# Competition Between Cavitation and Flow in Amorphous Solids


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**postdoc opportunity!**

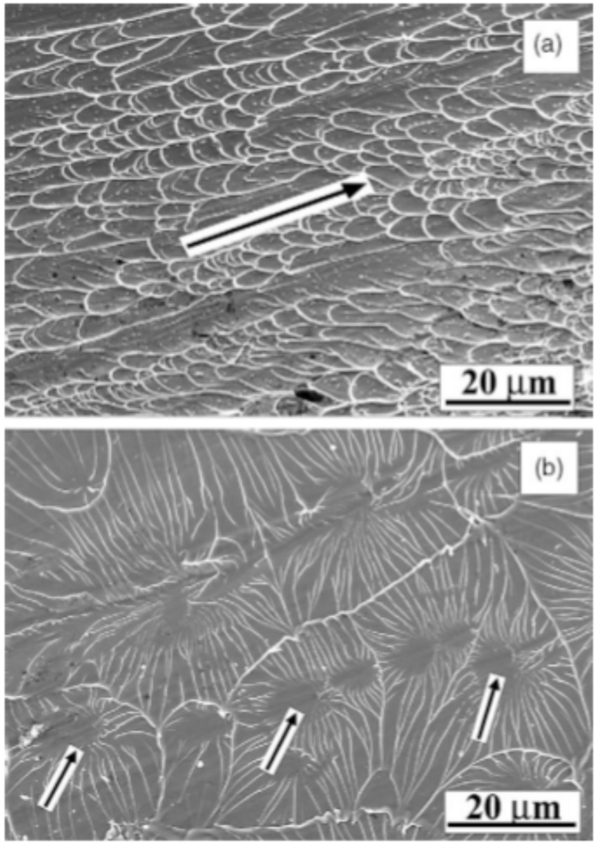
# Bulk Metallic Glasses

Douglas Hoffman, E-Science News 1998

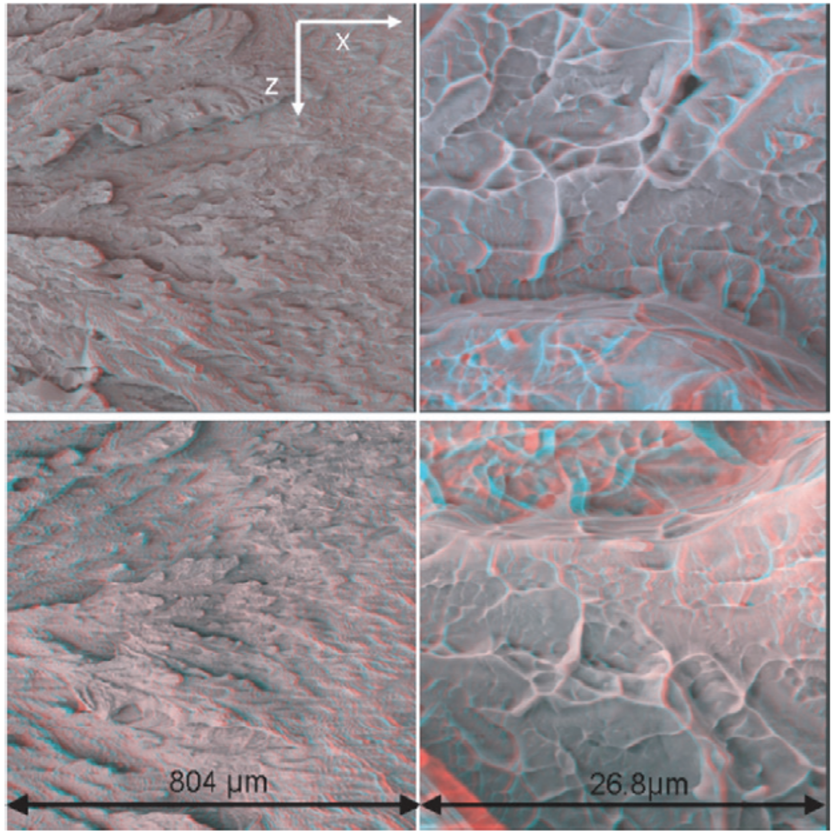
- Unique material with promising properties, but disordered structure.
- What can molecular dynamics simulation tell us about the mechanical response of these materials?

# Fracture in Metallic Glass

- Phenomenology of fracture in metallic glass



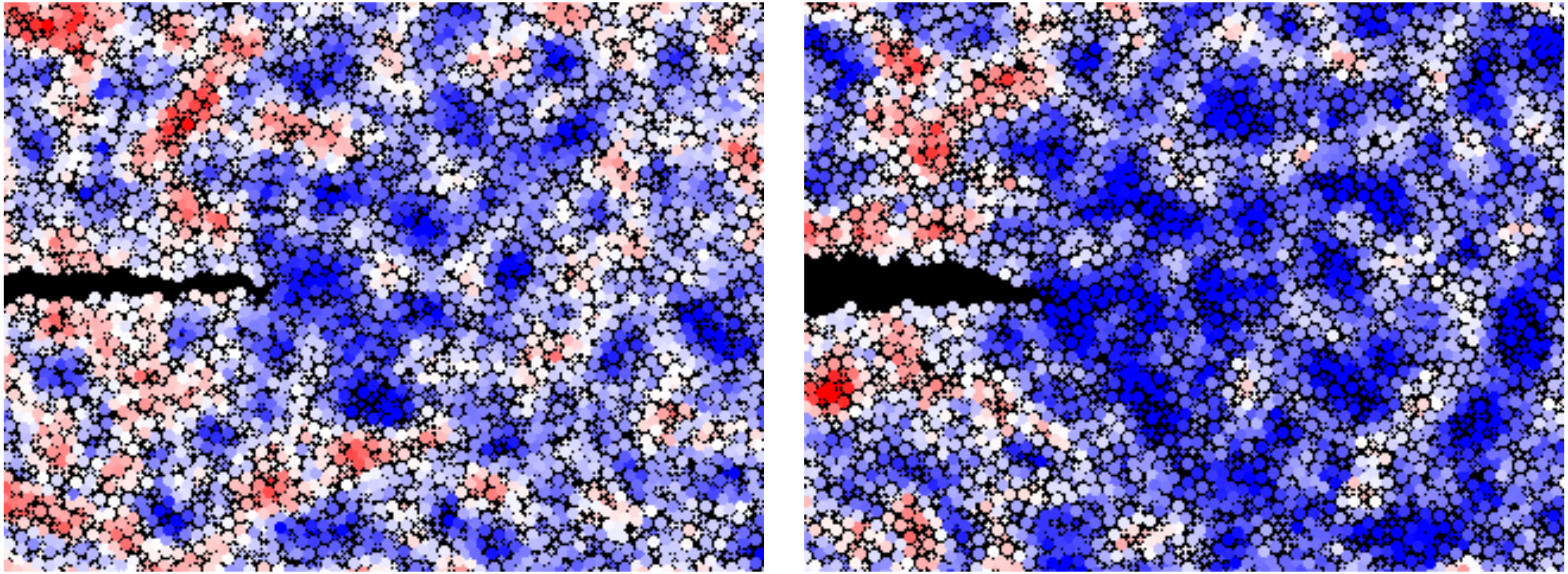

Compressive and Tensile Fracture in
$Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$
Zhang, Eckert and Schultz
Acta Materialia, 51, pp.1167 (2003)




Tensile fracture in Vitreloy 1
Bouchaud, Boivin, Pouchou, Bonamy, Poon and Ravichandran
Europhysics Letters, V83, pp. 66006 (2008)

# MD Simulations of Fracture

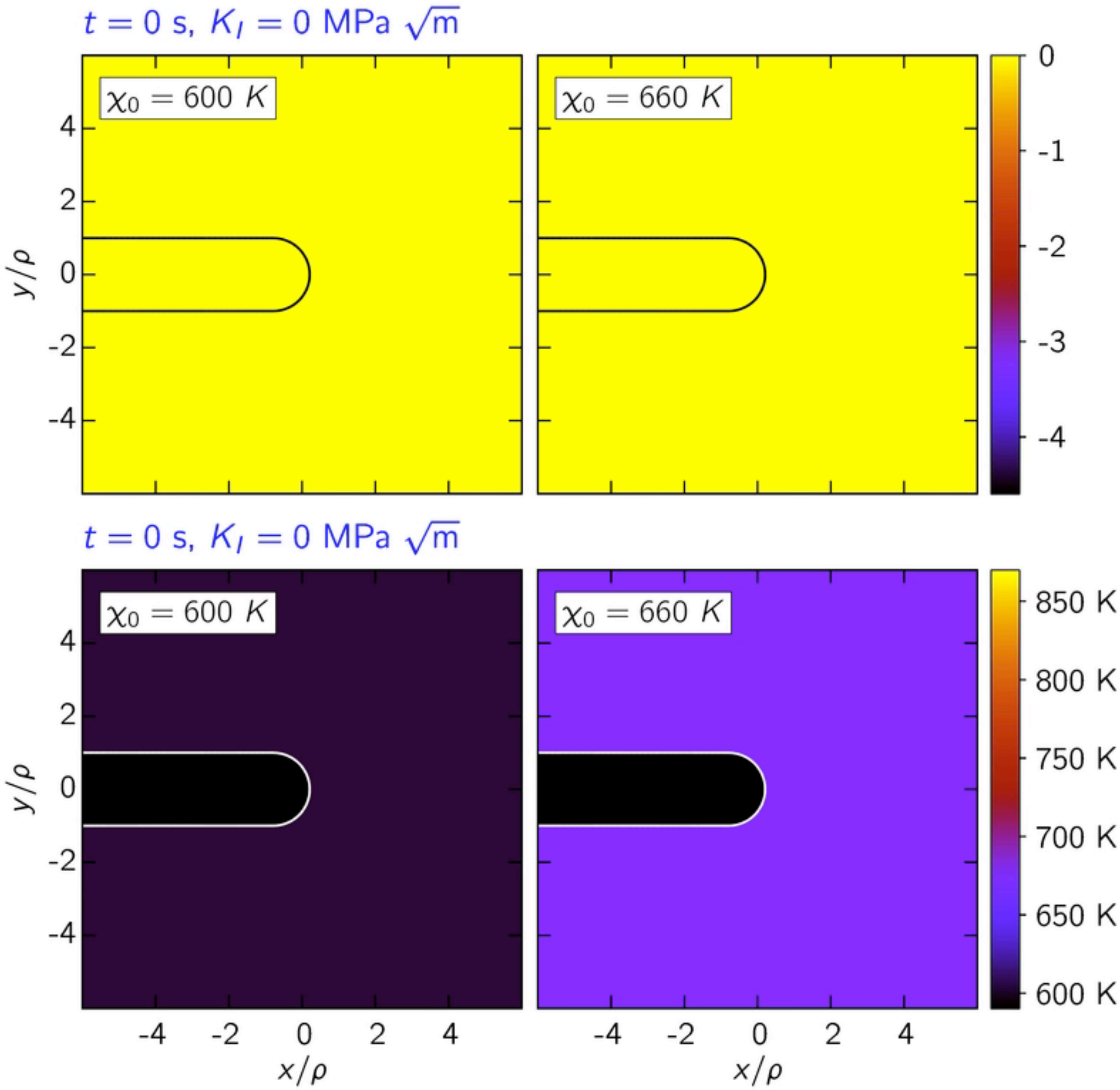
- Simple model of a polydisperse system interacting with pairwise potential
- Both "ductile" and "brittle" simulations exhibit cavitation ahead of crack tip.



ML Falk, PRB,V60, 7062 (1999)

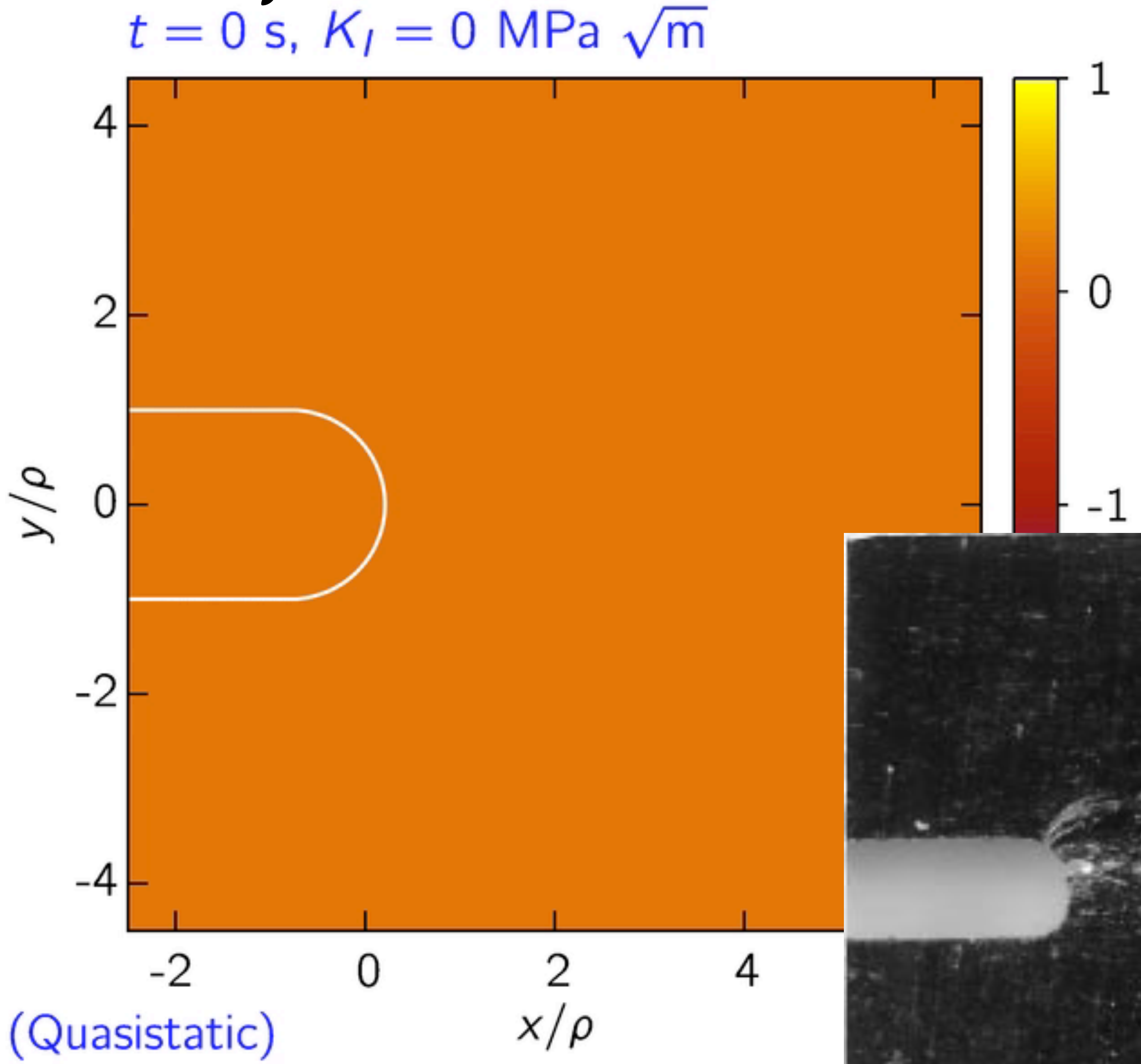
# STZ Crack Tip

Chris Rycroft, UC Berkeley

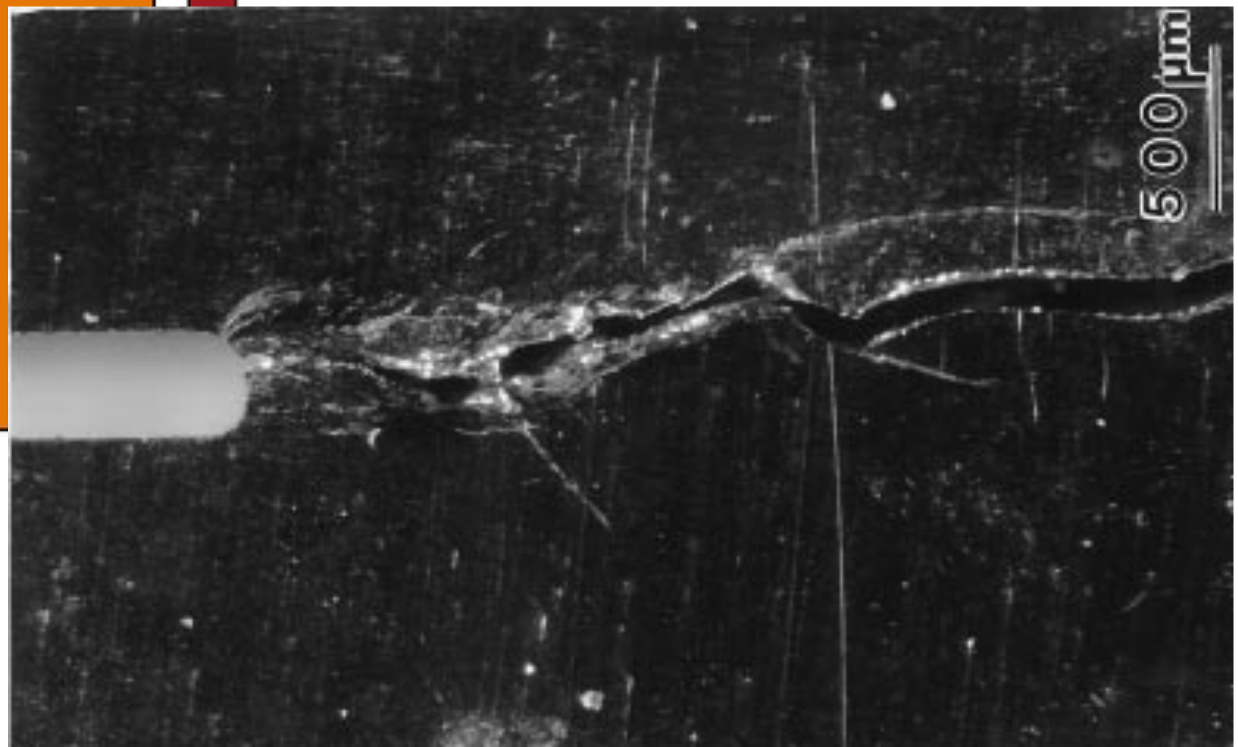


# Fracture with Cavitation

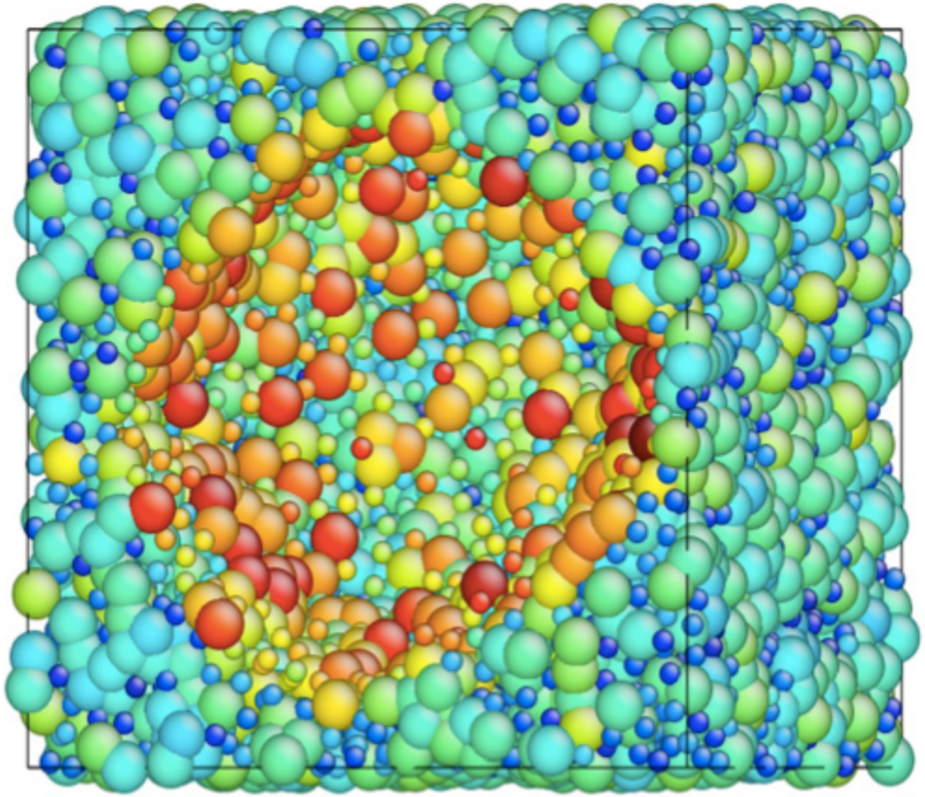
## Rycroft, Bouchbinder PRL 109, 194301 (2012)



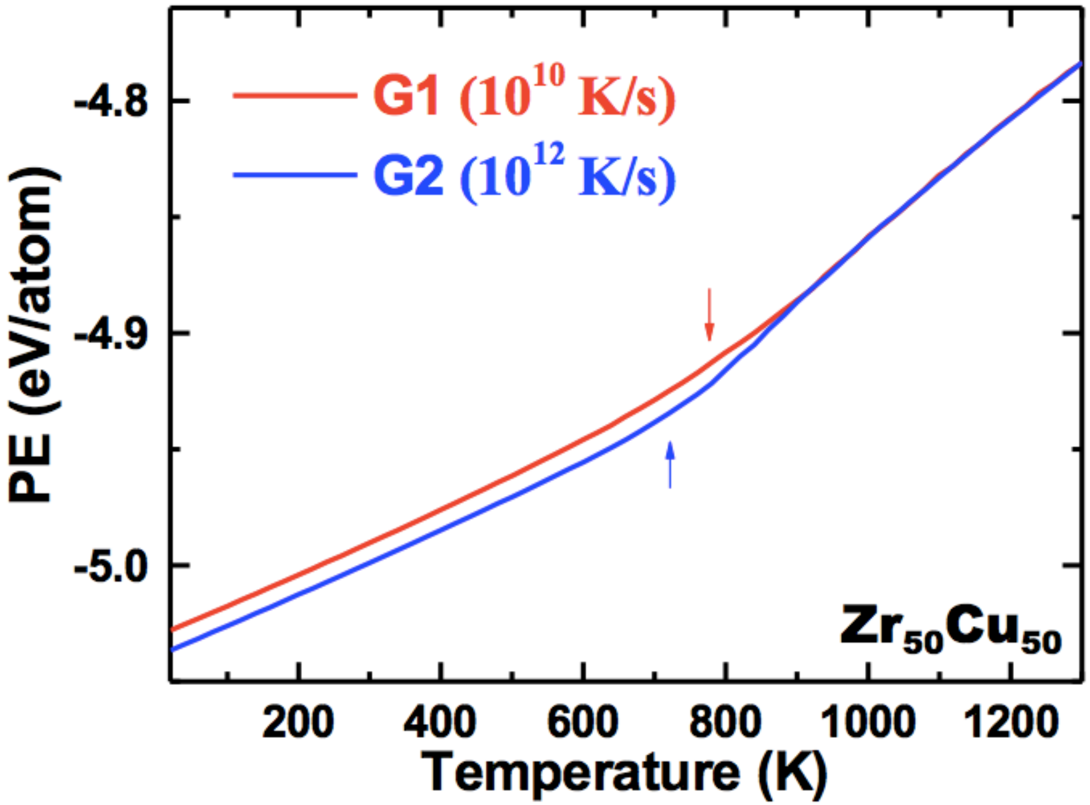

Lowhaphandu and Lewandowski
Scripta Materialia 38, 1811 (1998)



# Simulated System: $Cu_{50}Zr_{50}$

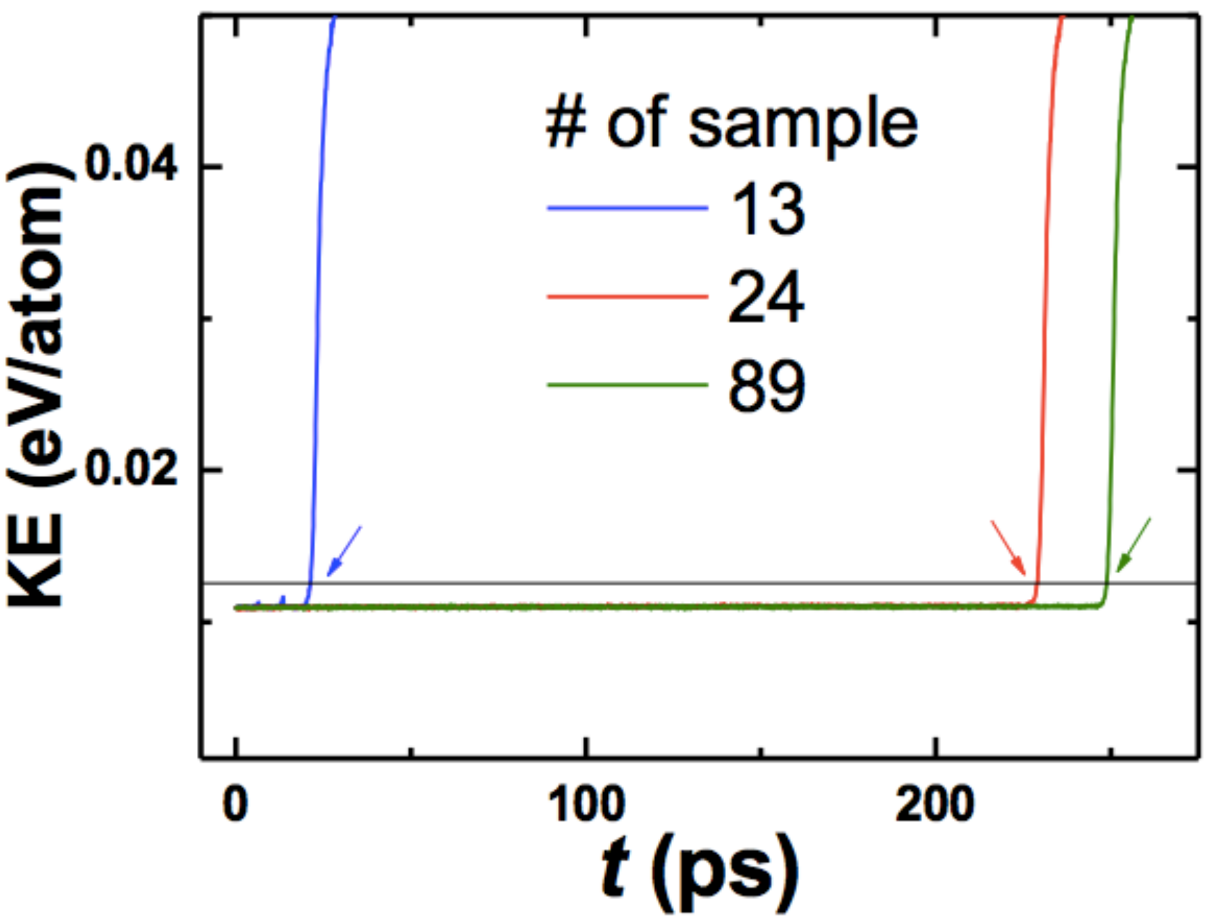


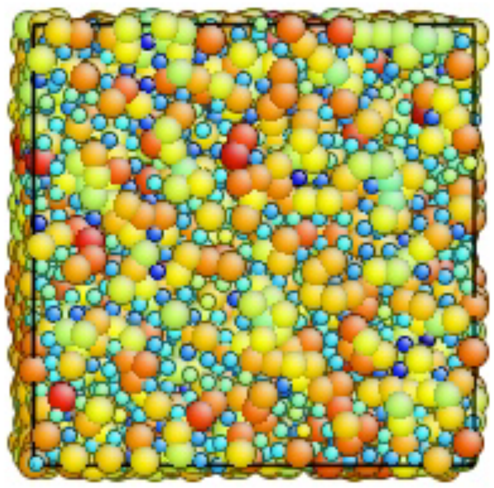
- EAM Potential
  Y. Q. Cheng and E. Ma, Prog. Mater. Sci. 56, 379 (2011)
- 16,000 atoms
- Quench rates 1K/ps and 0.01K/ps

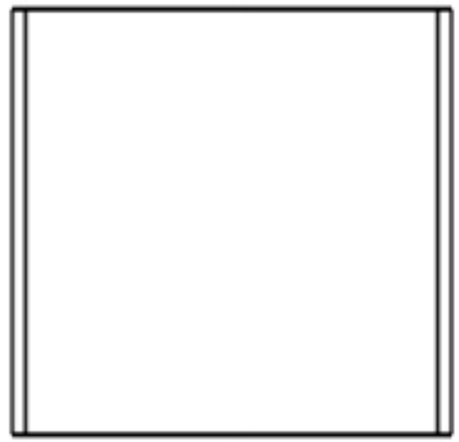



- Unlike crystalline systems, it is not possible to skip simulating the processing step

# Cavitation At Constant Strain





# Homogeneous or Heterogeneous?

- Macroscopically glasses appear isotropic and homogeneous.
- Structurally glasses are in many ways structurally similar to a liquid.
- However, cavitation in structurally identical samples with randomized initial velocities occurs at the same location implying heterogeneous nucleation.

➡ Use MD to test theories of nucleation.

➡ Measure the critical cavity size and determine how it compares to the CNT prediction.

# Classical Nucleation in Solids

- For a cavity nucleus to be unstable, the incremental elastic energy released must exceed the incremental surface energy and plastic work required to grow.

$$dF_e > dF_s + \delta W_p$$

$$4\pi K \epsilon_\infty r^2 dr > 8\pi\gamma r dr + \delta W_p(r, \dot{r})$$

- An estimate of the plastic work depends on assumptions regarding constitutive response, thermal softening and other difficult to ascertain details.

# Classical Nucleation in Solids

- We make 3 assumptions:
  - spherical cavity
  - rate independence of plastic work
  - plastic work scales with volume

$$4\pi K\epsilon_\infty r^2 dr > 8\pi\gamma r dr + \delta W_p(r,\dot{r})$$

- Under these conditions plastic work can be captured by a single parameter that determines the critical strain below which cavitation is impossible

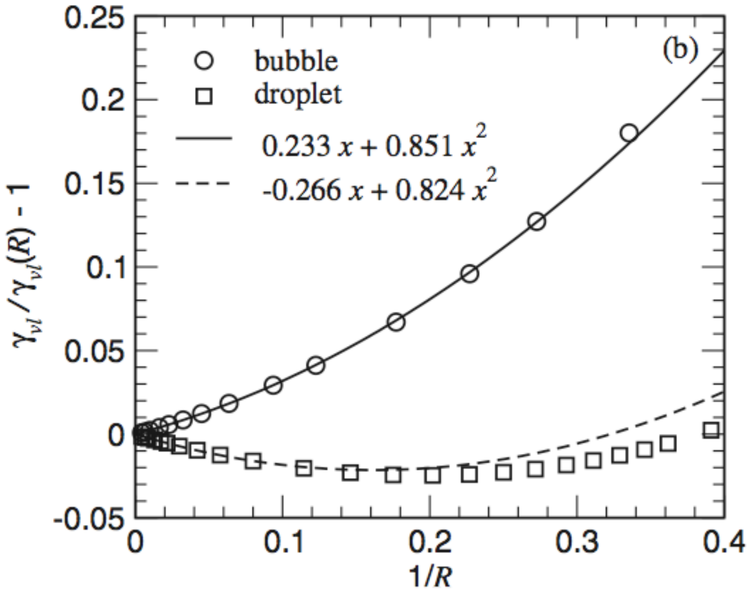
$$4\pi K\left(\epsilon_\infty - \epsilon_c\right) r^2 dr > 8\pi\gamma r dr$$

# Radius Dependence of Surface Energy "Tolman Length"

- It is known that for small nuclei (bubbles) the surface energy varies with bubble size

$$\gamma = \frac{\gamma_\infty}{1 + \frac{2\delta}{r}}$$

For work on Tolman length in liquid see An, Garrett, Samwer, Liu, Zybin, Luo, Johnson, Goddard, Journal of Physical Chemistry Letters, 2, 1320-1323 (2011)




Block, Das, Oettel, Viranu and Binder, *Curvature dependence of surface free energy of liquid drops and bubbles: A simulation study*, JCP, 133, 154702 (2010)

# Classical Nucleation in Solids

$$\gamma = \frac{\gamma_\infty}{1 + \frac{2\delta}{r}}$$

- We can infer a critical cavity size

$$r^* = \frac{2\gamma_\infty}{K\left(\varepsilon - \varepsilon_c\right)}$$

$$r_c = r^*\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{4\delta}{r^*}} - \frac{2\delta}{r^*}\right)$$

- And a critical free energy fluctuation for nucleation

$$F_c \equiv 4\pi\gamma r_c^2 - \frac{4}{3}\pi K(\epsilon_\infty - \epsilon_c) r_c^3$$

# Parameters in Theory

$$R = f \exp\left(-\frac{F_c}{k_B T}\right)$$

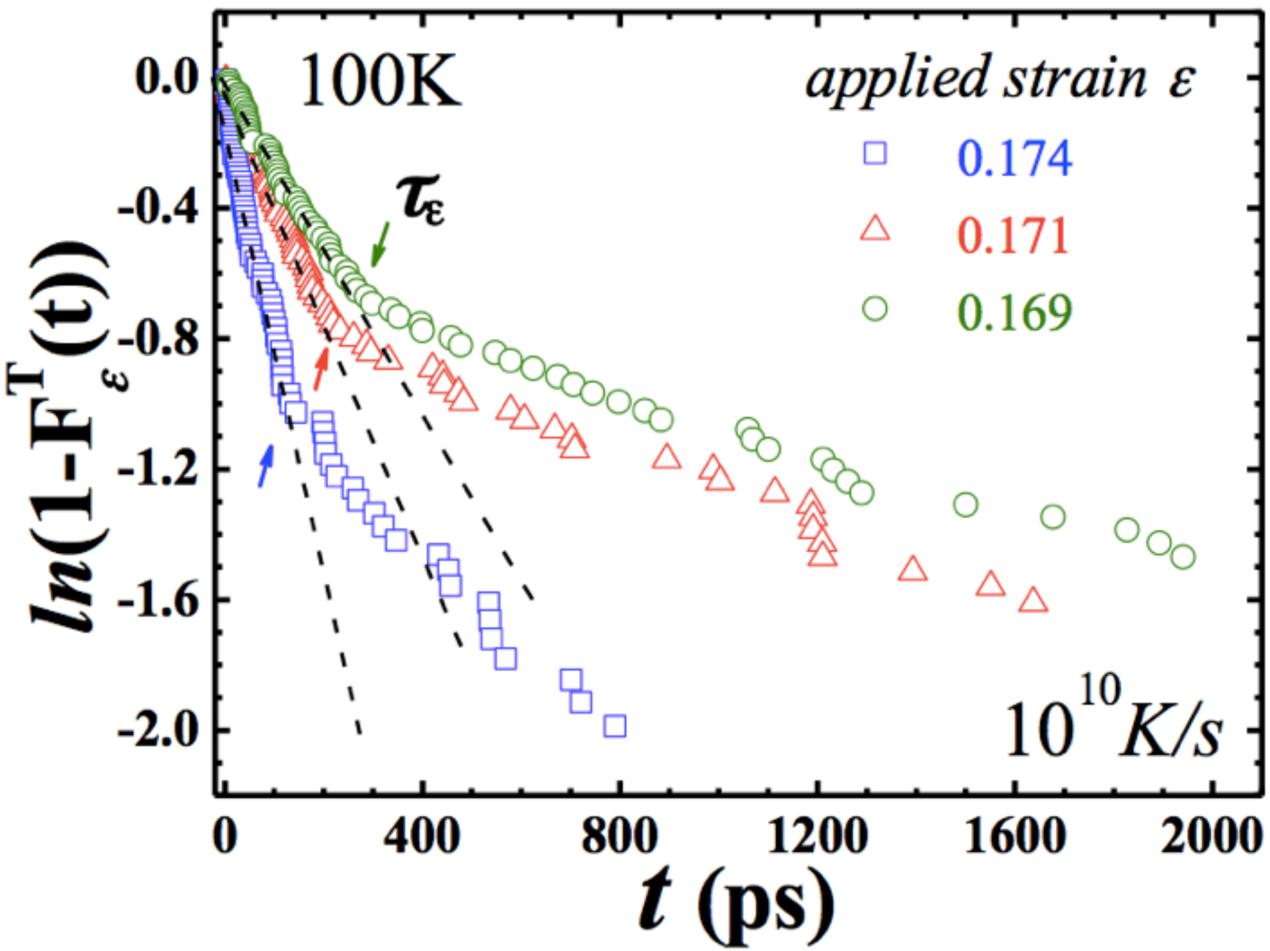
$$F_c \equiv 4\pi\gamma r_c^2 - \frac{4}{3}\pi K(\epsilon_\infty - \epsilon_c) r_c^3$$

$$r^* = \frac{2\gamma_\infty}{K(\varepsilon - \varepsilon_c)} \qquad r_c = r^*\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{4\delta}{r^*}} - \frac{2\delta}{r^*}\right)$$

- Independent variables $k_B T, \epsilon_\infty$
- Directly measurable parameters $\gamma_\infty$=0.080 eV/Å$^2$
  $K$=106 GPa
- From T scaling $f = 0.1 ps^{-1}$
- From dKE/d(PV) during expansion $\varepsilon_c = 0.02$
- Tolman Length is fitted $\delta$=1.15Å

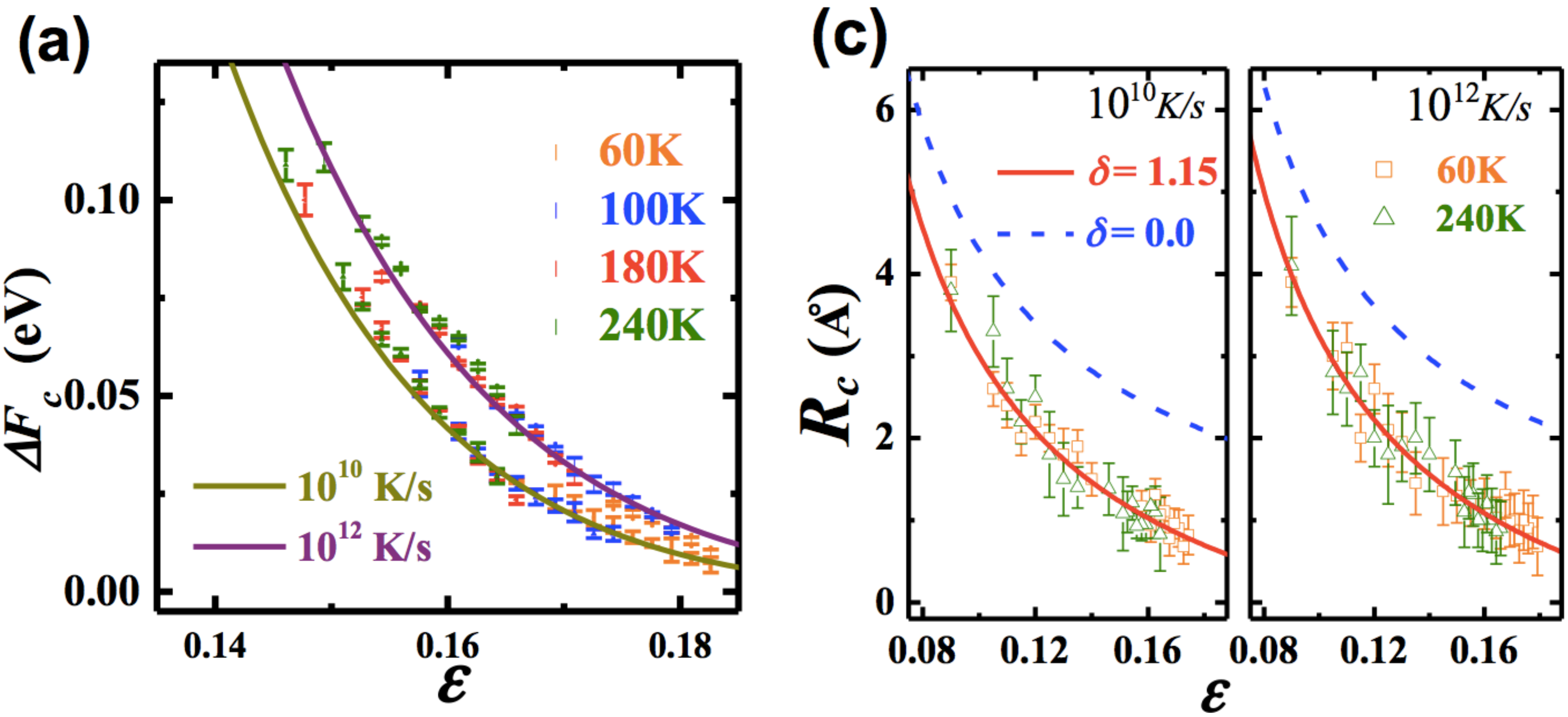
# Cavitation: Strain and Hold

Log of fraction of samples not yet cavitated at a given time for a given applied remote strain.




Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)

# Theory vs. Simulation: Prior to Aging




Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)

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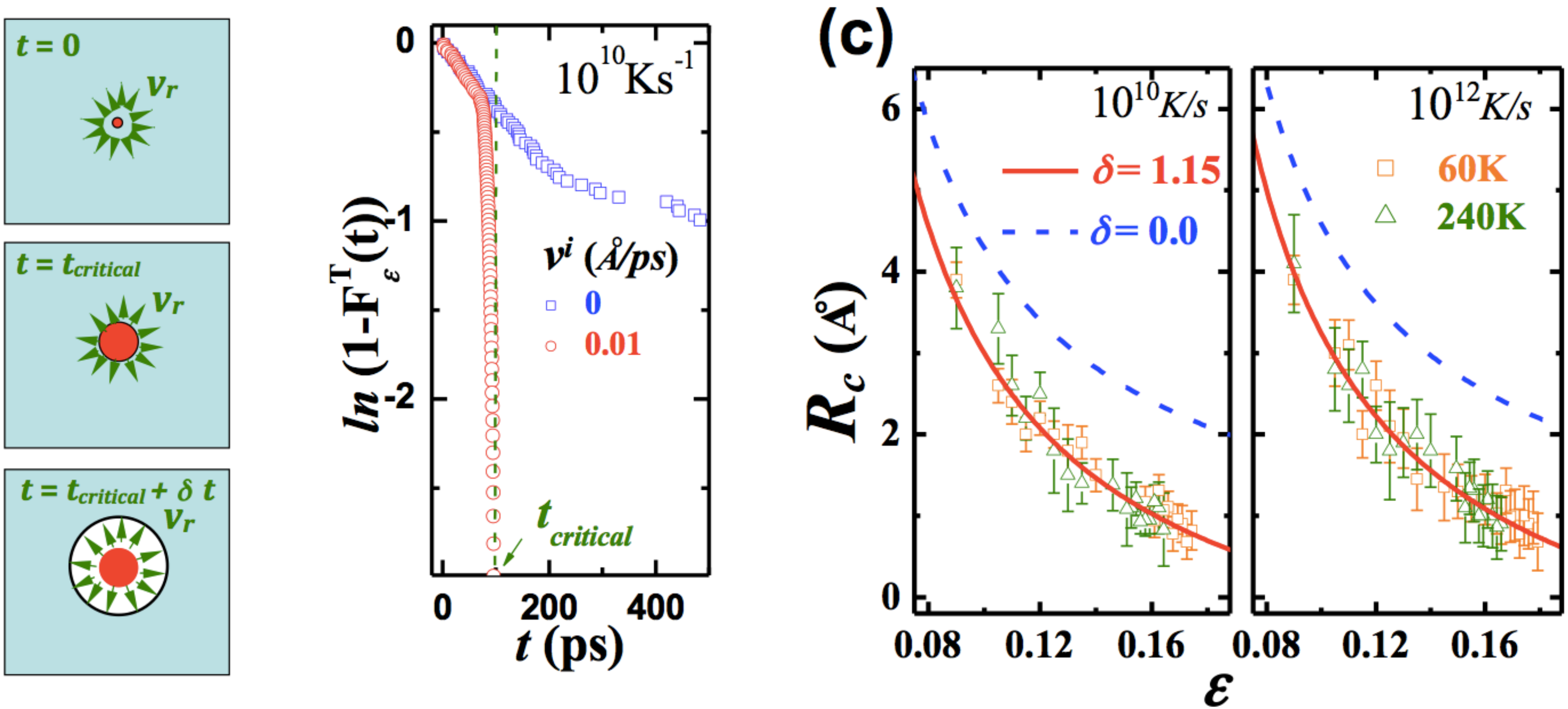
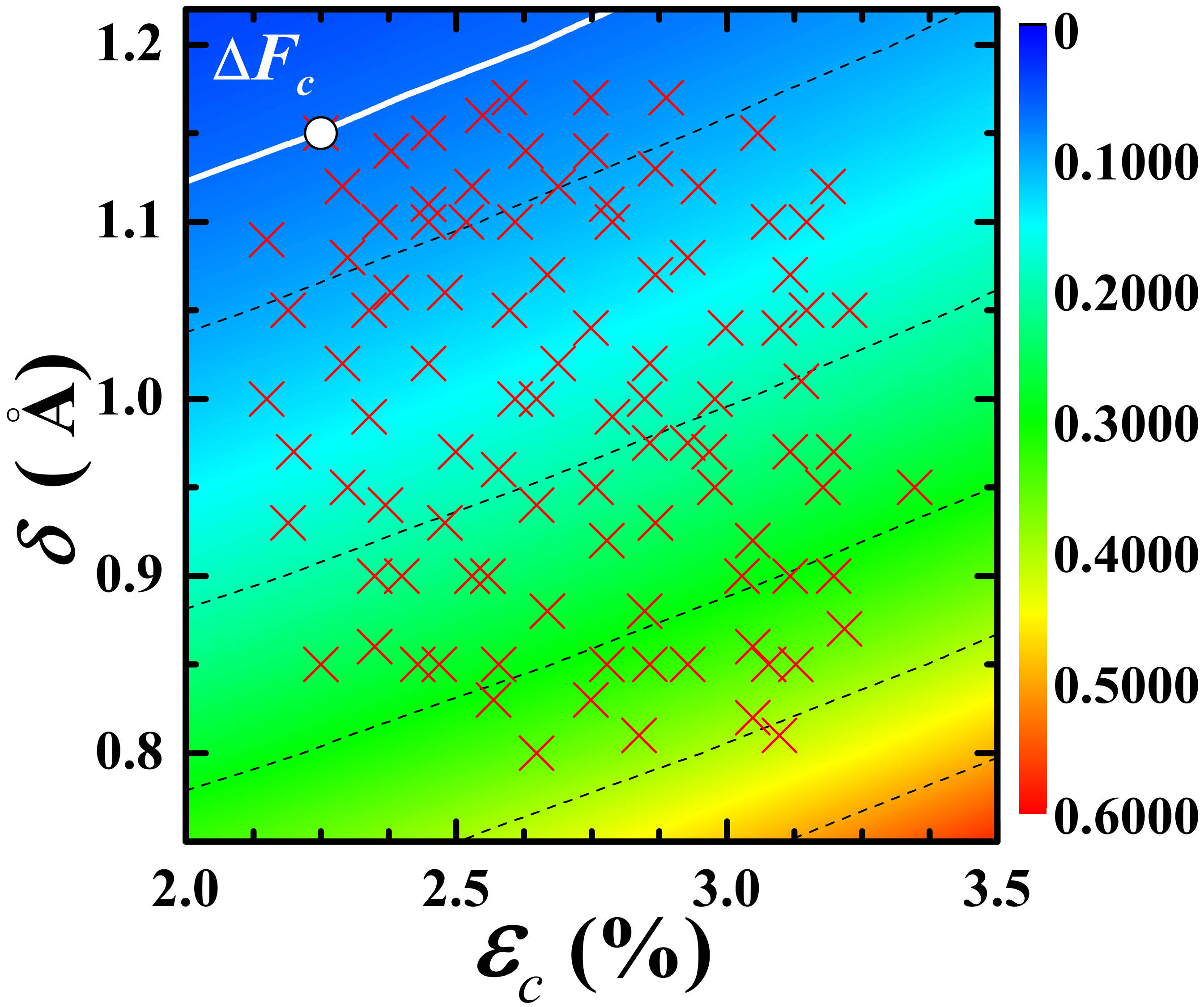



Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)

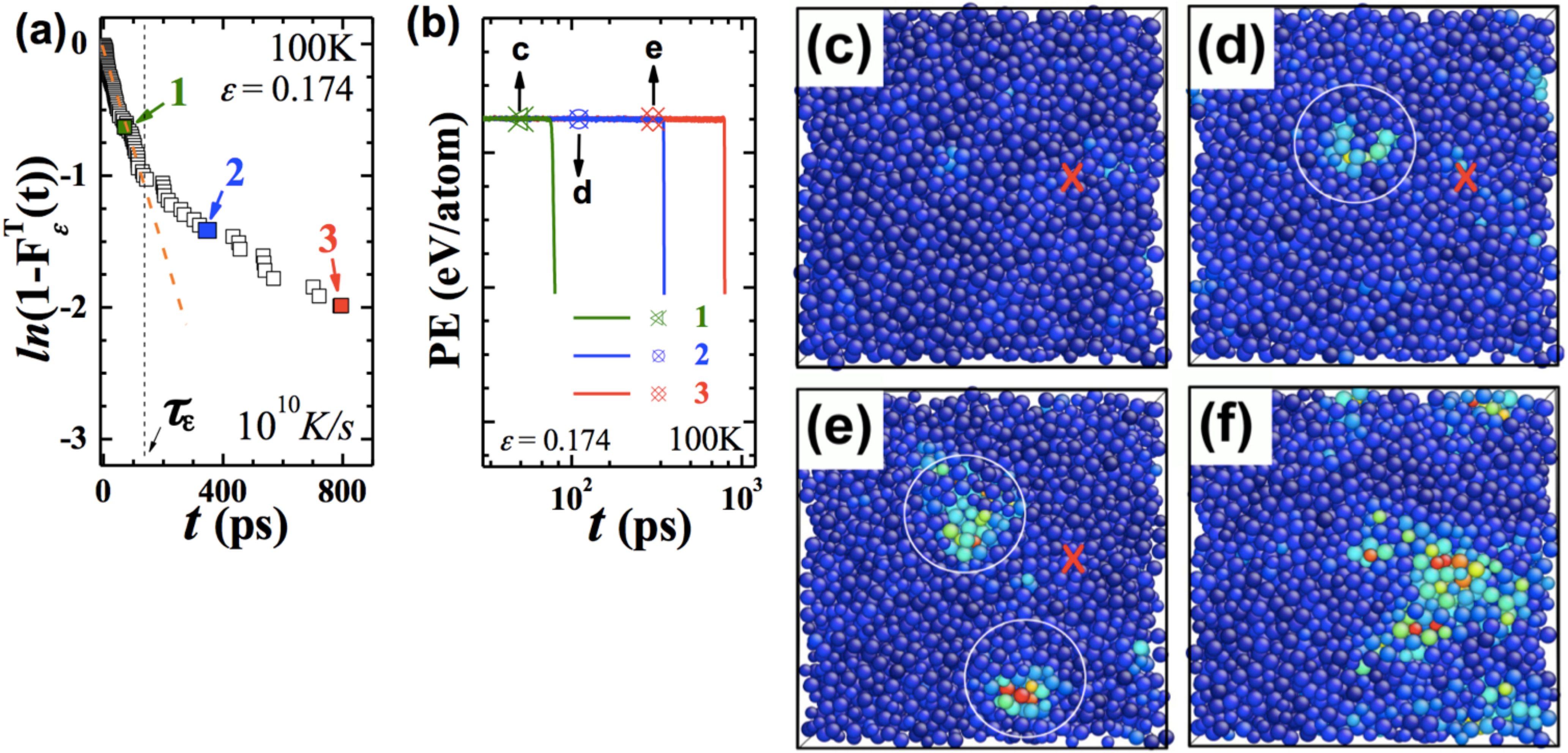
# Nature of Local Fluctuations




- Low correlation between Tolman length and critical strain (<0.13)
- 3.4 times more sensitive to Tolman length than critical strain.

Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)

# Onset of Aging: STZ activity

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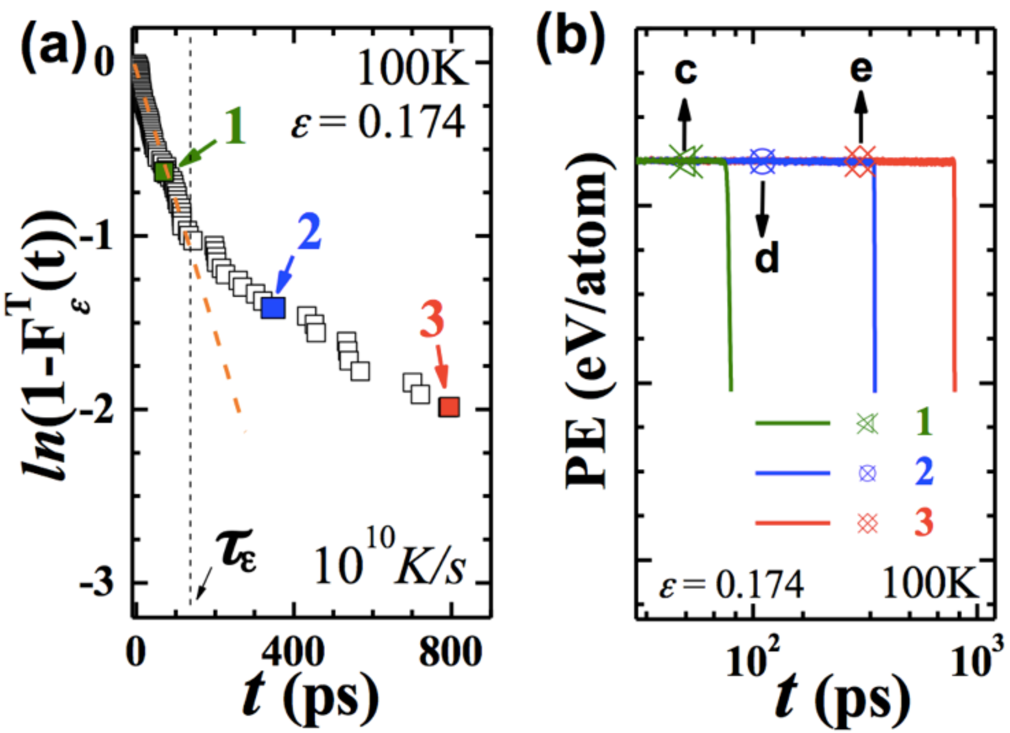
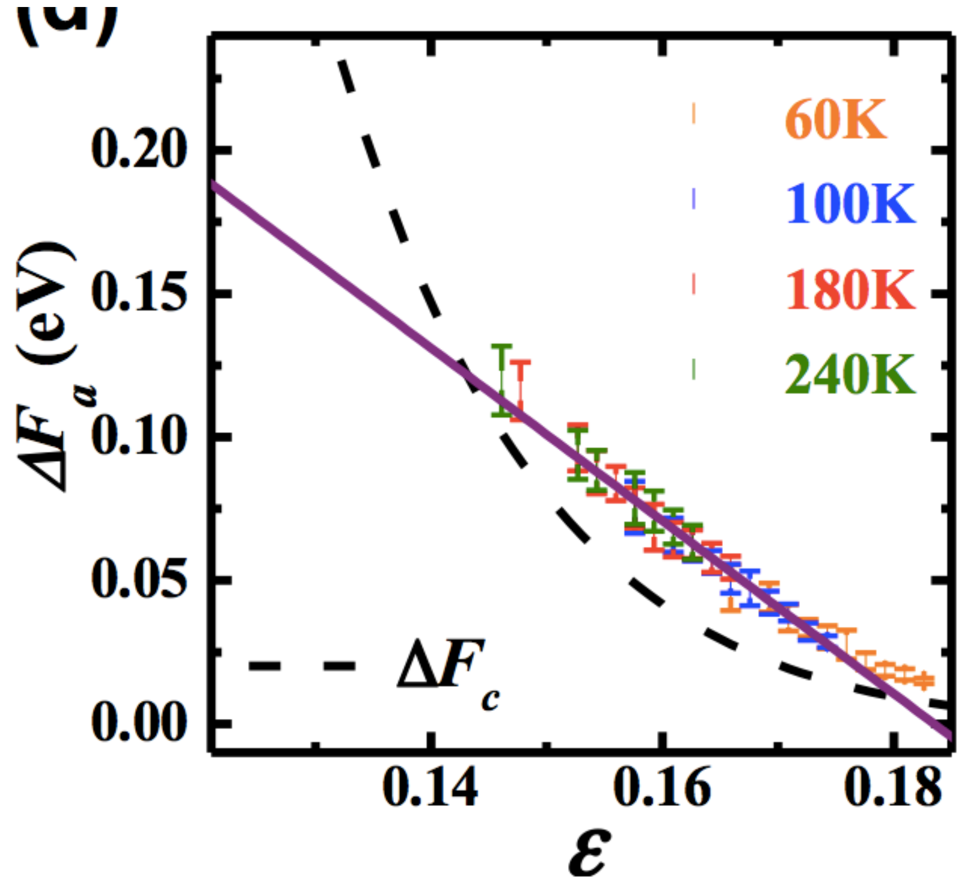
# Onset of Aging: STZ activity




$$R_a = f_a \exp\left(\frac{-\Delta F_a}{k_B T}\right)$$




- Measured activation volume: 4.5Å$^3$
- Extrapolated zero strain activation energy: 0.55eV

Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)

# Conclusions

- Cavitation may play a crucial role in the fracture process zone.
- Plastic dissipation suppresses cavitation at low strains.
- Barrier to cavitation is reduced due to "Tolman Length" effects that decrease surface energy at small radii.
- At short time scales Poissonian rate is predicted by CNT.
- The critical radius under hight tensile strain 14%-18% is very small (1Å-4Å) as confirmed by comparison to simulation.
- Spatial fluctuations in surface energy and, to a lesser degree, susceptibility to plasticity result in heterogeneous nucleation.
- Aging coincides with STZ activity for which we extract an activation barrier and activation volume.

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- STZ activation is favored over cavitation at low strains.
- Acknowldegement: NSF DMR 0808704 and 1107838

Guan, Lu, Spector, Valavala, Falk, PRL 110, 185502 (2013)