SAND2020-3671PE

Computational Disordered Materials

Dr. Thomas J. Hardin

President Harry S. Truman Fellowship in National Security Science and Engineering

tjhardi@sandia.gov

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

My Background

2006-2011

Bachelor of Science:
Mechanical Engineering
Mathematics

National Merit Scholar

Brent L. Adams

2011-2012

Master of Science:
Mechanical Engineering

NASA
Space Technology
Research Fellow

Eric R. Homer

2012-2018

Doctor of Philosophy:
Materials Science
and Engineering

National Defense Science
& Engineering Graduate
Fellow

Christopher A. Schuh

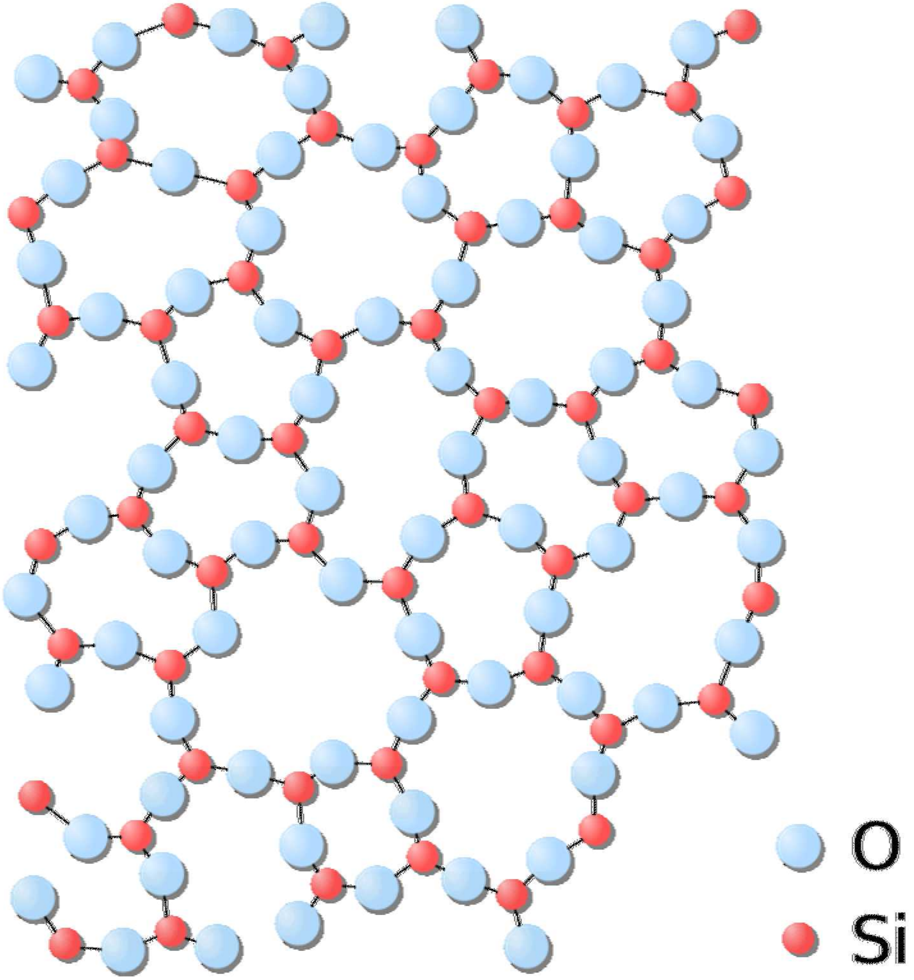
2019-Present

President Harry S.
Truman Fellowship in
National Security Science
and Engineering

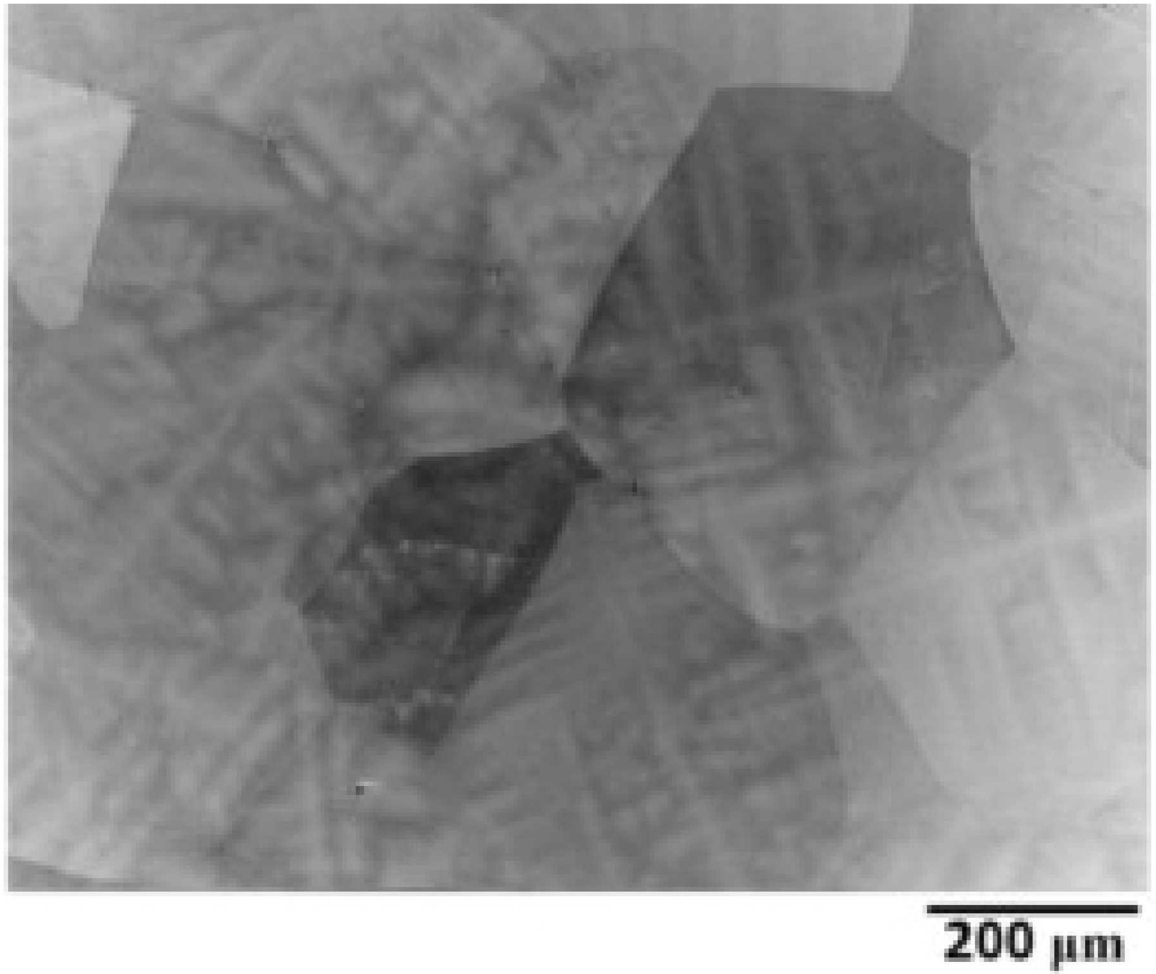
PI on $780k LDRD

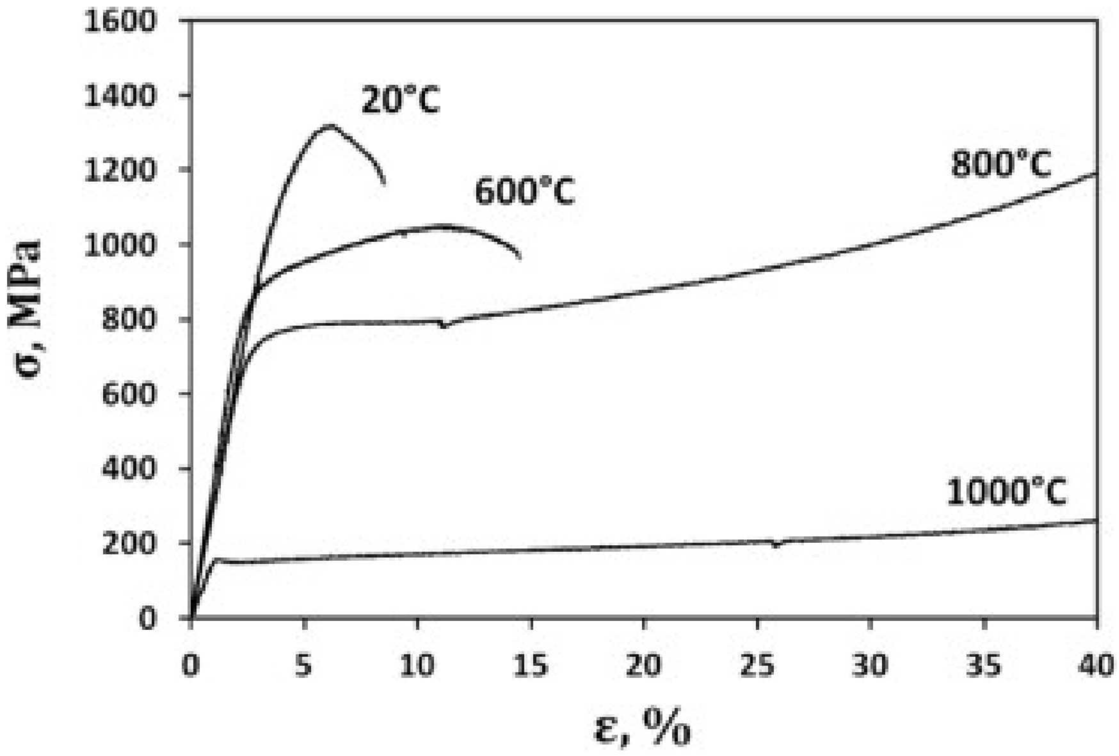
Disordered Materials for Energy

Disordered Materials for Energy: Silicate Glass



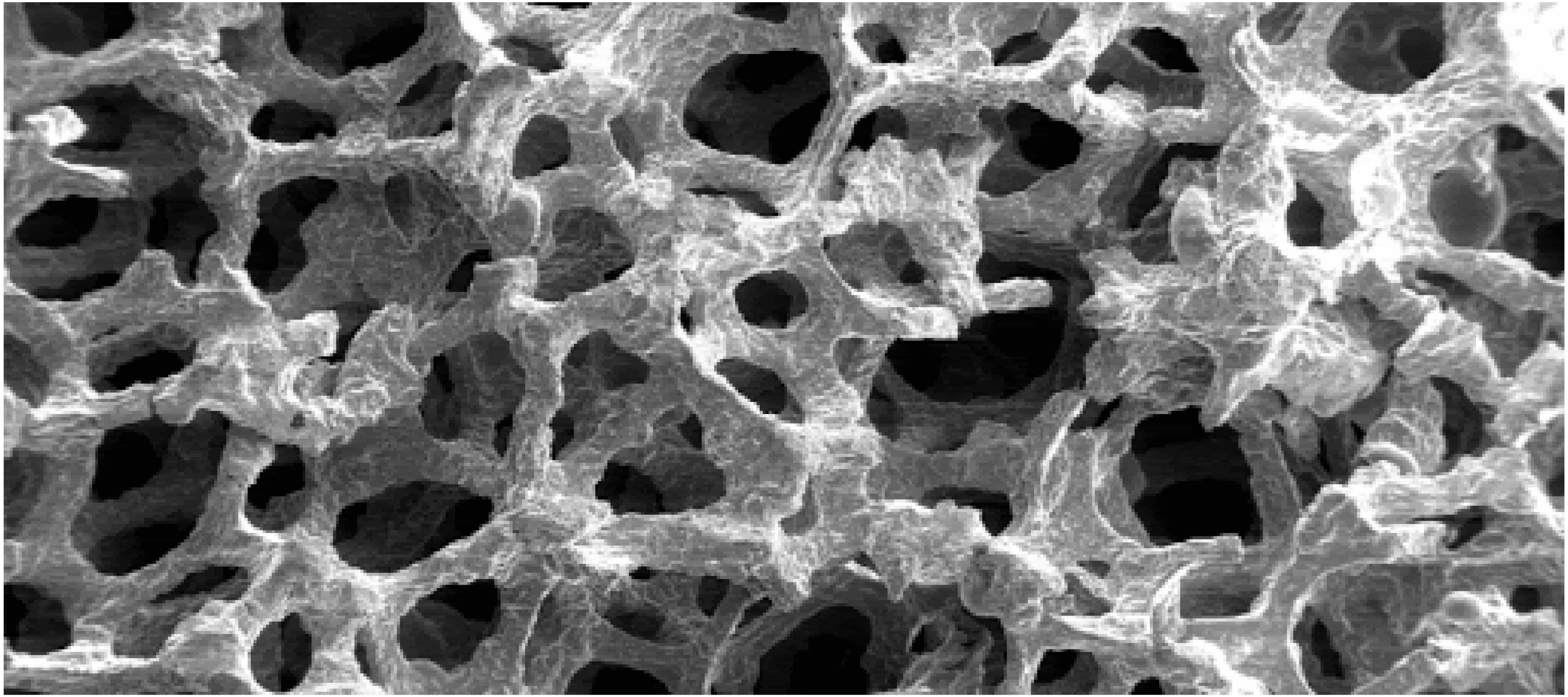
Disordered Materials for Energy: High Entropy Alloys





Stepanov, N. D., et al. "Structure and mechanical properties of a light-weight AlNbTiV high entropy alloy." *Materials Letters* 142 (2015): 153-155.

Disordered Materials for Energy: Metallic Glass



Li, Jinyang, et al. "Recent advances in metallic glass nanostructures: synthesis strategies and electrocatalytic applications." *Advanced materials* 31.7 (2019): 1802120.
http://www.yalescientific.org/2016/03/will-cars-run-on-hydrogen-bulk-metallic-glasses-make-electrocatalysts-cheaper-and-more-efficient/

Disordered Materials for Energy: Borosilicate Glass

United States Patent [19]

Chickering et al.

[54] **NUCLEAR WASTE ENCAPSULATION IN BOROSILICATE GLASS BY CHEMICAL POLYMERIZATION**

[75] Inventors: **Ronald W. Chickering,** Hempfield Township, Westmoreland County; **Bulent E. Yoldas,** Churchill; **Bruce H. Neuman,** Salem Township, Westmoreland County, all of Pa.

[73] Assignee: **Westinghouse Electric Corp.,** Pittsburgh, Pa.

https://phys.org/news/2016-11-radioactive-immobilized-glass-millions-years.html

Disordered Materials for Energy: Borosilicate Glass

In this 2019 photo, a sign at the Hanford Nuclear Reservation is posted near Richland. (AP Photo/Elaine Thompson, file)

Hanford nuclear waste cleanup efforts could be delayed

A new report does not mention the Dept. of Energy moving radioactive capsules to safer storage.

Wednesday, March 11, 2020 9:04am NORTHWEST

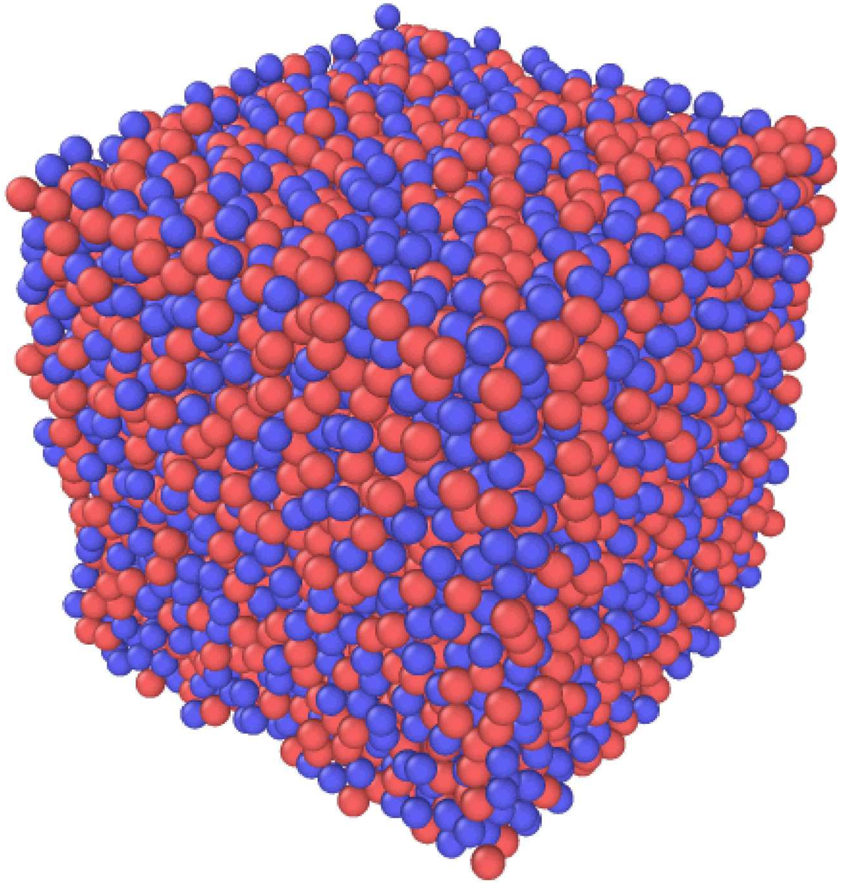
Wednesday, March 11, 2020 9:04am

https://www.heraldnet.com/northwest/hanford-nuclear-waste-cleanup-efforts-could-be-delayed/

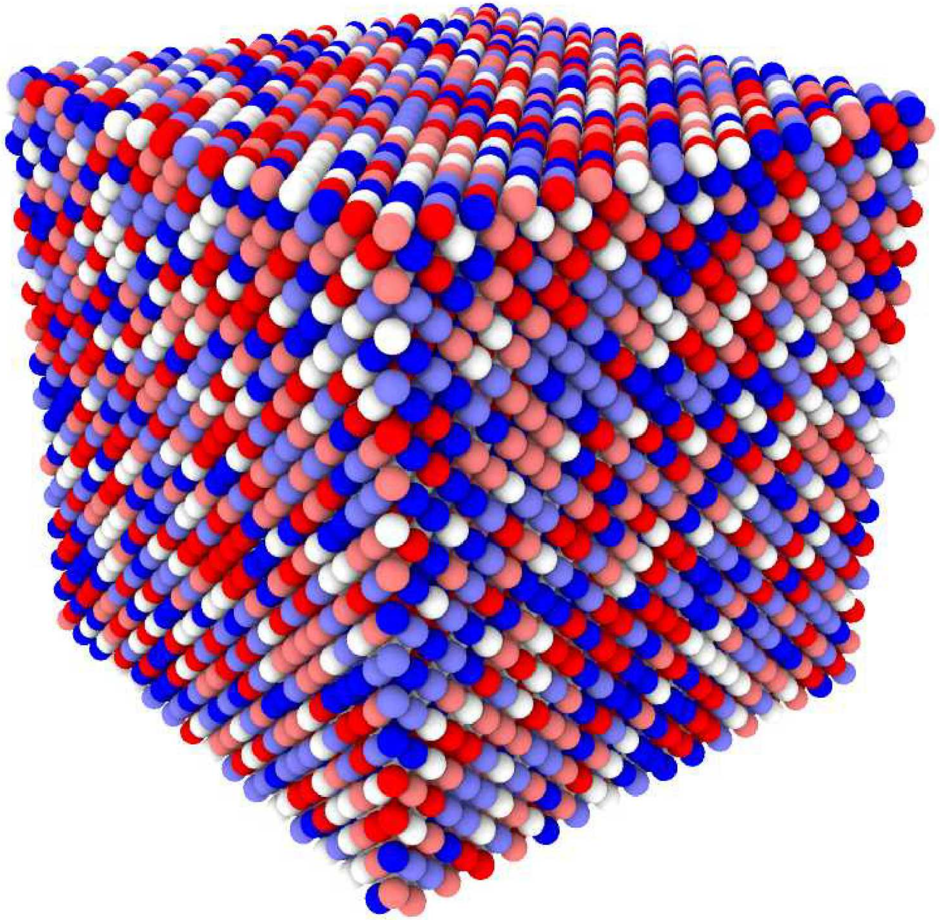
Disordered Materials for Energy

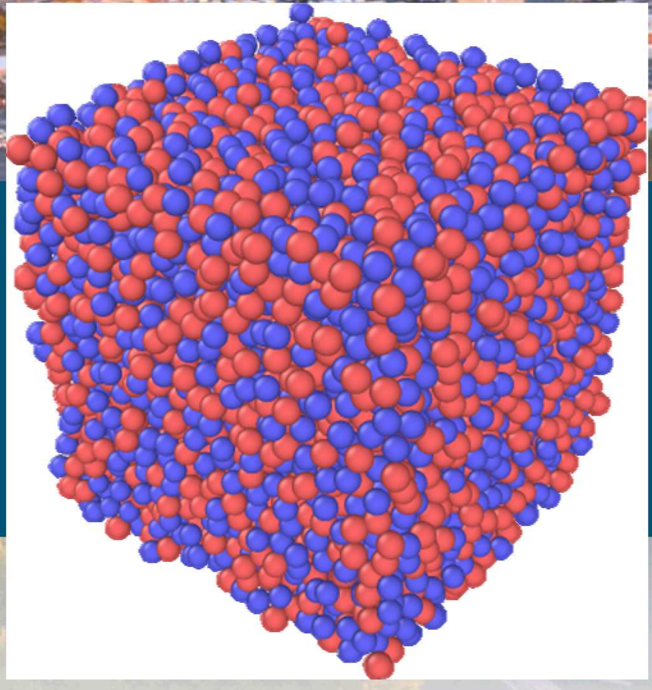
Two Case Studies

Bulk Metallic Glass



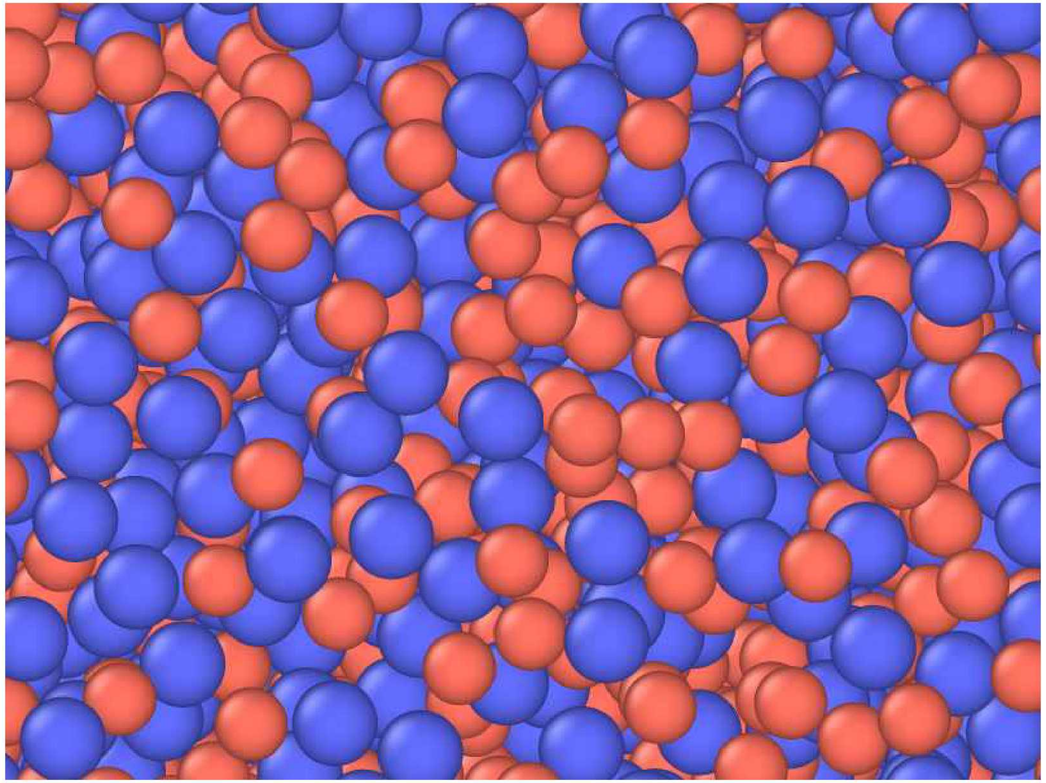
High Entropy Alloys

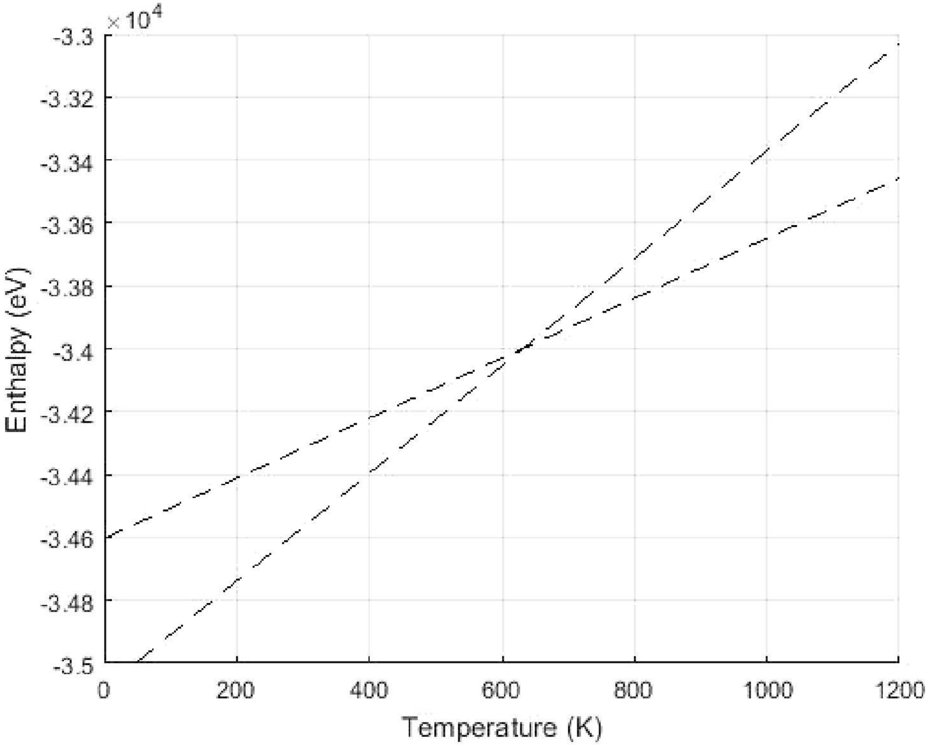




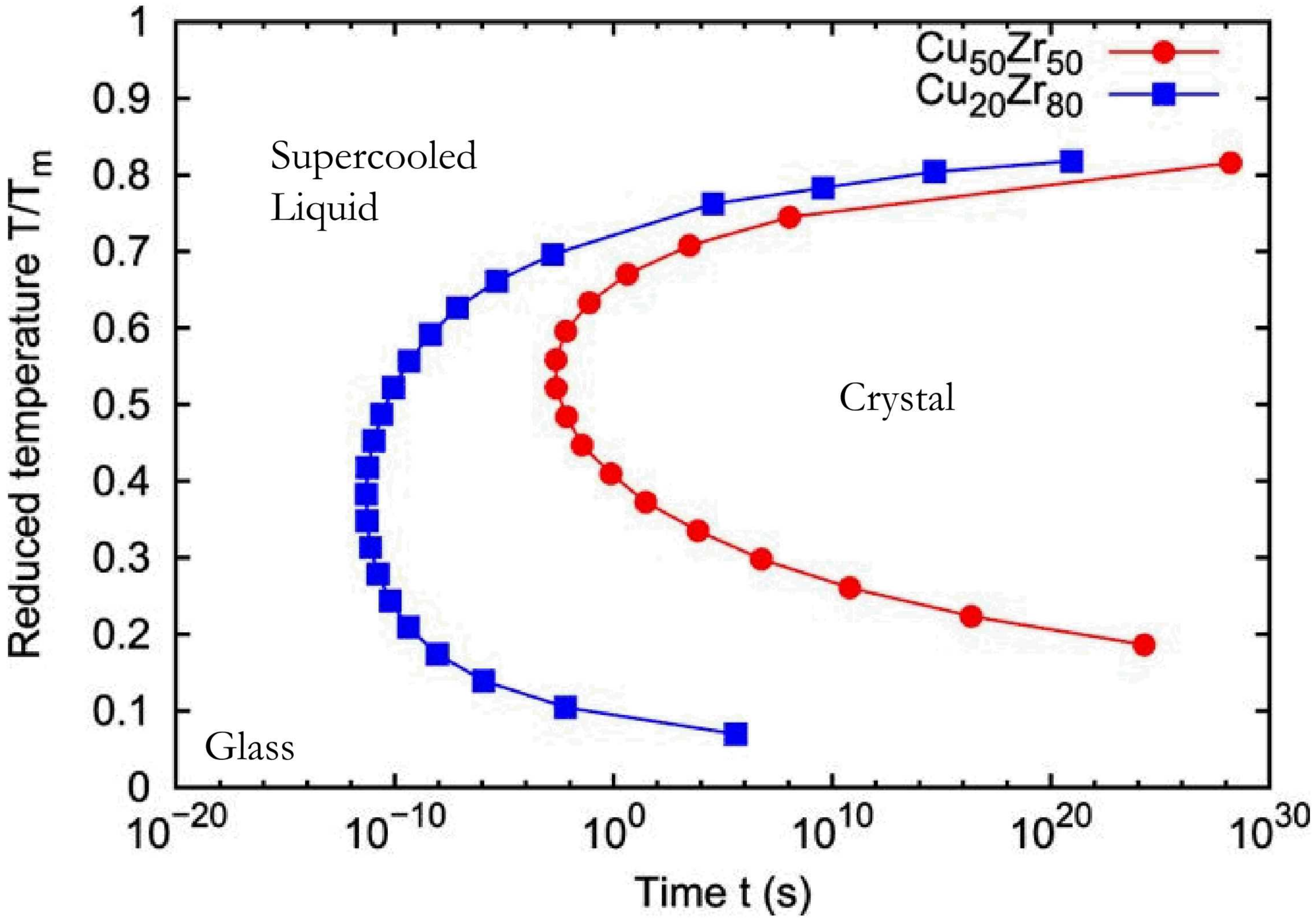
Bulk Metallic Glass

The Glassy State



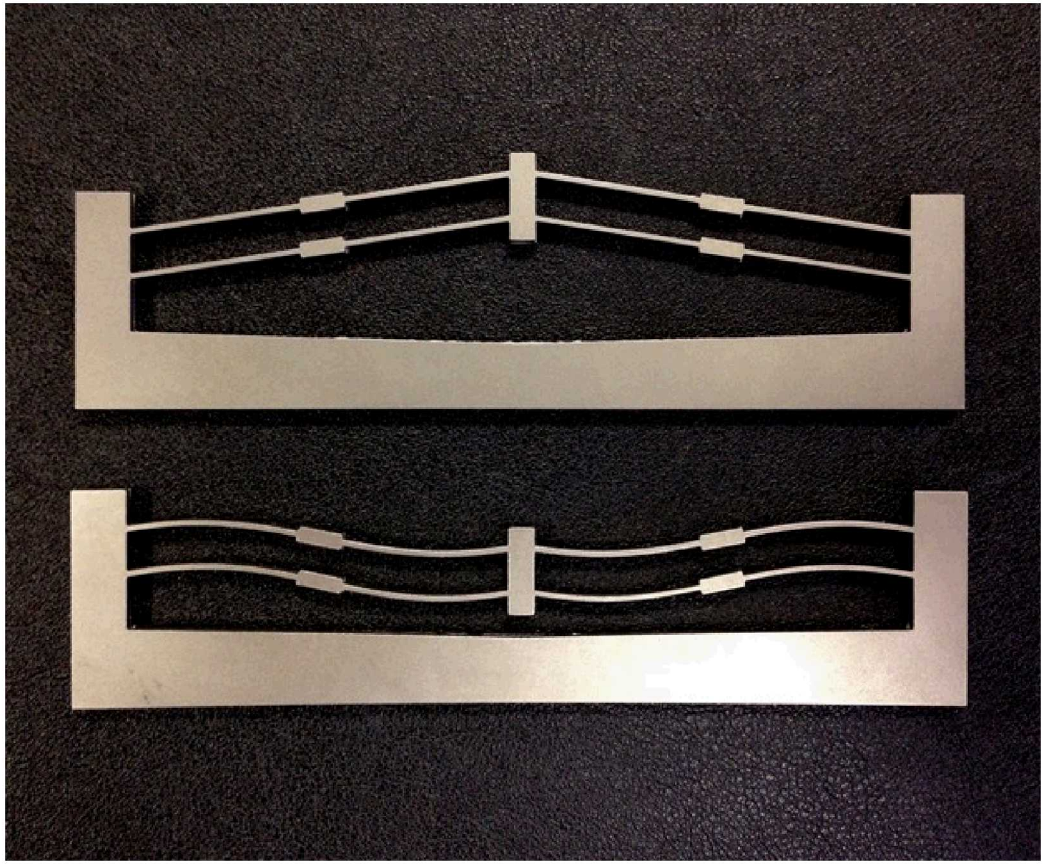


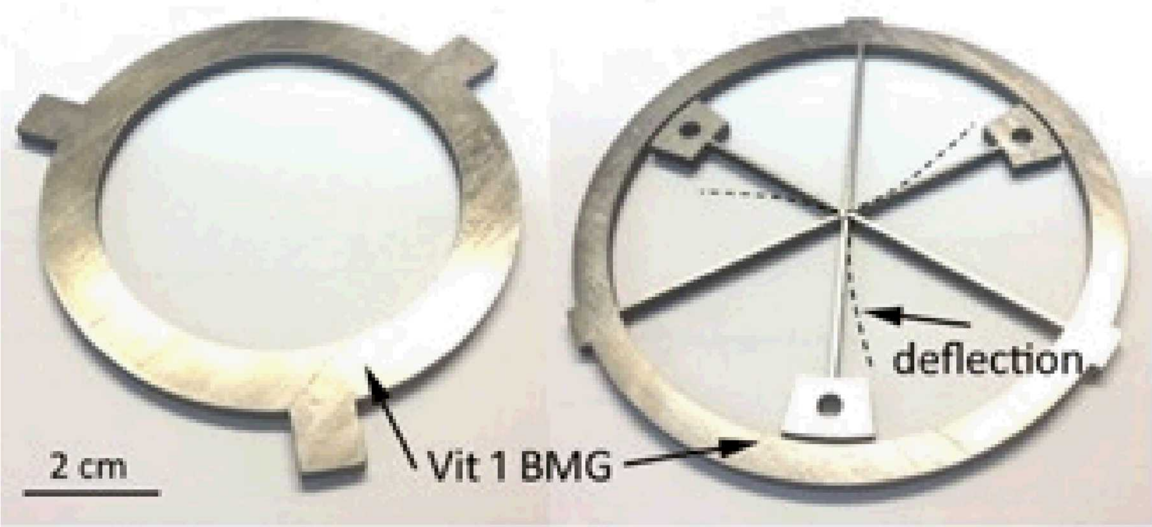
Downside to Bulk Metallic Glass



Sato, Yuji, et al. "Predictive modeling of Time-Temperature-Transformation diagram of metallic glasses based on atomistically-informed classical nucleation theory." *Scientific reports* 7.1 (2017): 1-9.

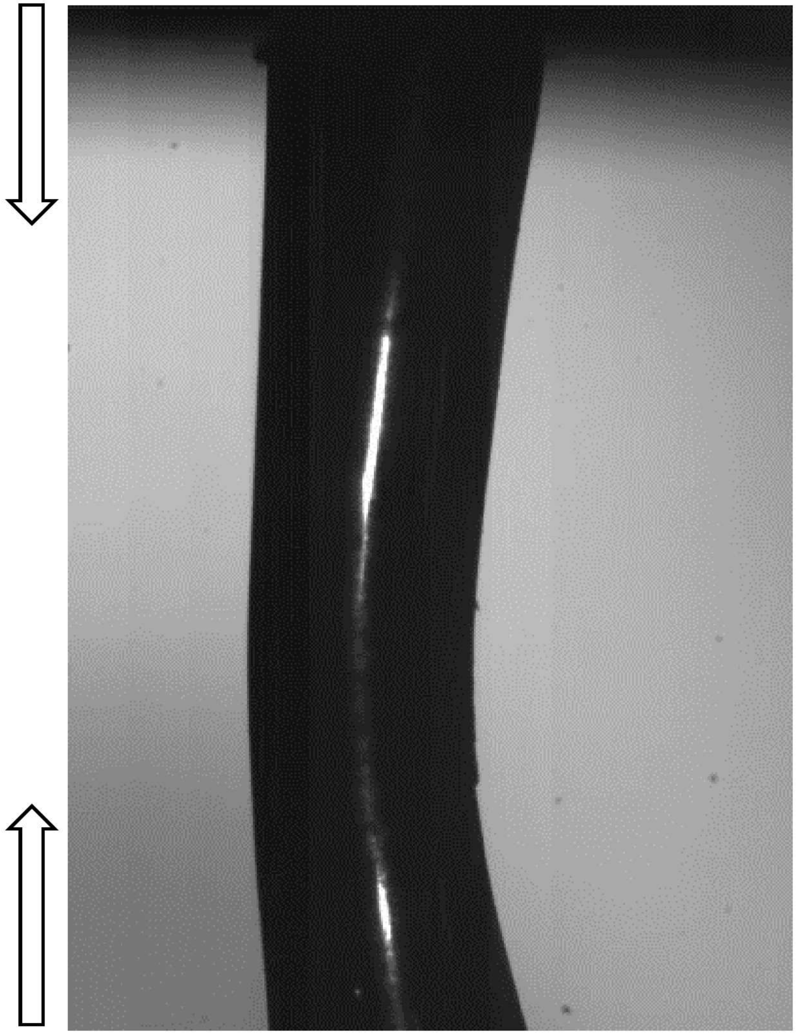
Bulk Metallic Glass for Compliant Mechanisms

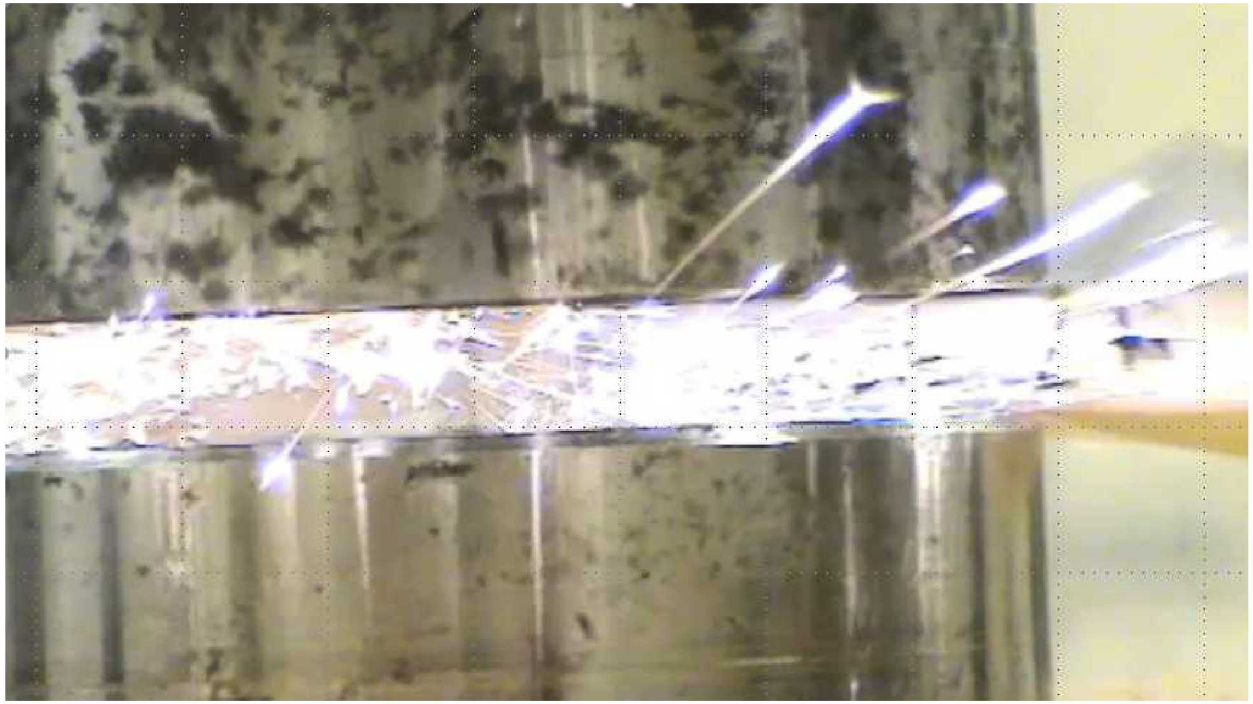




Homer, Eric R., et al. "New methods for developing and manufacturing compliant mechanisms utilizing bulk metallic glass." Advanced Engineering Materials 16.7 (2014): 850-856.

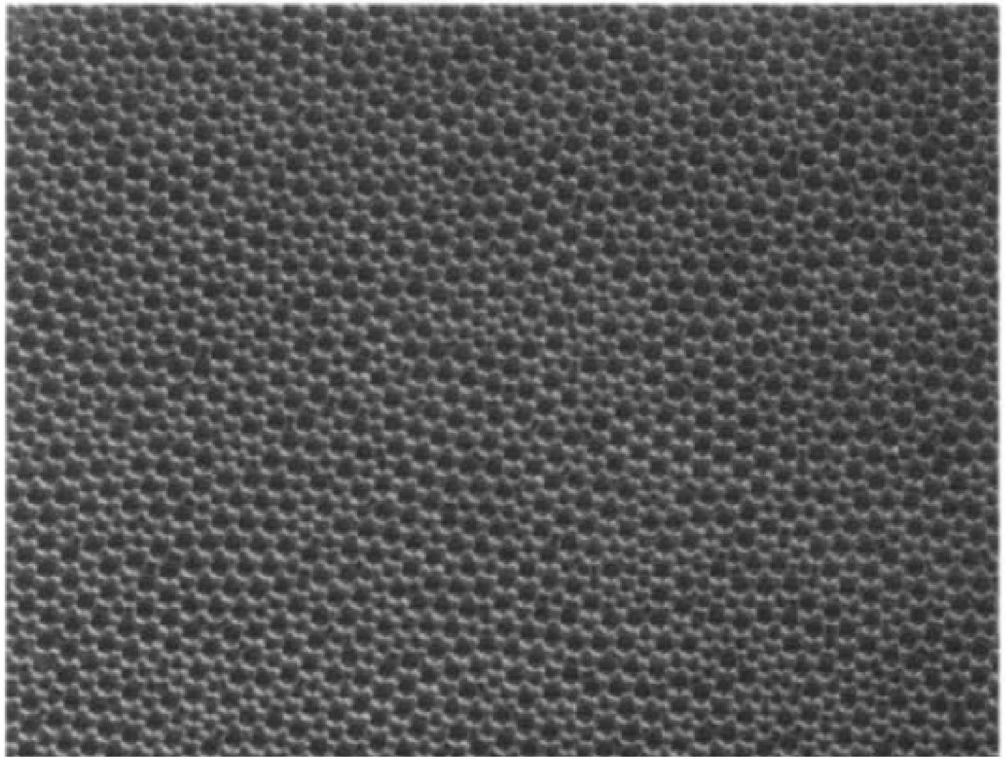
Downside to Bulk Metallic Glass

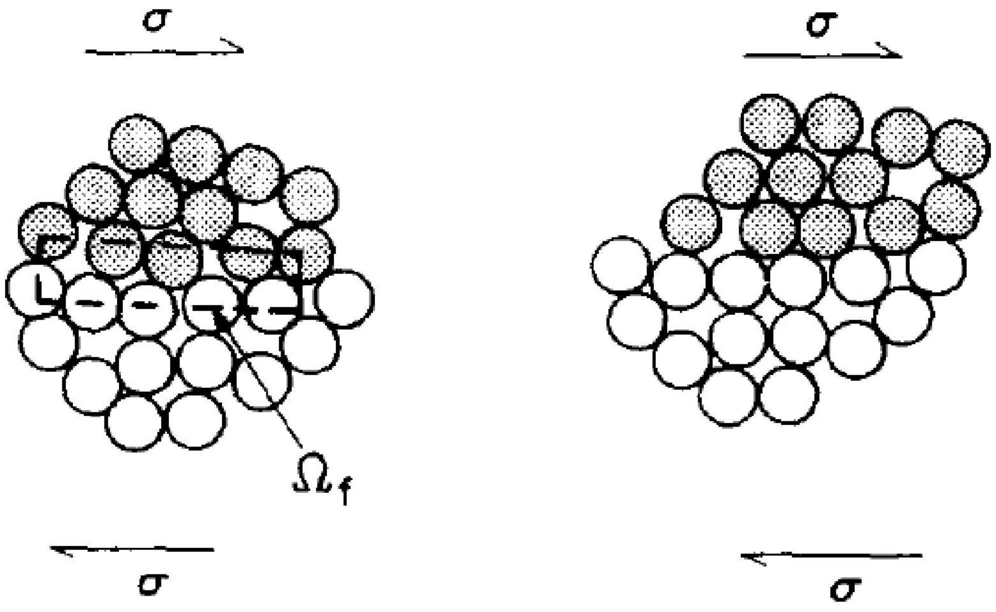




Unpublished – Courtesy of Prof. Eric Homer.

Glassy Structure on Two Scales

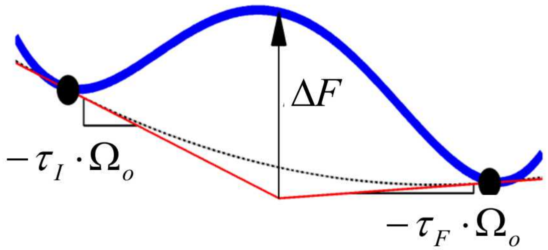




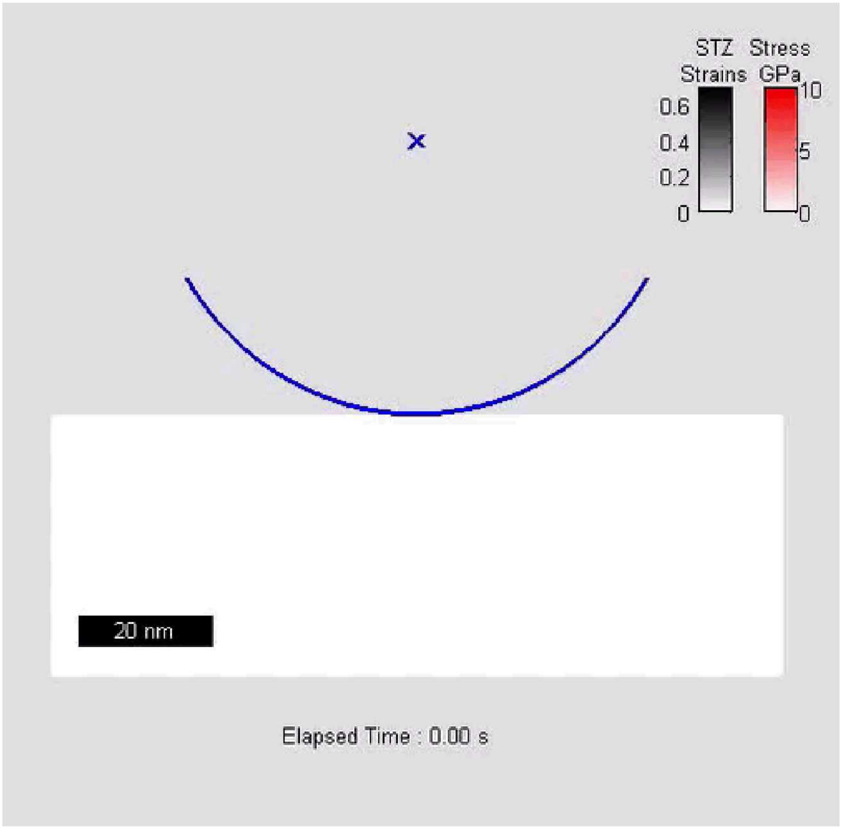
Argon, A. S., and H. Y. Kuo. *Materials science and Engineering* 39.1 (1979): 101-109.

STZ Dynamics

1. Load applied to finite element model, calculate stress.
2. Each element/node is a potential shear transformation zone. Calculate stress-biased activation rate for each potential STZ.

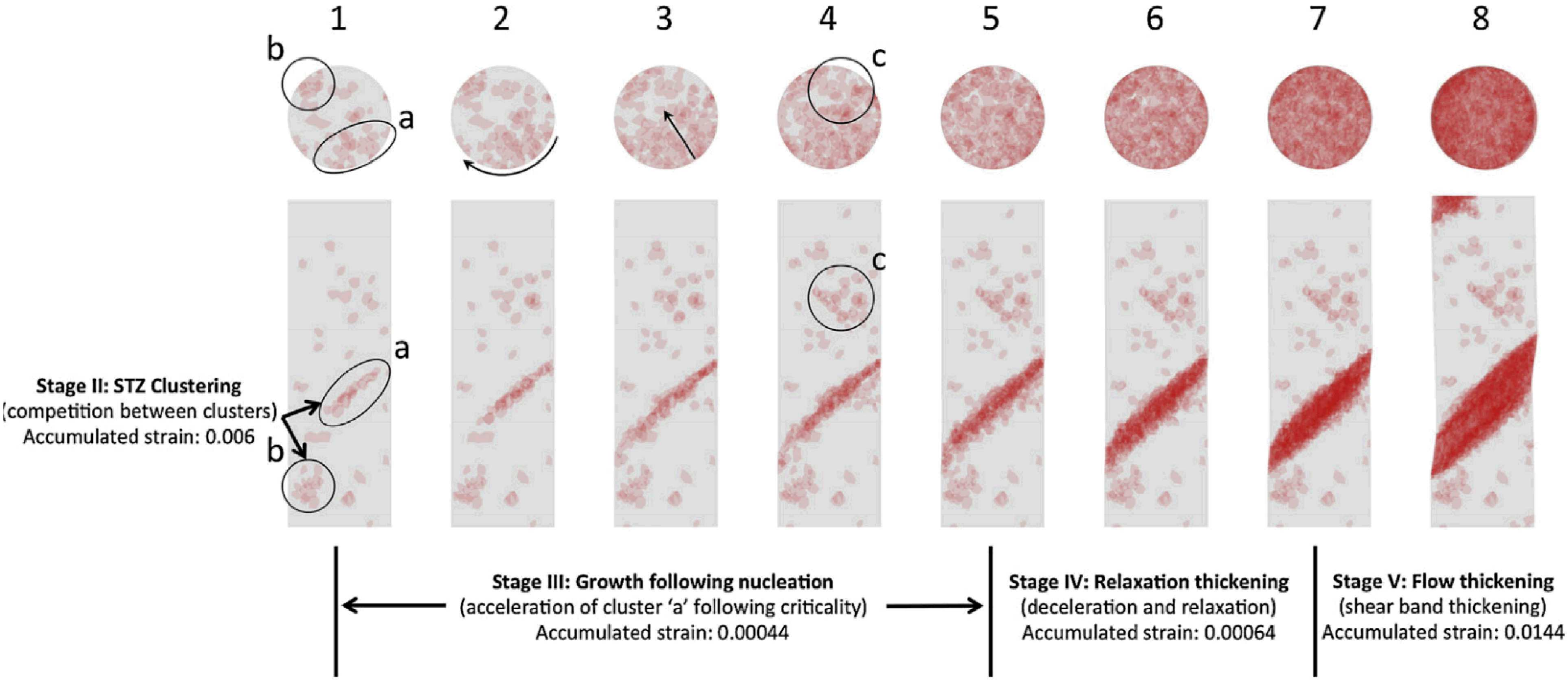


3. Select one shear transformation and a time step via kinetic Monte Carlo.
4. Apply local plastic shear strain to finite element mesh. Return to 1.



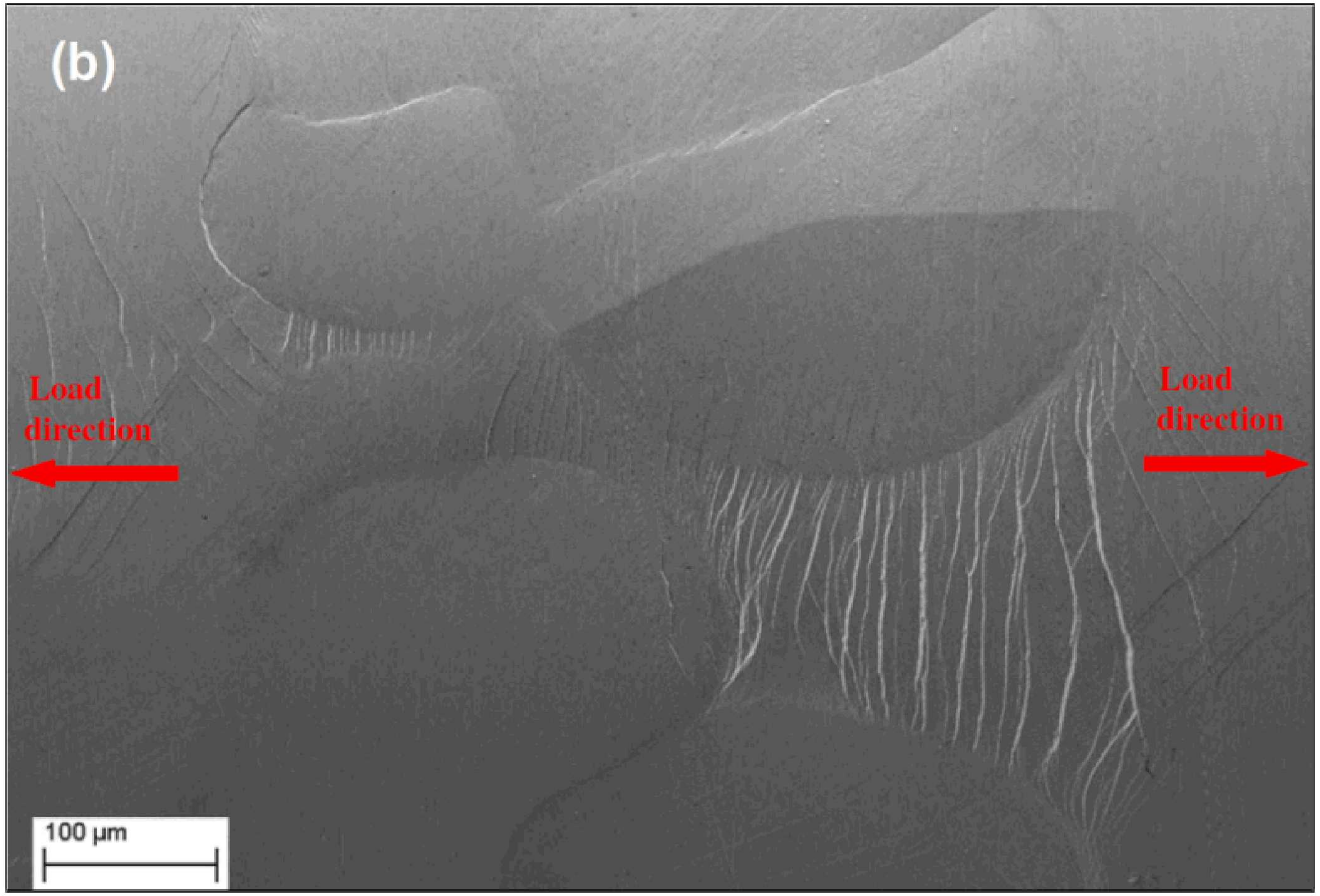
Packard, C. E., et al. "Cyclic hardening of metallic glasses under Hertzian contacts: Experiments and STZ dynamics simulations." *Philosophical Magazine* 90.10 (2010): 1373-1390.

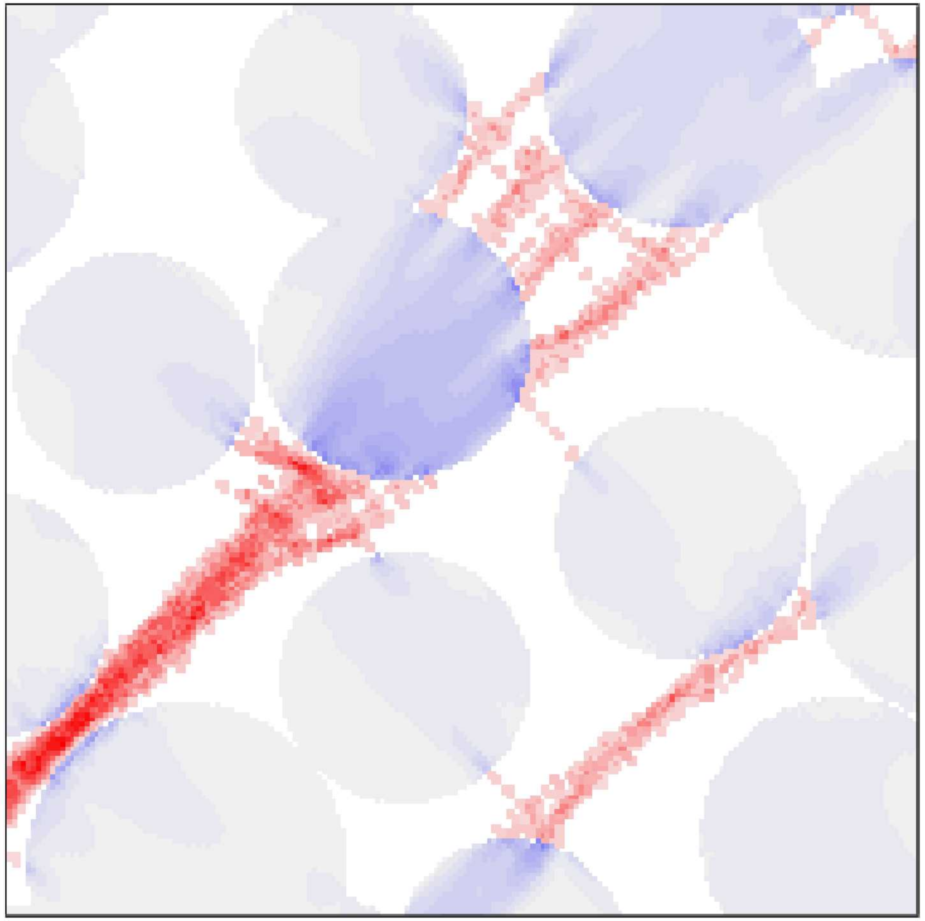
STZ Dynamics: Successes



Homer, Eric R. "Examining the initial stages of shear localization in amorphous metals." *Acta Materialia* 63 (2014): 44-53.

Metallic Glass Matrix Composites





Wu, Y., et al. "Formation of Cu–Zr–Al bulk metallic glass composites with improved tensile properties." *Acta Materialia*59.8 (2011): 2928-2936.

Hardin, Thomas J., and Eric R. Homer. "Microstructural factors of strain delocalization in model metallic glass matrix composites." *Acta Materialia* 83 (2015): 203-215.

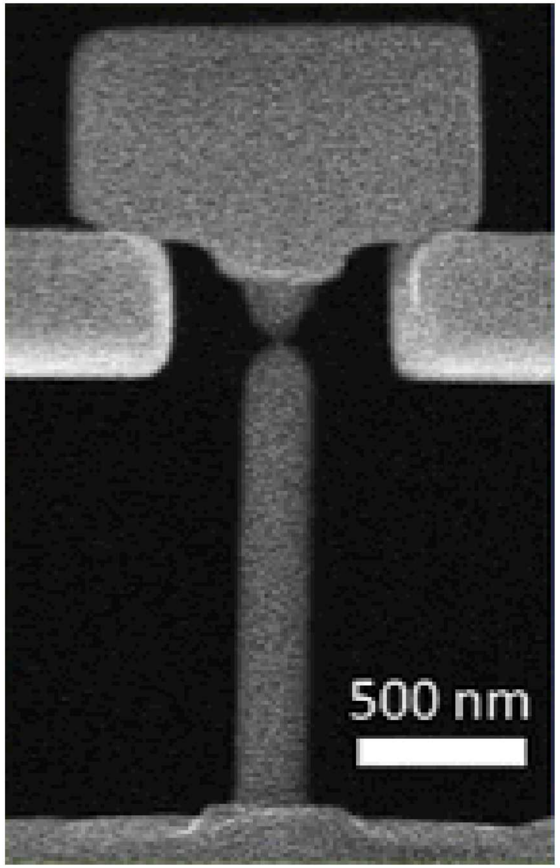
Impact of Recent Research

Two modern developments spurred the development of next-generation mesoscale metallic glass models

Proliferation of nanomechanical testing

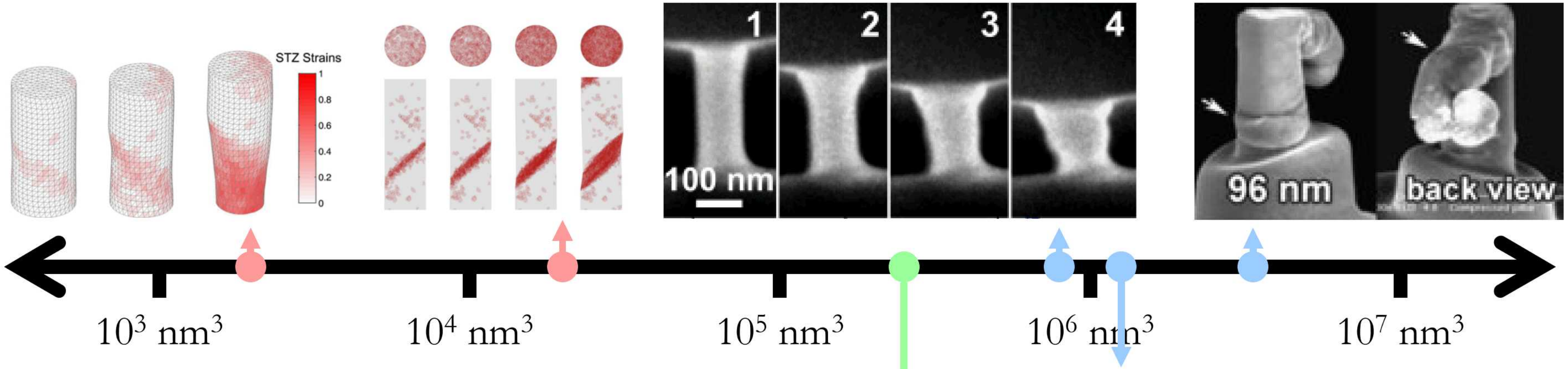
Appreciation of importance of the structure of glass

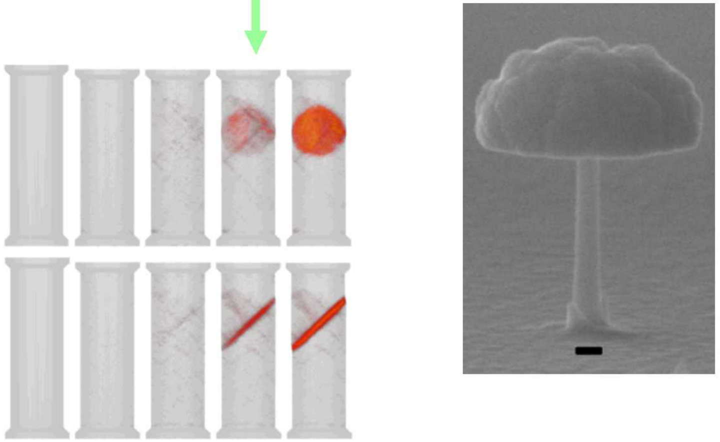
- MD & experimental insights on atomic configurations
- Glass viewed as heterogeneous nanocomposite



Liontas, Rachel, et al. *Acta Materialia* 118 (2016): 270-285.

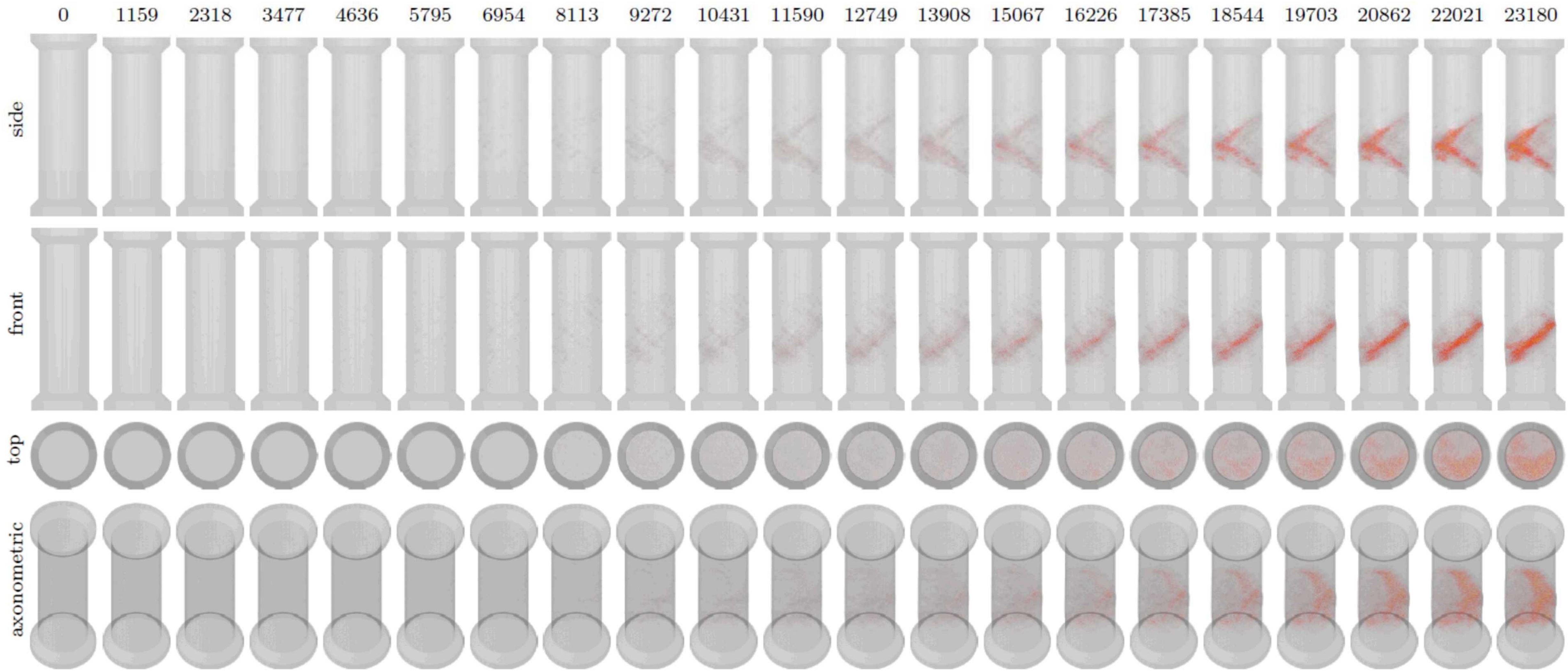
200x Speedup, 18x Sizeup





Homer, Eric R. *Acta Materialia* 63 (2014): 44-53..
Homer, Eric R., and Christopher A. Schuh. *Modelling and Simulation in Materials Science and Engineering* 18.6 (2010): 065009.
Harris, Matthew B., Lars S. Watts, and Eric R. Homer. *Acta Materialia* 111 (2016): 273-282.
Homer, Eric R., and Christopher A. Schuh. *Acta Materialia* 57.9 (2009): 2823-2833.
Hardin, Thomas J. *Computational Mechanics* (2018): 1-10.
Chen, C. Q., Y. T. Pei, and J. Th M. De Hosson. *Acta Materialia* 58.1 (2010): 189-200..
Gu, X. Wendy, et al., *Nano letters* 14.10 (2014): 5858-5864.
Chen, Chang Qiang, et al. *Physical Review B* 83.18 (2011): 180201.

Competitive Shear Localization



Hardin, Thomas J. "Accelerating coupled finite element-kinetic Monte Carlo models: 200x speedup of shear transformation zone dynamics simulations.“ *Computational Mechanics* (2018): 1-10.

Potential Energy Landscape Ansatz

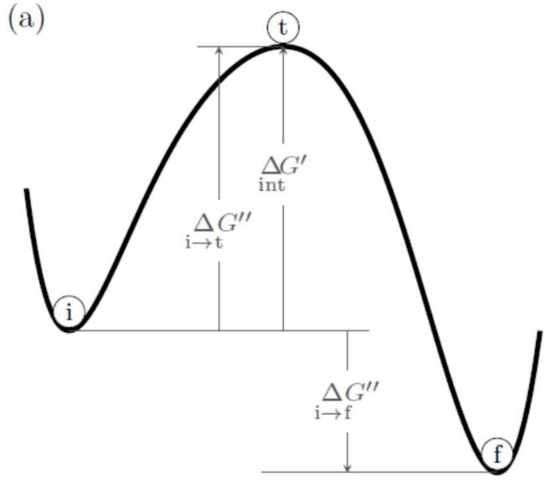
1. Configurational potential energy decompose into a portion which correlates with molar volume (dilatative CPE), and one which does not (isochoric CPE). Experiments have shown that shear modulus maps to total CPE.

$$U^\star = U_\mathrm{I}^\star + U_\mathrm{D}^\star$$

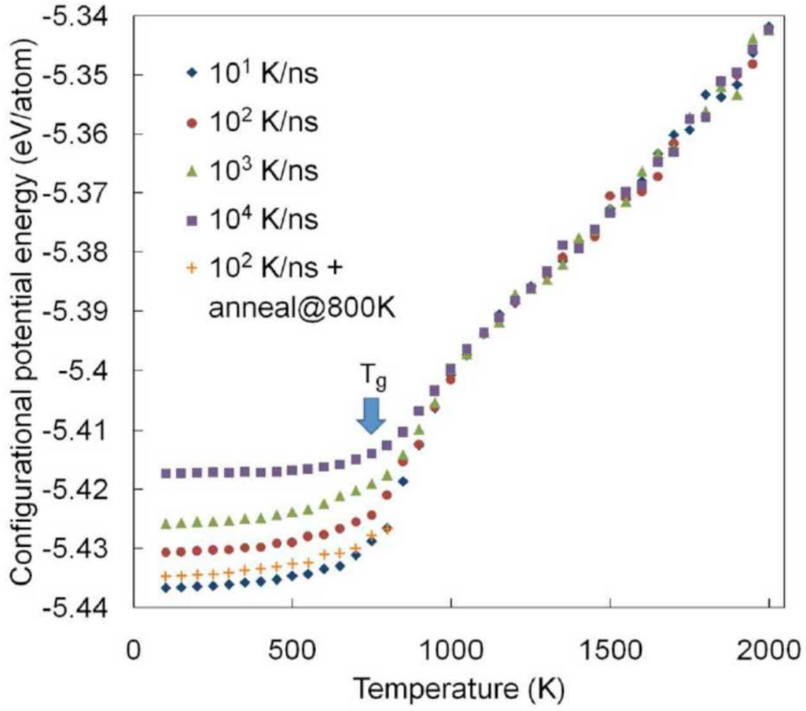
2. The density of "polyamorphs" of the glass plotted on the isochoric x dilatative axes can be represented by this simple combinatorial density of states.

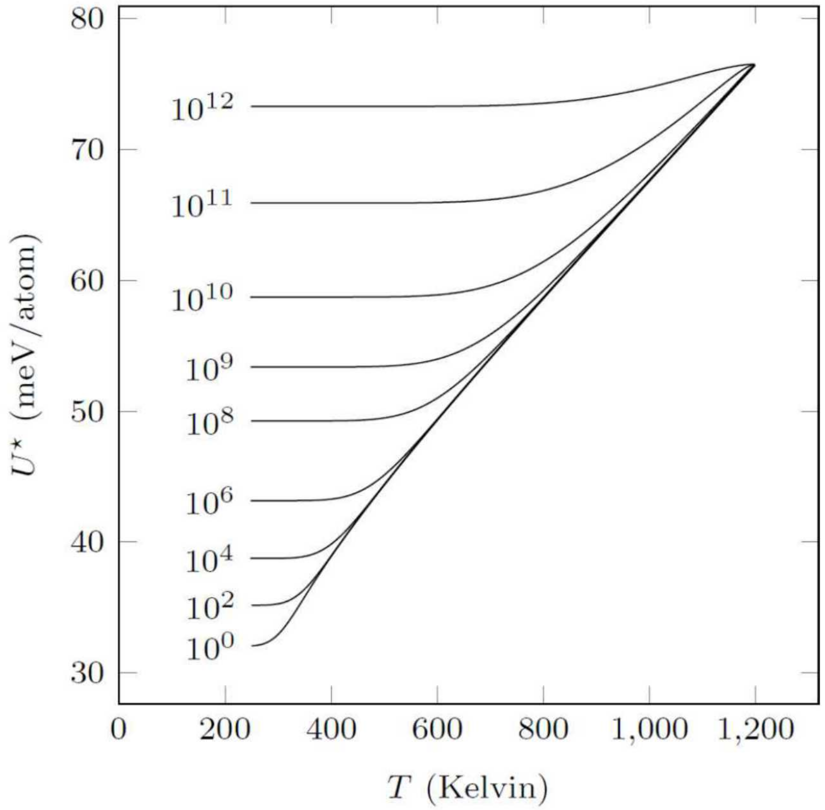
$$D(U_\mathrm{I}^\star, U_\mathrm{D}^\star) = \frac{n^\mathrm{Ref}}{(U^\mathrm{Ref})^2} \frac{\Gamma(3+a+b)}{\Gamma(1+a)\Gamma(1+b)} \left(\frac{U_\mathrm{I}^\star}{U^\mathrm{Ref}}\right)^a \left(\frac{U_\mathrm{D}^\star}{U^\mathrm{Ref}}\right)^b$$

3. The glass can transition between any two "polyamorphs," and the transition state barrier height is constant.



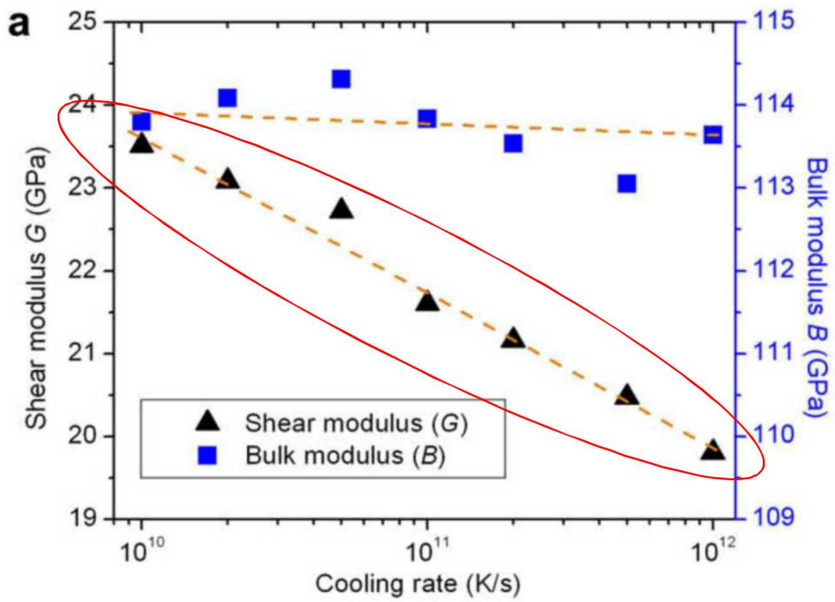
STZ Dynamics with Potential Energy Landscape

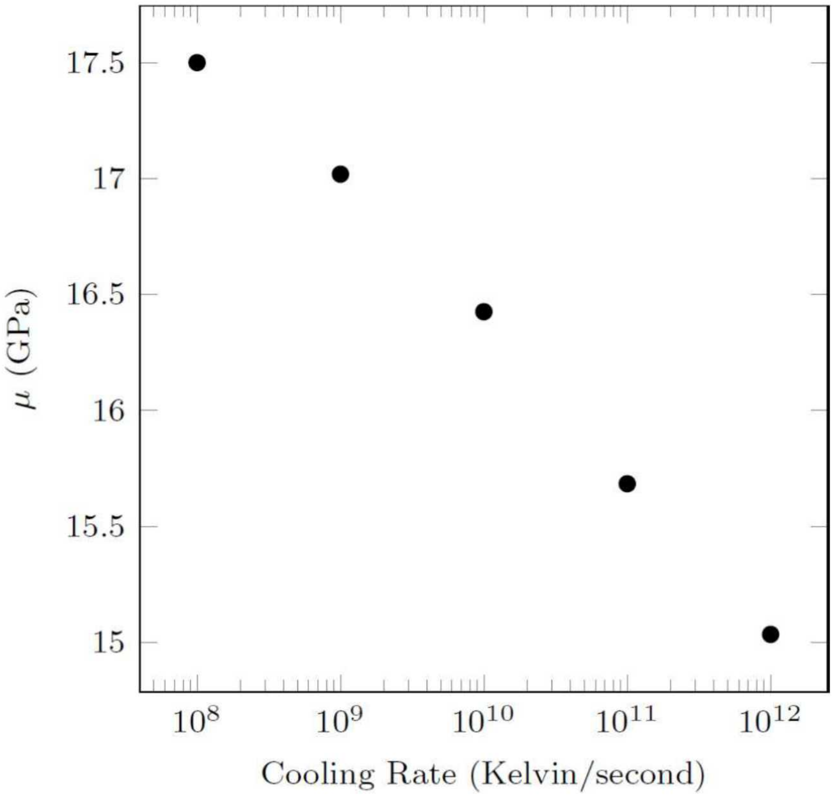




Y. Q. Cheng, E. Ma, *Applied Physics Letters*, vol. 93, art. 051910, 2008.

STZ Dynamics with Potential Energy Landscape





Y. Q. Cheng, A. J. Cao, E. Ma, Acta Materialia, vol. 57, pp. 3253-3267, 2009.

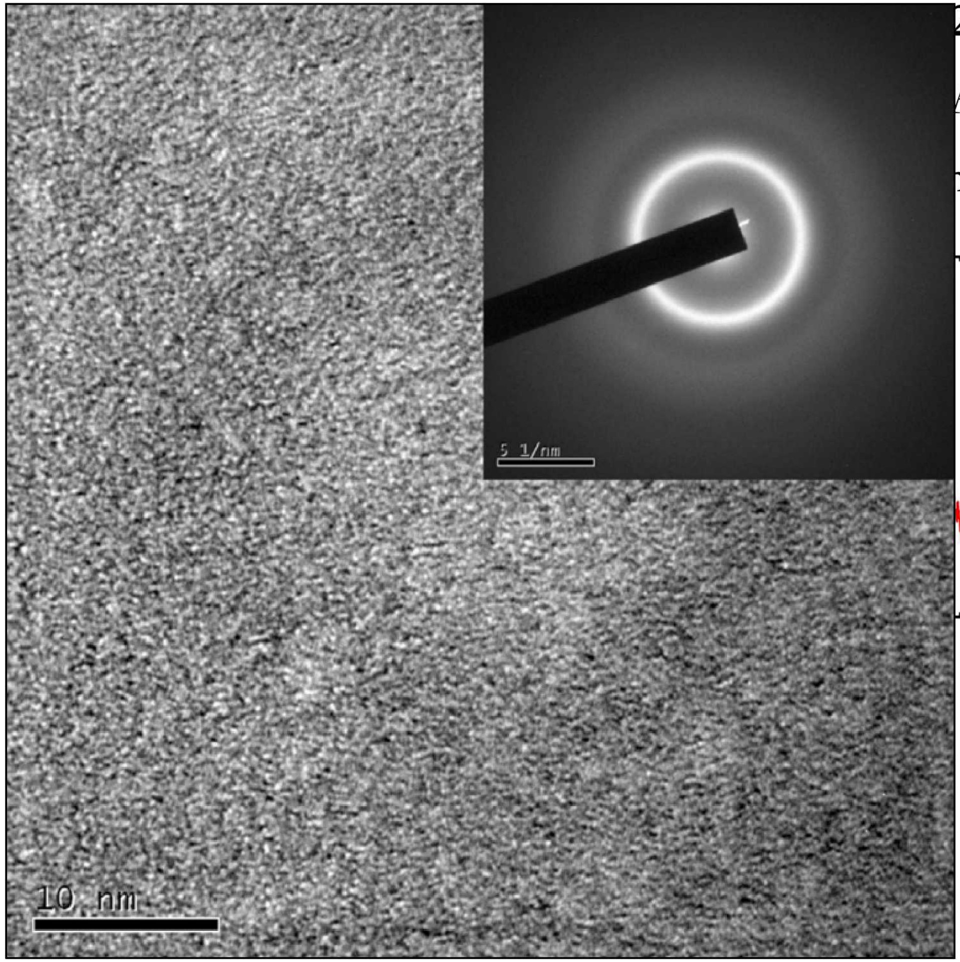
Looking Forward: Bridging Scales, a Tale of Two Samples

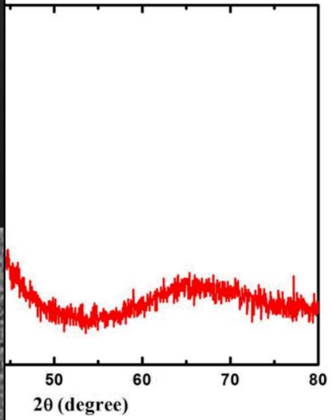
2

Composition Al_{10}

Molar Volume m^3/mol

XRD



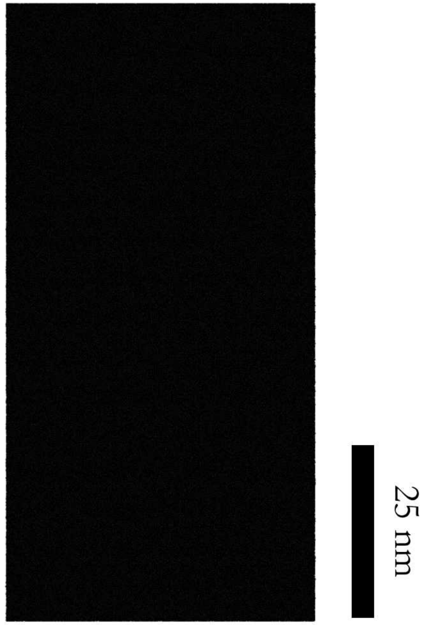


Adapted from Miyazaki, Narumasa, et al. "Prediction of pressure-promoted thermal rejuvenation in metallic glasses." *npj Computational Materials* 2 (2016): 16013.

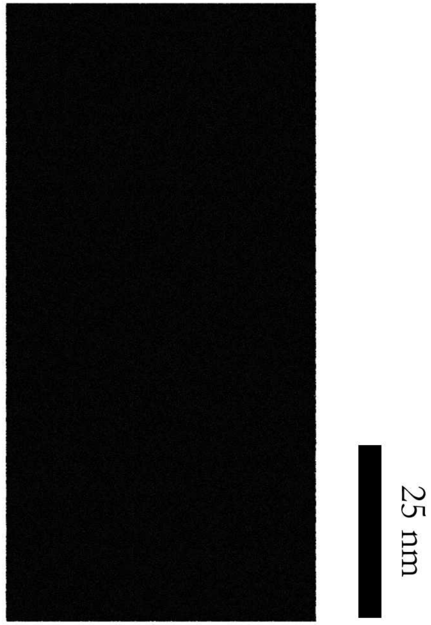
Gao, Qian, et al. "Crystallization kinetics of the Cu50Zr50 metallic glass under isothermal conditions." *Journal of Solid State Chemistry* 244 (2016): 116-119.

Looking Forward: Bridging Scales, a Tale of Two Samples

Sample 1



Sample 2

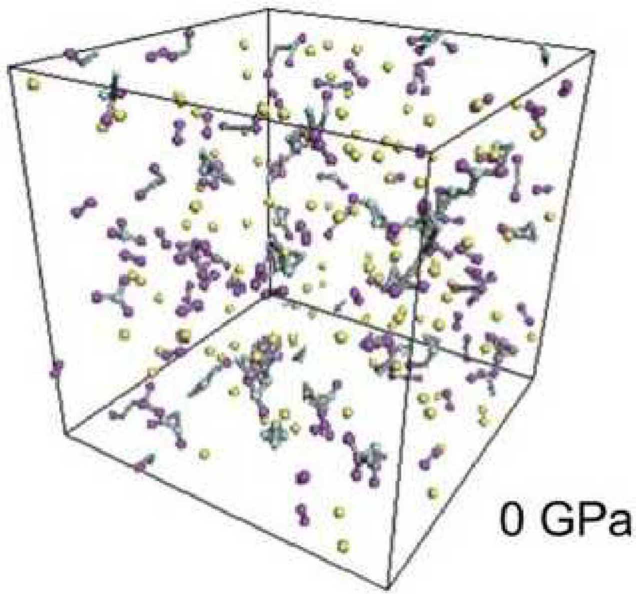


Von Mises Atomic Strain distributions in uniaxial tensile tests. Strain rate = 10^8 /s, Temperature = 300 K in both cases.

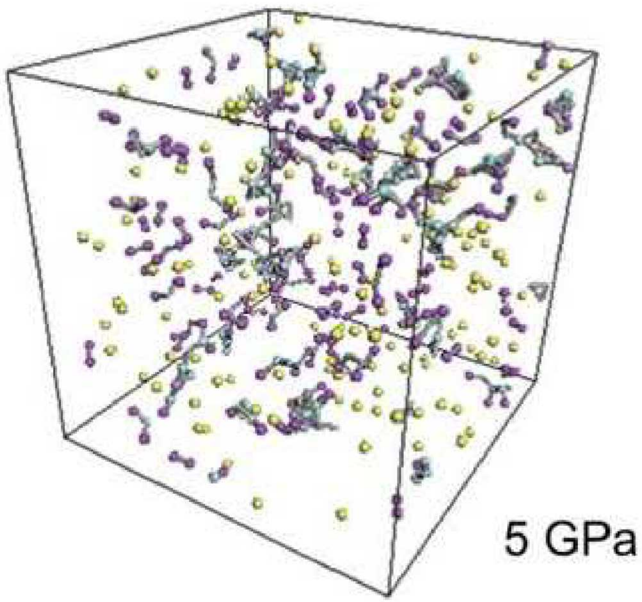
Adapted from Miyazaki, Narumasa, et al. "Prediction of pressure-promoted thermal rejuvenation in metallic glasses." *npj Computational Materials* 2 (2016): 16013.

Looking Forward: Bridging Scales, a Tale of Two Samples

Sample 1



Sample 2



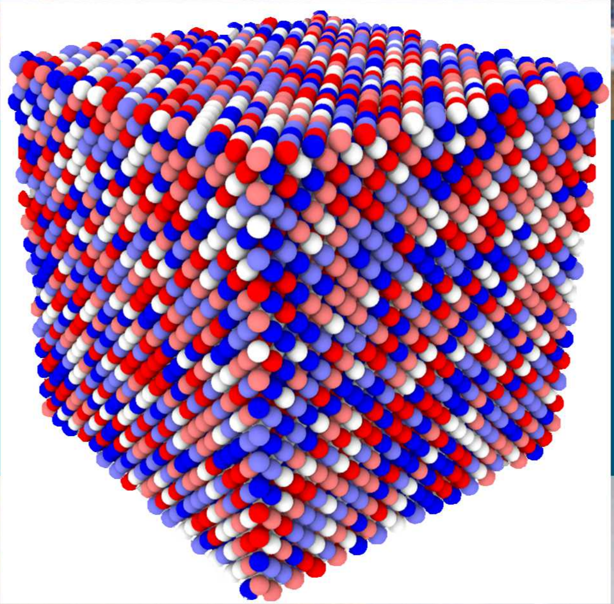
Locations of icosahedral short-range atomic clusters

Adapted from Miyazaki, Narumasa, et al. "Prediction of pressure-promoted thermal rejuvenation in metallic glasses." *npj Computational Materials* 2 (2016): 16013.

Loose Ends

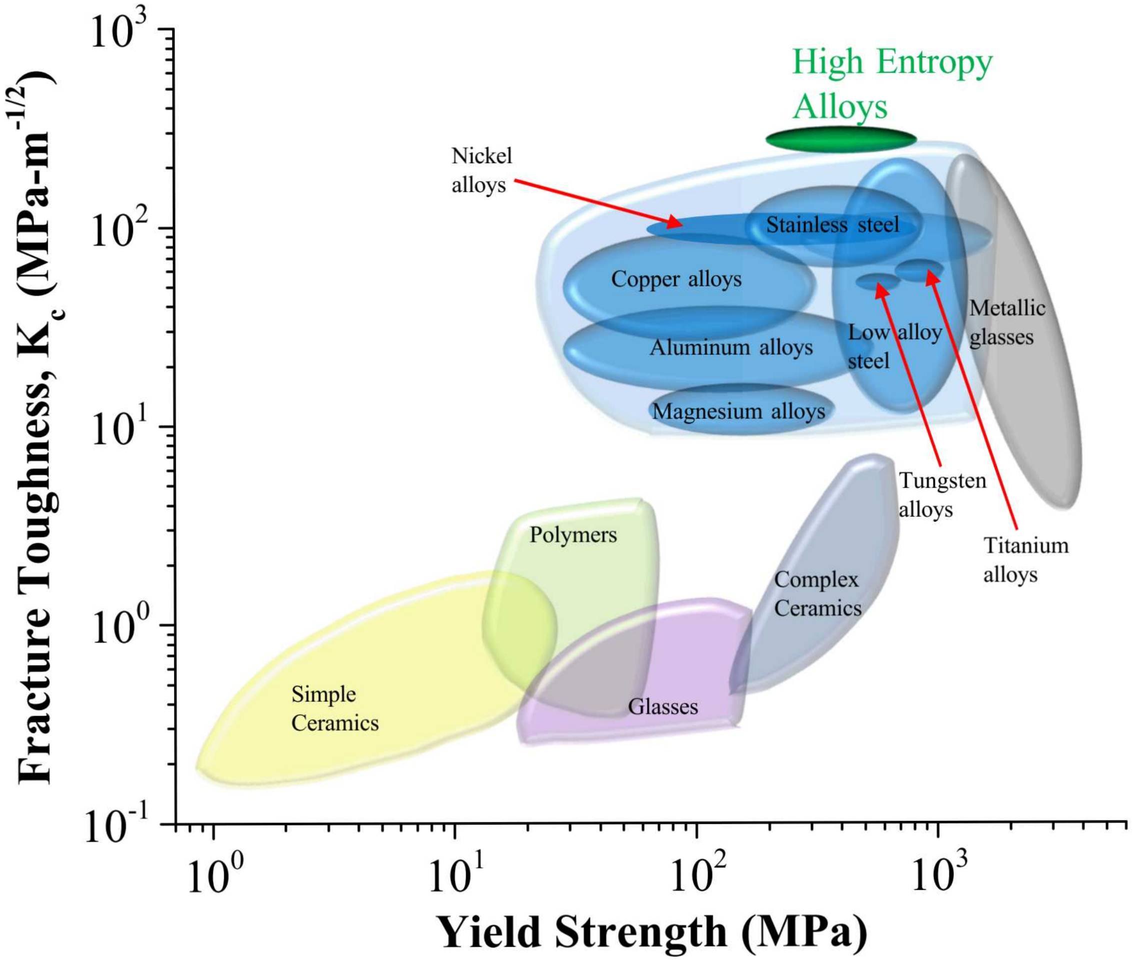
1. How does the glass change as we do [process] to it?

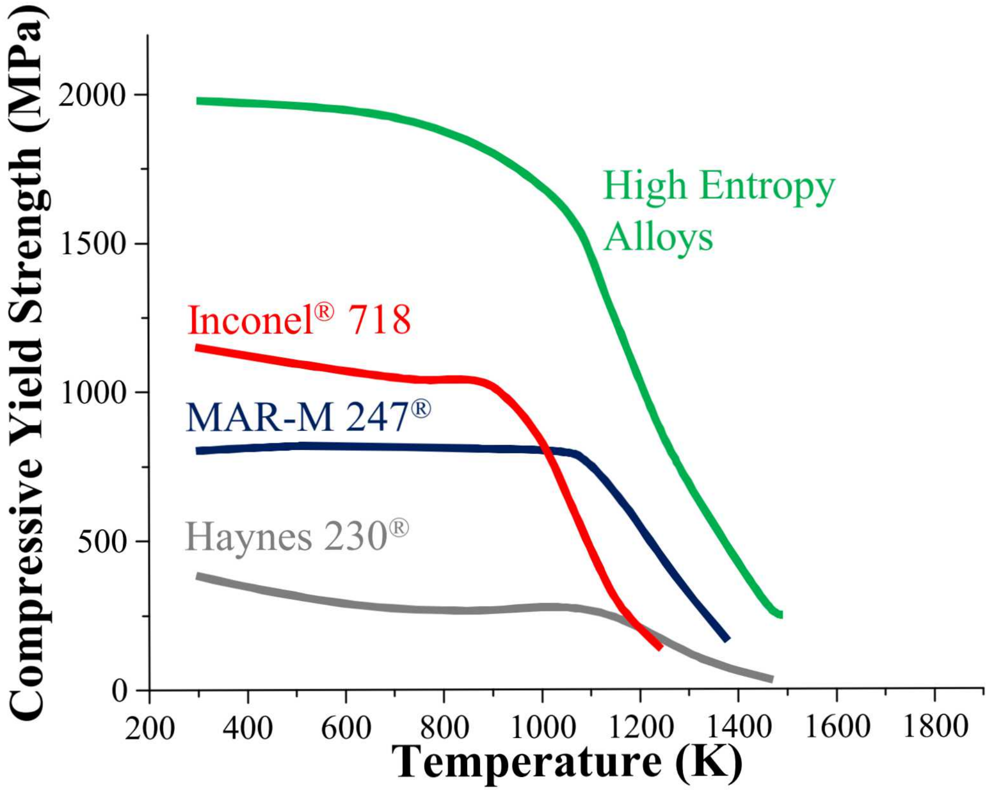
2. How does the structure of the glass impact its [property]?



High Entropy Alloys

Why Bother?



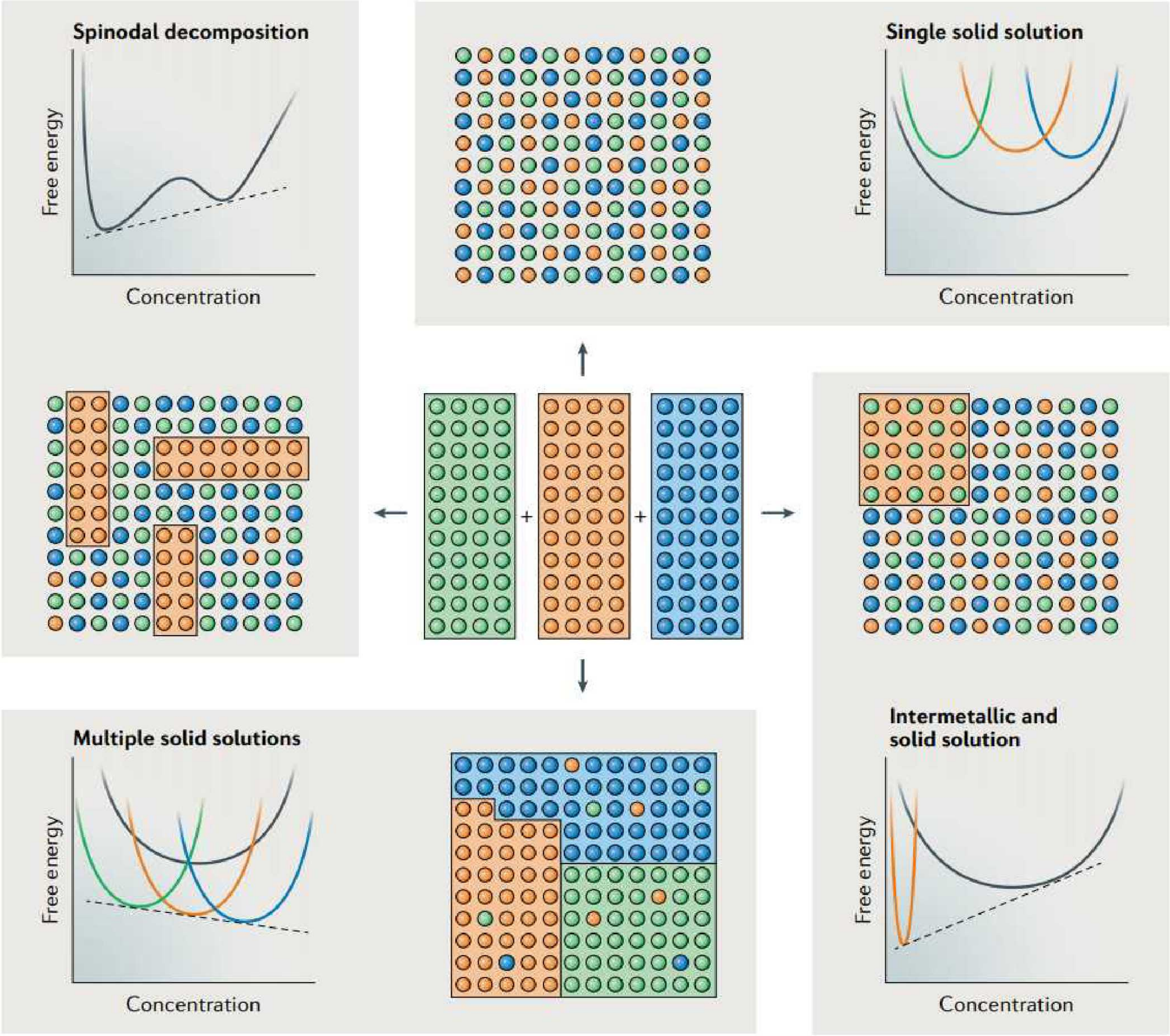


Courtesy of Dr. Andrew Kustas, Sandia.

Miracle, Daniel B., and Oleg N. Senkov. "A critical review of high entropy alloys and related concepts." *Acta Materialia* 122 (2017): 448-511.

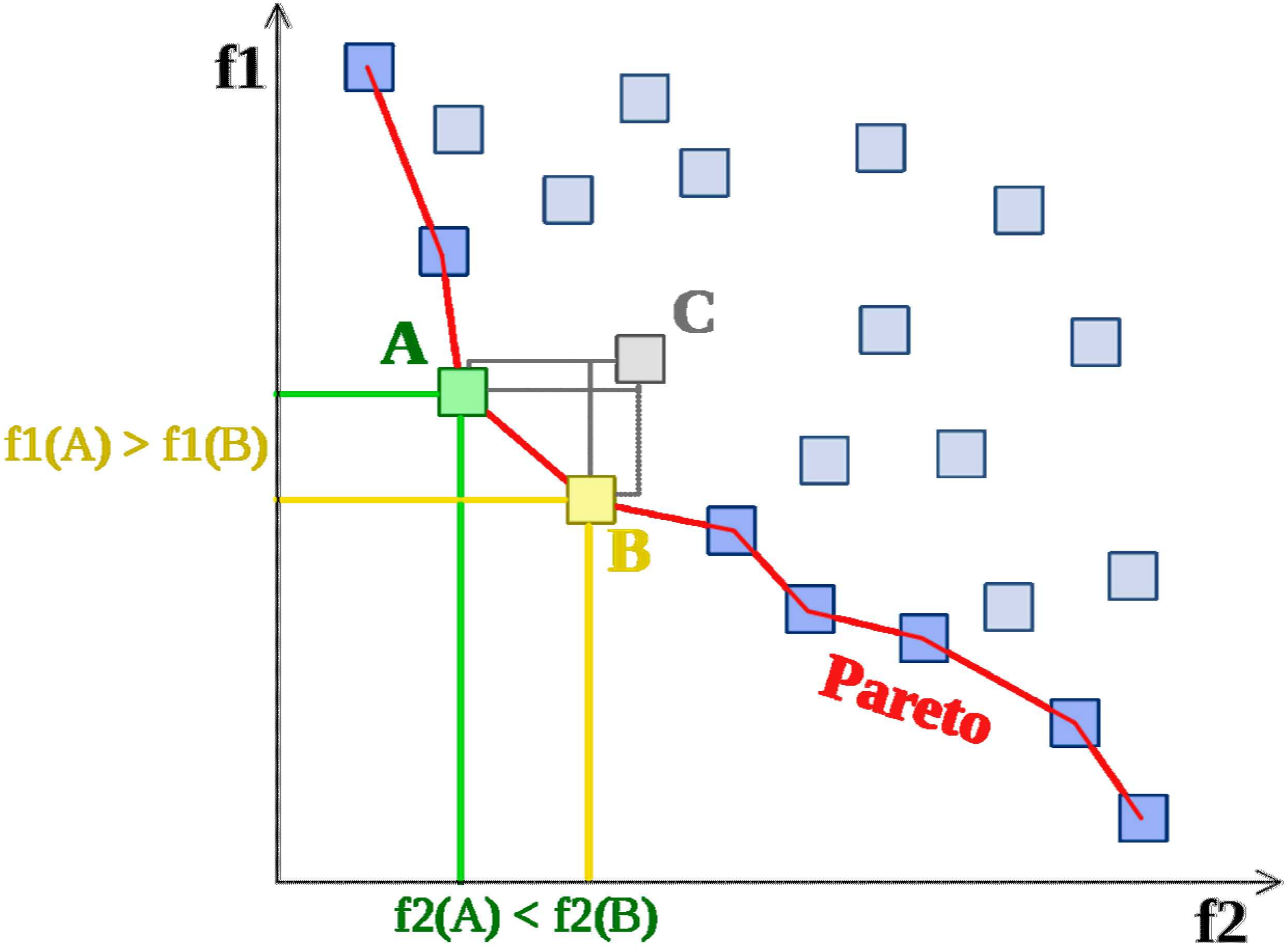
Gludovatz, Bernd, et al. "A fracture-resistant high-entropy alloy for cryogenic applications." *Science* 345.6201 (2014): 1153-1158.

Thermodynamic Rationale



George, Easo P., Dierk Raabe, and Robert O. Ritchie. "High-entropy alloys." *Nature Reviews Materials* 4.8 (2019): 515-534.

Pareto Front

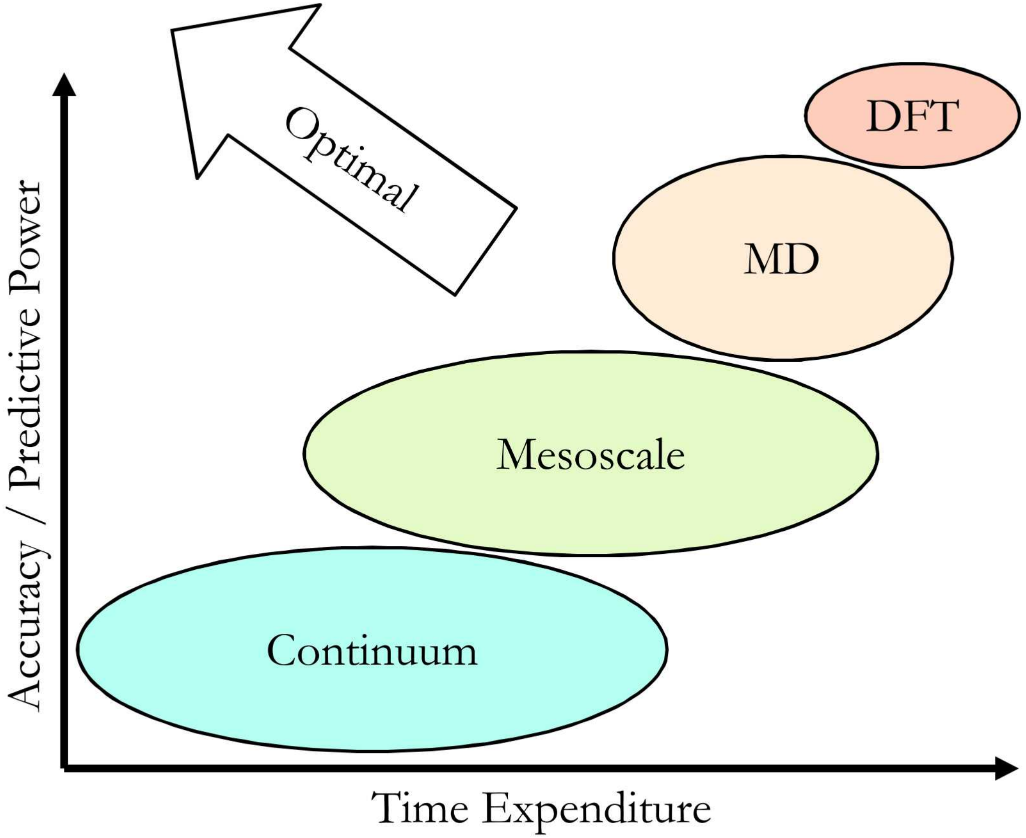


"… we must begin to think differently about the scope of complex concentrated alloy studies. A small handful of equiatomic or near-equiatomic compositions are commonly used as a proxy for all the alloys in a multi-component phase diagram. We need to explore a broader range of compositions in promising alloy systems."

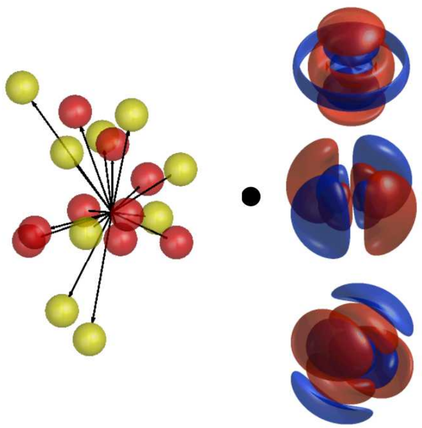
Miracle, D. B. "High entropy alloys as a bold step forward in alloy development." *Nature communications* 10.1 (2019): 1-3.

Problems with Direct High-Throughput Simulation of HEA

1. Random nature of HEAs requires large cells to capture representative properties.
2. Large cell size implies first principles not an option; so MD is the best we can do.
3. Large number of constituents implies challenging construction of empirical potential.
4. Even with perfect empirical potential, difficulty of constructing meaningful simulations within performance constraints.



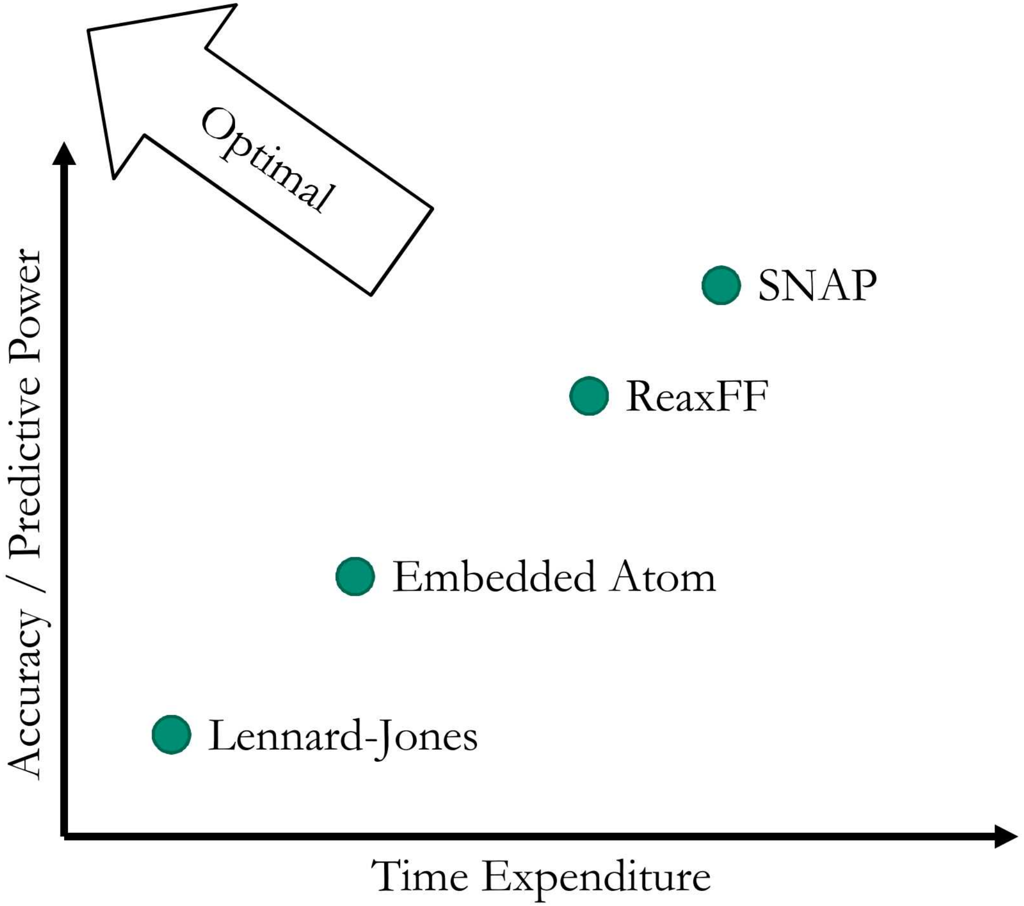
Spectral Neighbor Analysis Potential (SNAP)



$$\cdot \quad = \begin{bmatrix} c_{0,0,0} \\ c_{0,1,-1} \\ c_{0,1,0} \\ c_{0,1,-1} \\ c_{1,0,0} \\ c_{1,1,-1} \\ c_{1,1,0} \\ c_{1,1,1} \\ c_{1,2,-2} \\ c_{1,2,-1} \\ \vdots \end{bmatrix}$$

$$E_{SNAP}(\mathbf{r}^N) = N\beta_0 + \boldsymbol{\beta} \cdot \sum_{i=1}^{N} \mathbf{B}^i$$

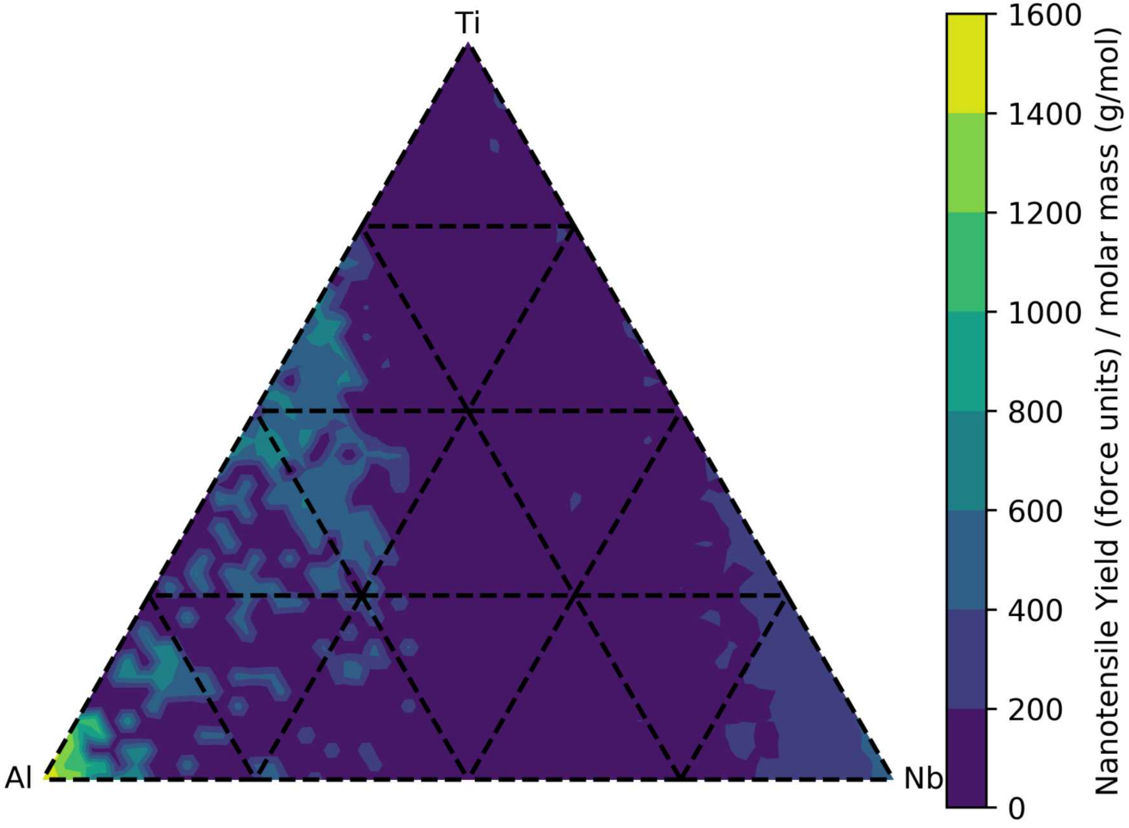
github.com/FitSNAP/FitSNAP
By Dr. Aidan P. Thompson et al.



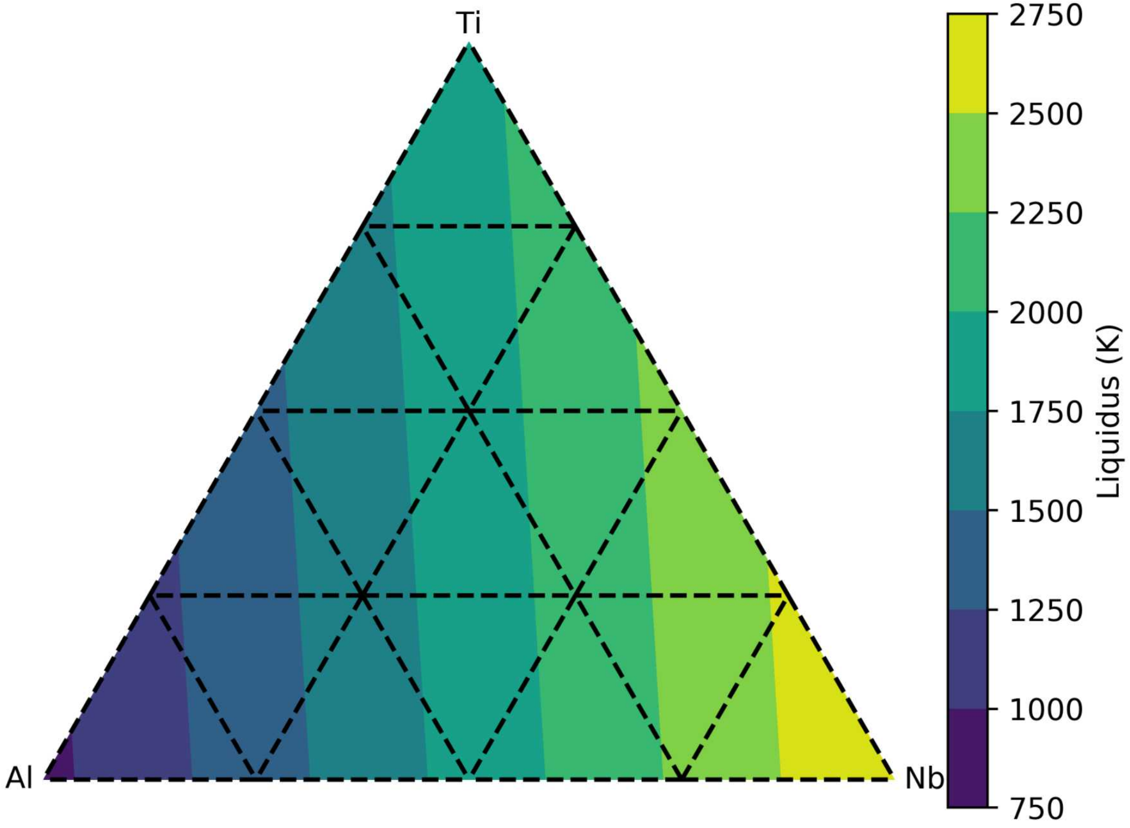
Thompson, Aidan P., et al. "Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials." *Journal of Computational Physics* 285 (2015): 316-330.

High-Throughput Analysis of Al-Ti-Nb System w/SNAP potential

Quasistatic Nanotensile Test

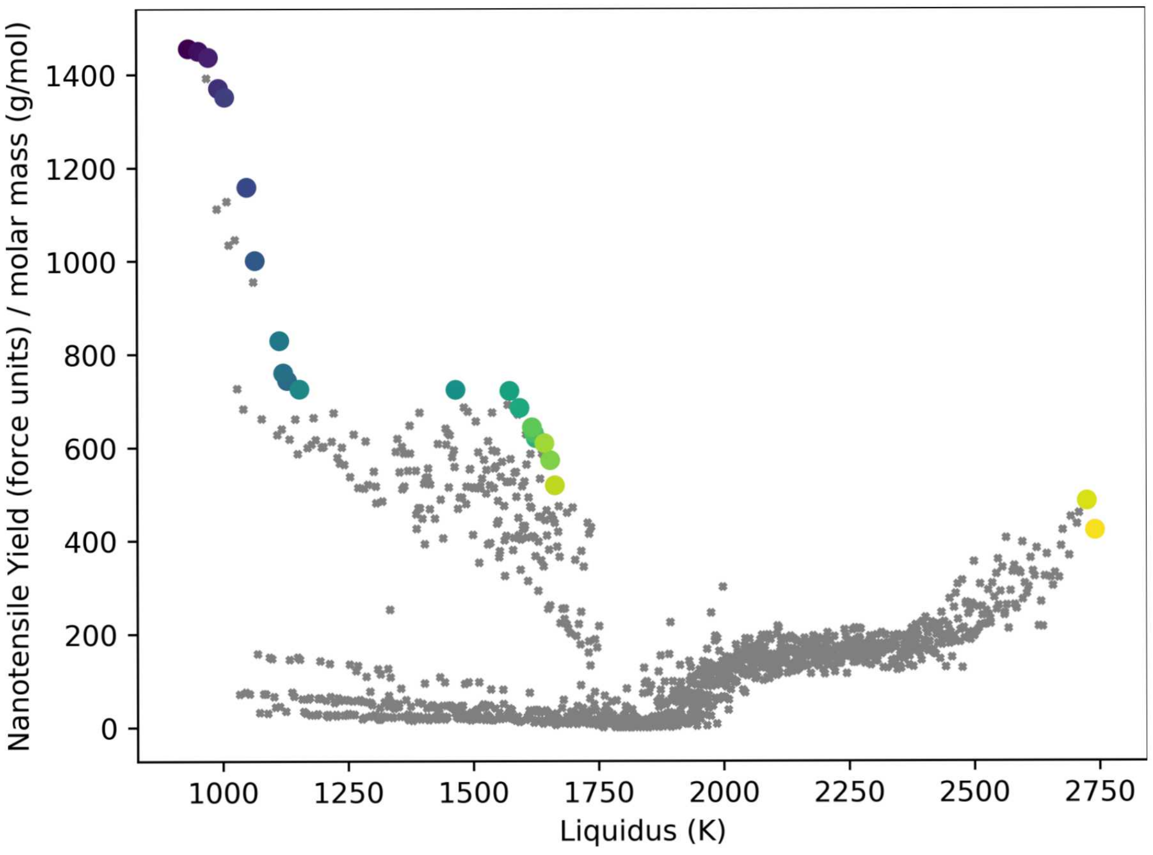


Rough Estimate of Liquidus Temp

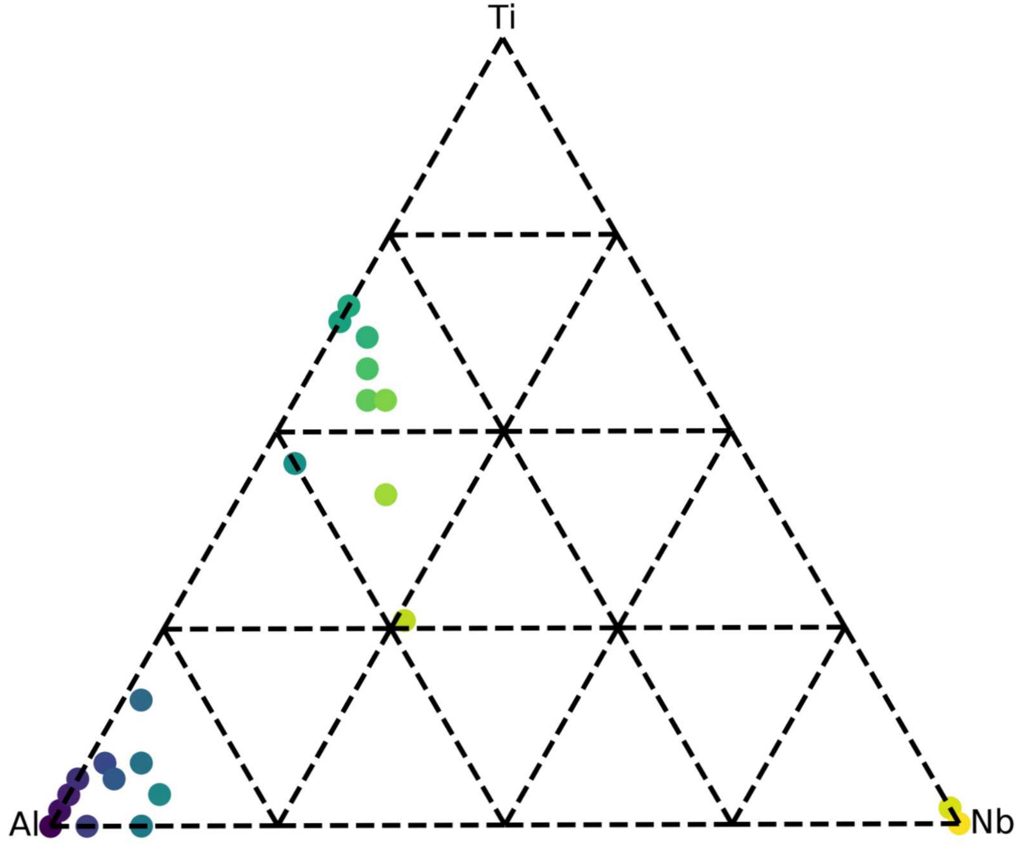


High-Throughput Analysis of Al-Ti-Nb System w/SNAP potential

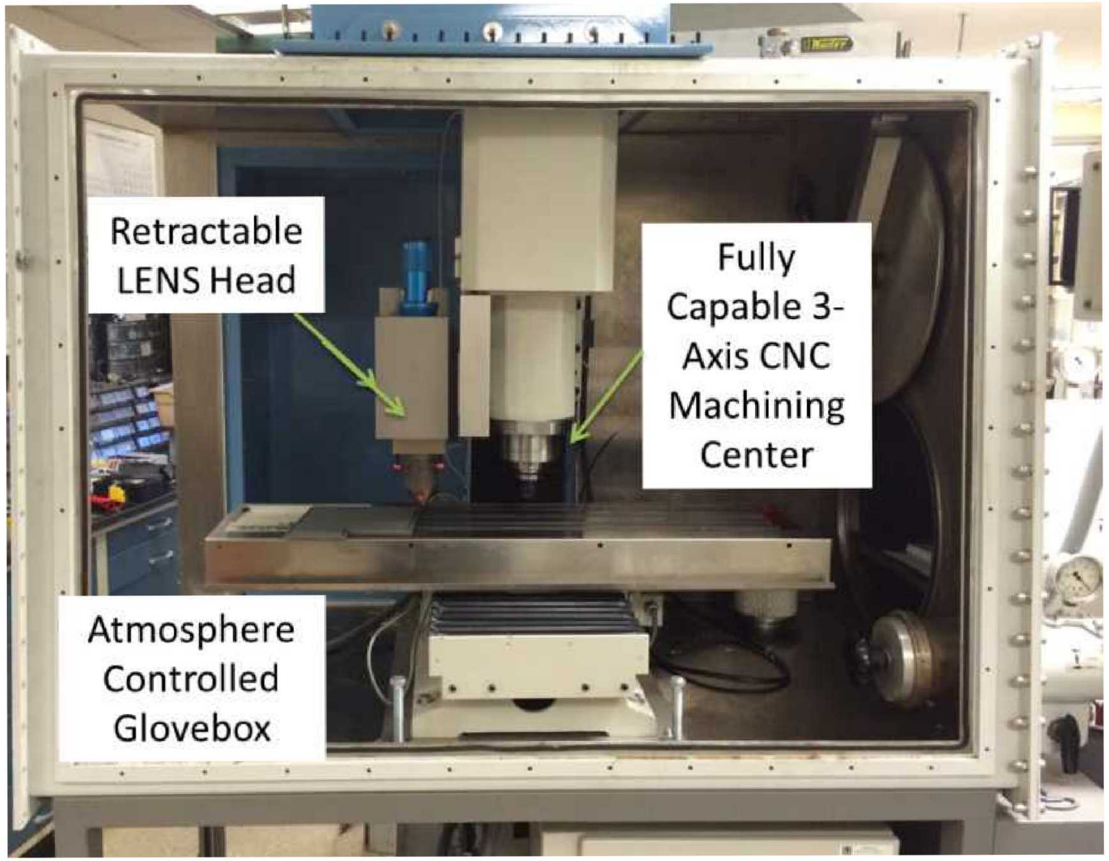
Scatter Plot of Objectives

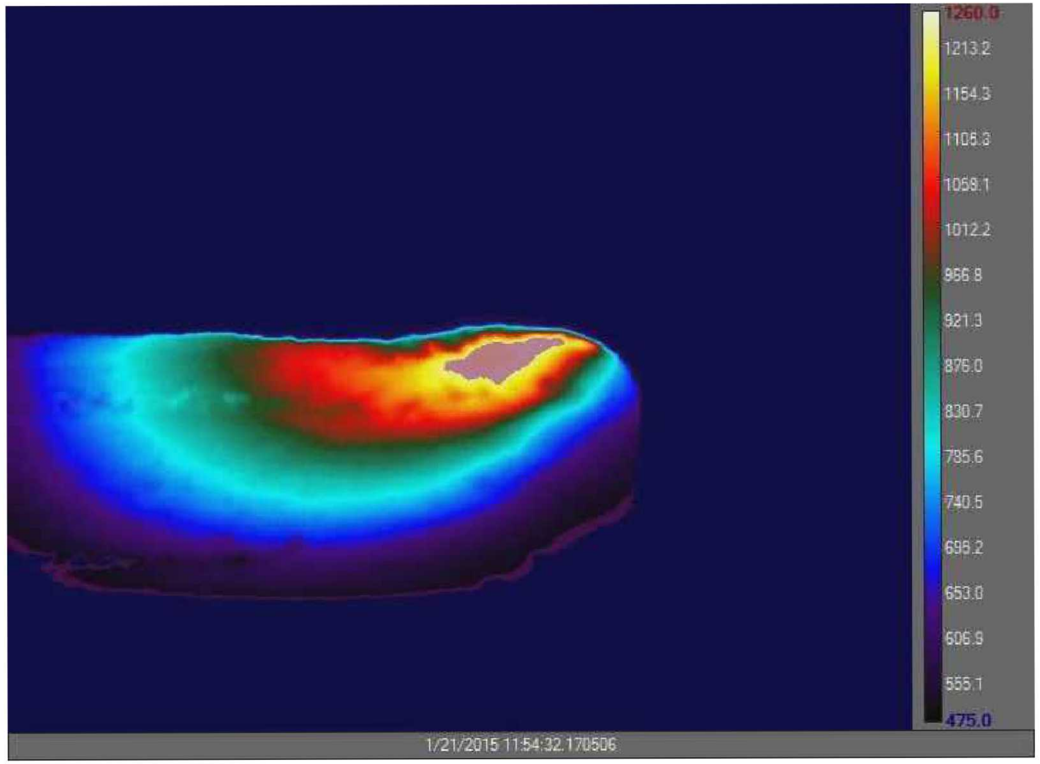


Compositions of Pareto Optimal Designs



Attempts at Additively Manufacturing HEAs





Courtesy of Dr. Andrew Kustas, Sandia.

Attempts at Additively Manufacturing HEAs

Courtesy of Dr. Andrew Kustas, Sandia.

Credit to Collaborators

MIT:	Christopher Schuh	**My Students:**
	Eric Homer (currently at BYU)	Jonathan Paras
	Mostafa Hassani (currently at Cornell)	Carlos Cruz
	David Veysset	Laura Malhotra
	Keith Nelson	Madelyn Payne
SNL:	Michael Chandross	
	Scotty Bobbitt	Timothy Ruggles
	Andrew Kustas	Joshua Rackers