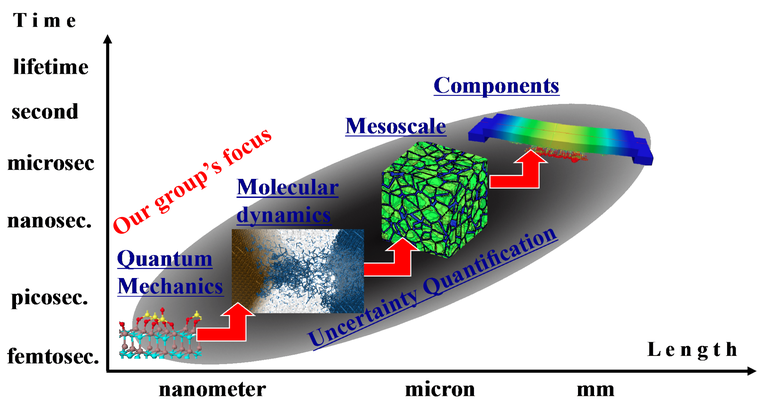
RESEARCH HIGHLIGHTS

PURDUE MATERIALS ENGINEERING

Predictive modeling of materials

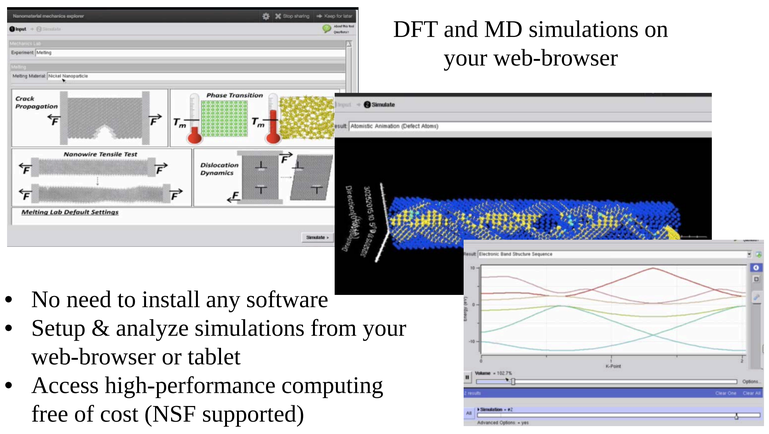
Research highlights of the Strachan Group

Overview



- Uncover and characterize the molecular-level mechanisms that govern materials
- Contribute to the design and certification of materials
- Quantify uncertainties and confidence in the predictions for decision-making

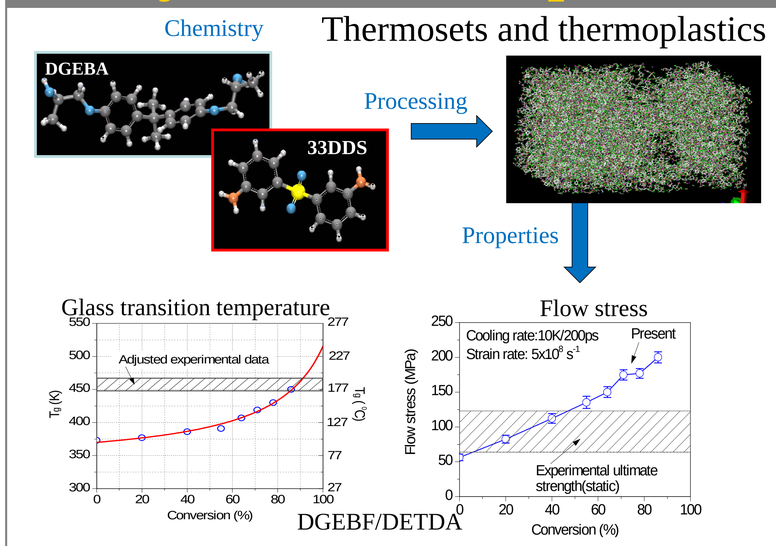
Online simulation tools in NSF's nanoHUB



DFT and MD simulations on your web-browser

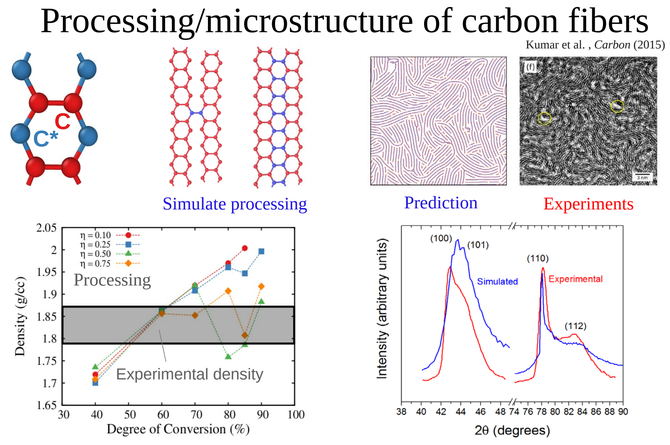
- No need to install any software
- Setup & analyze simulations from your web-browser or tablet
- Access high-performance computing free of cost (NSF supported)

Polymers & composites



- *Li, Medvedev, Lee, Kim, Caruthers, & Strachan, Polymer, 53, 4222-4230 (2012).*
- *Li & Strachan Polymer 97, 456-464 (2016).*

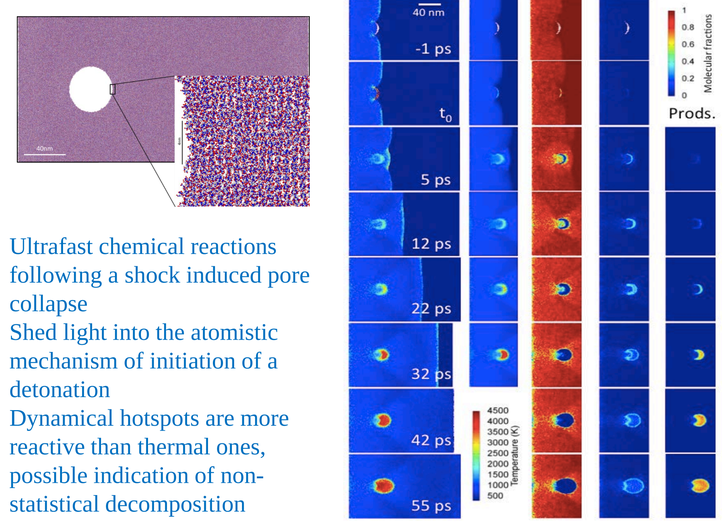
Processing/microstructure of carbon fibers



- Algorithm predicts transverse microstructure and resulting properties
- Atomic-scale insight into microstructure evolution and transverse modulus

Materials at extreme conditions

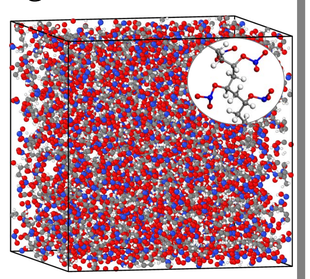
Shock to deflagration transition in high energy density materials



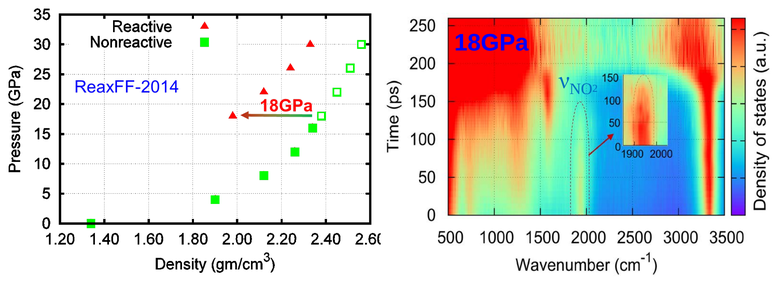
- Ultrafast chemical reactions following a shock induced pore collapse
- Shed light into the atomistic mechanism of initiation of a detonation
- Dynamical hotspots are more reactive than thermal ones, possible indication of non-statistical decomposition

Wood, Cherukara, Kober, & Strachan. J. Phys. Chem. C, 119, 22008-22015 (2015).

Decomposition and reaction of Polyvinyl Nitrate under shock and thermal loading



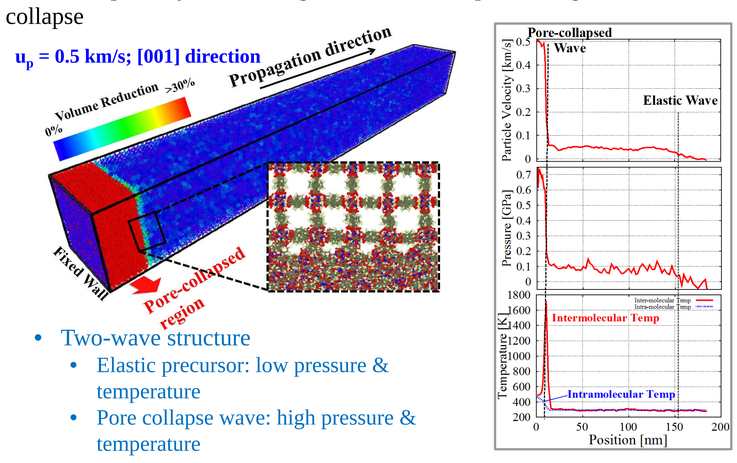
- Simulations capture the transition from the unreactive to reactive Hugoniots
- Disappearance of the NO_2 peaks is indicative to the rapid chemical reactions
- One-on-one matching between the simulation and experiment for both threshold shock strength required associated time scales for the decomposition reactions



Islam & Strachan. J. Phys. Chem. C 121.40 (2017): 22452-22464.

Shockwave attenuation for protection

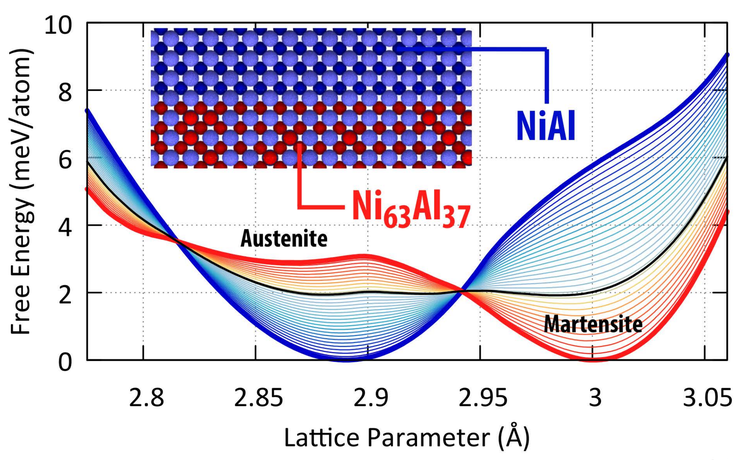
Endothermic, volume-collapsing reactions reduce pressure behind shock
Nanoscale porosity in metal organic frameworks provide significant volume collapse



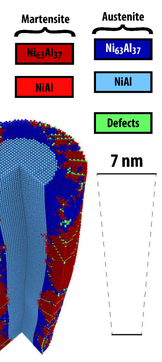
- Two-wave structure
  - Elastic precursor: low pressure & temperature
  - Pore collapse wave: high pressure & temperature

K Banlusan, and A Strachan, J. Chem. Phys. 146 , 184705 (2017)
K. Banlusan and A. Strachan, J. Phys. Chem. C, 120 12463–12471 (2016).

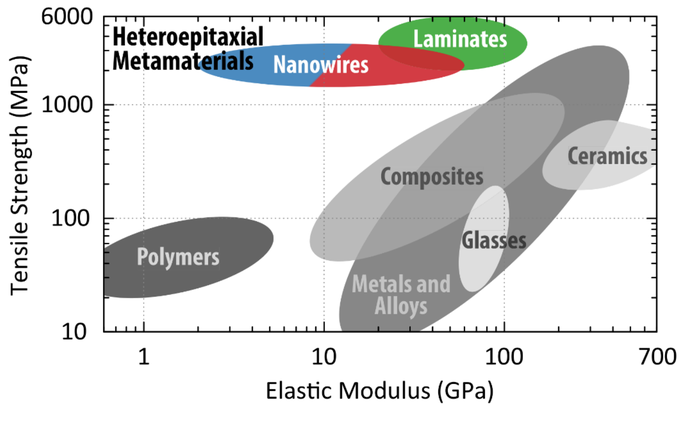
Design of ultra-low stiffness metals



- Free energy landscape engineering: epitaxial combination of a martensitic alloy with a non-martensitic component to enable new properties including ultra-low stiffness



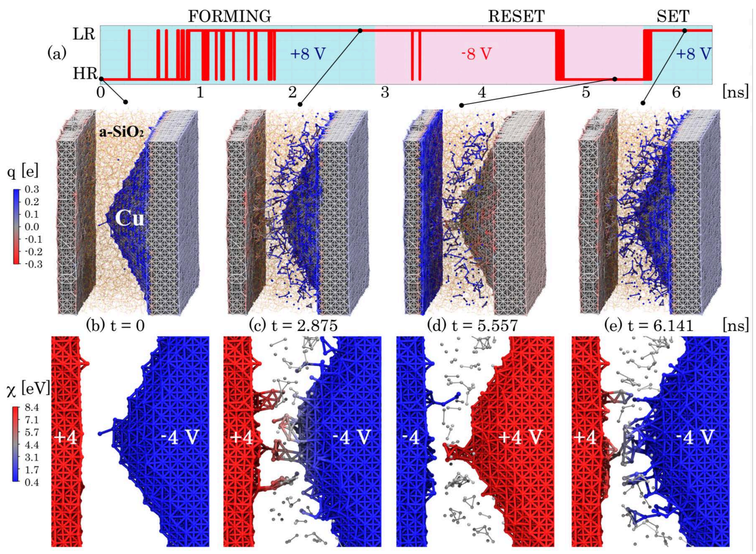
- Lowest stiffness metamaterial nanowire shows coexistence of austenite and martensite, with a wide range of stable lattice parameters due to the engineered free energy landscape



Reeve, Belessiotis-Richards, & Strachan. Nature Commun. 8, 1137 (2017).

Materials for electronic applications

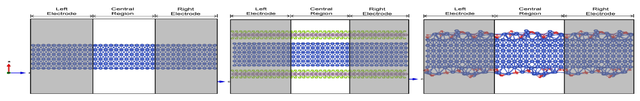
Novel memory devices: resistance switching



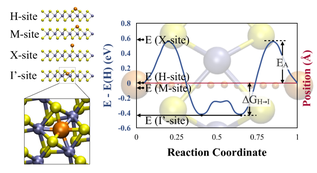
- Modeling the operation of an electrochemical electro-metallization cell
- Uncover mechanisms behind ultra-fast switching

Onofrio, Guzman, and Strachan, Nanoscale, 8, 14037-14047 (2016).
Onofrio, Guzman, and Strachan. Nature Mater. 14, 440–446 (2015).

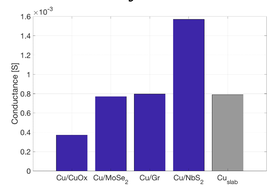
Two dimensional materials

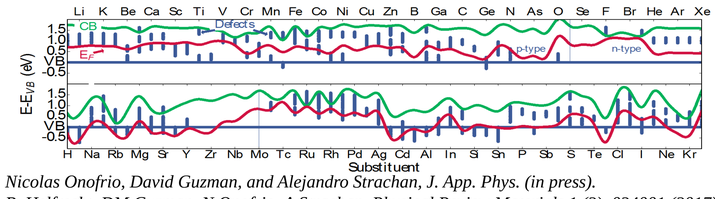


High-throughput study of doping



Cu/2D material hybrid interconnects





Nicolas Onofrio, David Guzman, and Alejandro Strachan, J. App. Phys. (in press).
B. Helfrecht, DM Guzman, N Onofrio, A Strachan, Physical Review Materials 1 (3), 034001 (2017).

Group and sponsors

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Postdocs and senior researchers: Chunyu Li, Benjamin Haley, Md Mahbubul Islam, Karthik Guda

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