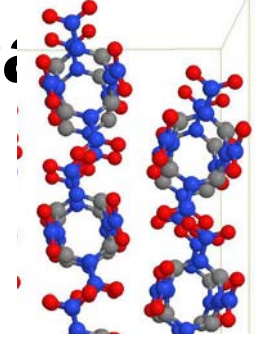

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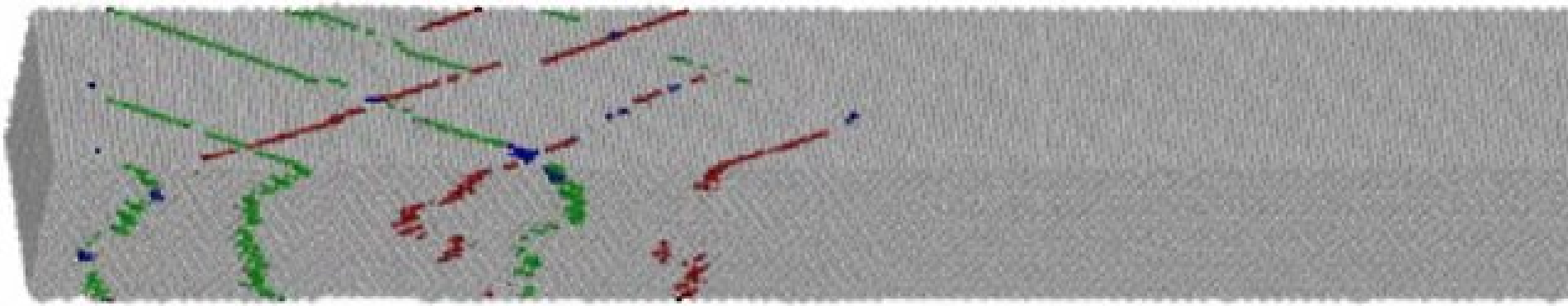

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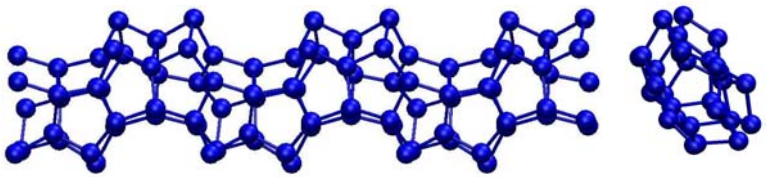
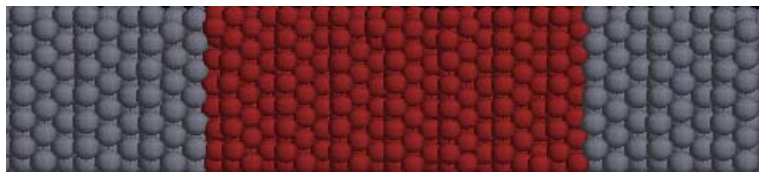
MD examples: nanoscale materials & phenomena

- **Prediction of atomic level structure, energetics and mechanical properties of Si nanotubes**



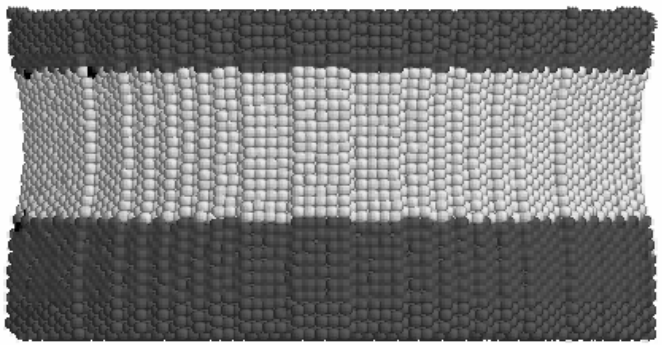
Palaria, Klimeck, and Strachan.

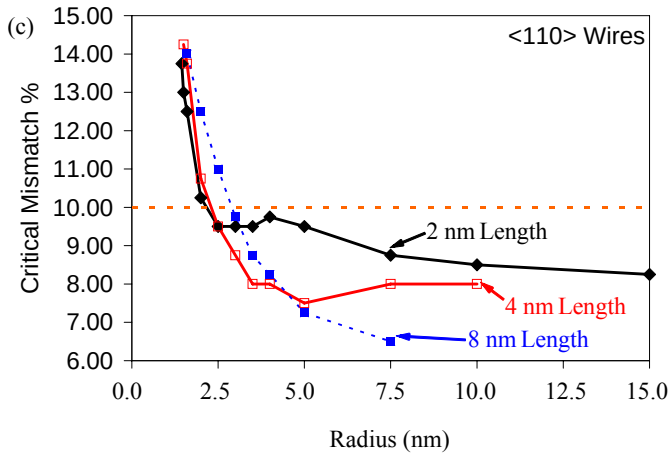
- **Size dependency of thermal transport in nano-heterostructures**

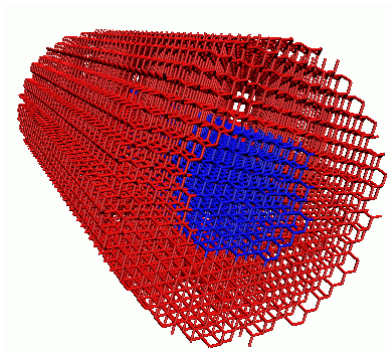


Zhou, Anglin and Strachan, J. Chem. Phys. (2007)

- **Coherency limit and relaxation mechanisms in hetero-epitaxial nanowires**







Park and Strachan

Arumbakkam, Davidson, and Strachan, Nanotechnology (2007)

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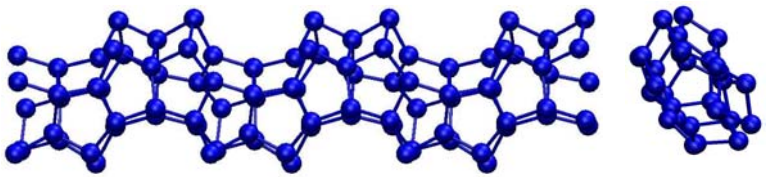

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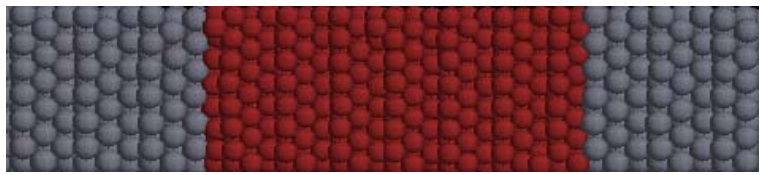

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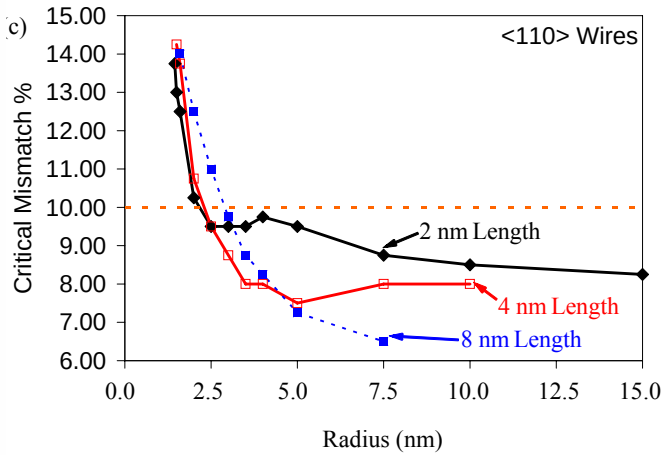
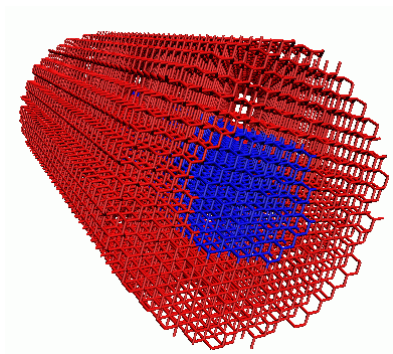




Park and Strachan

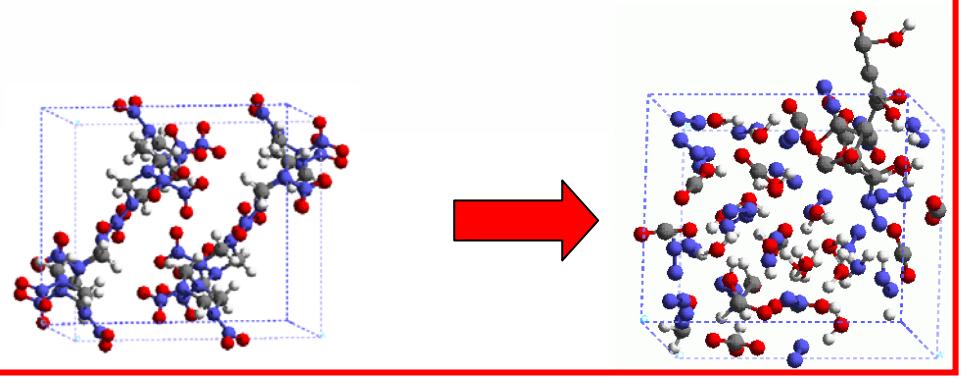
Arumbakkam, Davidson, and Strachan, Nanotechnology (2007)

MD examples: chemistry in condensed matter

Shock and thermal decomposition of high energy density materials

Phys. Rev. Lett. 91, 098301-1-4 (2003)

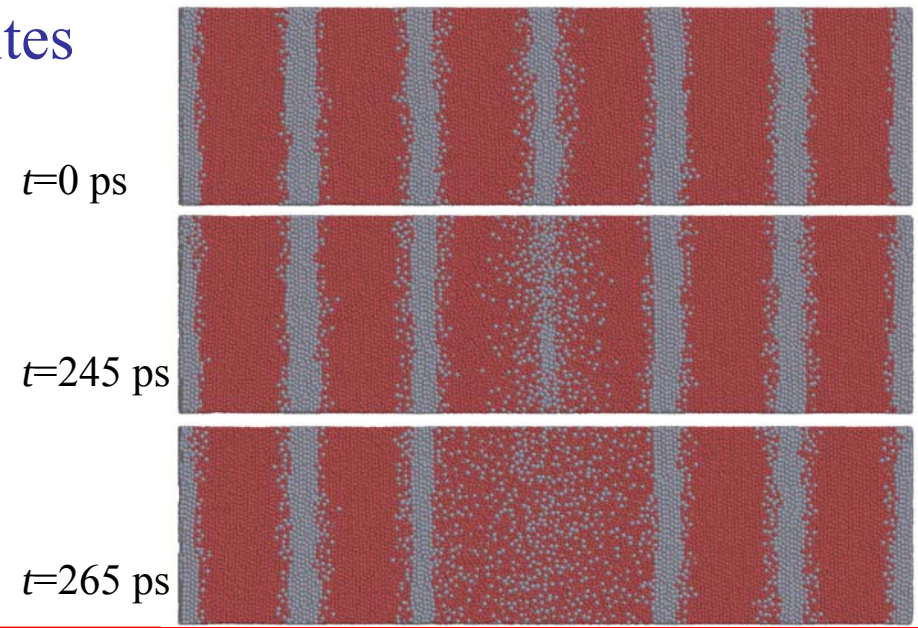
J Chem. Phys. 122, 54502-1-10 (2005)



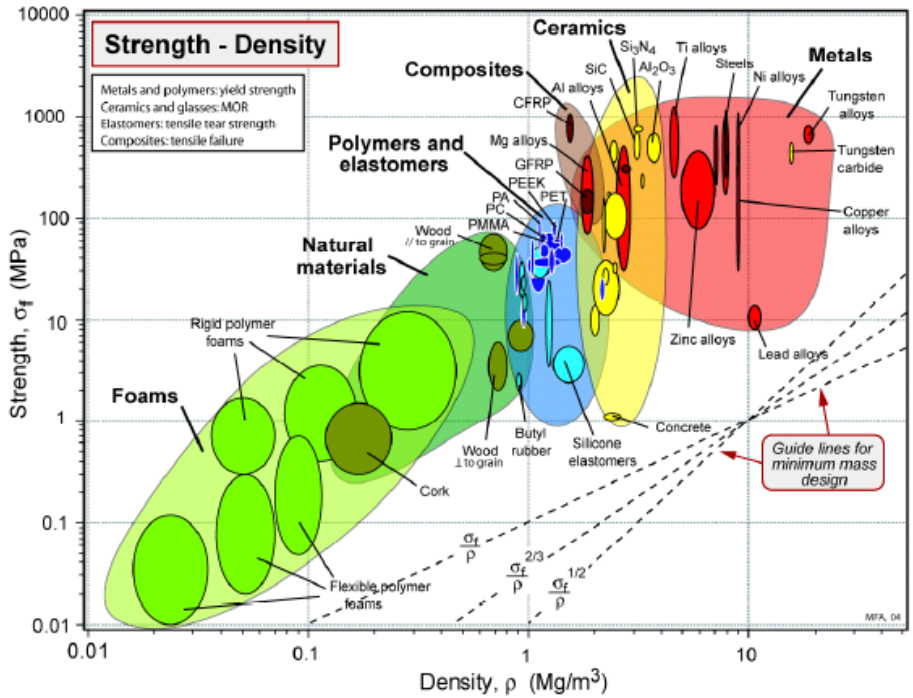
Metastable intermolecular composites

$$3Ni + Al \rightarrow Ni_3Al$$

Zhao, Germann, and Strachan, *Phys. Rev. B* **76**, 104105 (2007).
Zhao, Germann, and Strachan, *J. Chem. Phys.* **125**, 164707-1-8 (2006).



Why molecular dynamics?



Materials Selection in Mechanical Design (3rd edition)
by MF Ashby, Butterworth Heinemann, 2005

- Difference in bonding alone can not explain the enormous range in observed values for materials properties
- Atomic structure and microstructure (defects, interfaces, etc.) play a key role