KITP Nonequilibrium14, Sept. 22 – Dec. 12, 2014

Bridging the Mesoscale Gap

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Oct. 3, 2014

Workshop: Dislocations and Plasticity
ITP – UCSB, March 27-29, 1997

Explore commonalities of different problem -- connecting a few dots (→ JSL talks)

avalanches, intermittency, non- linear, non-equilibrium response

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primary example:

shear viscosity of supercooled liquids

additional examples:

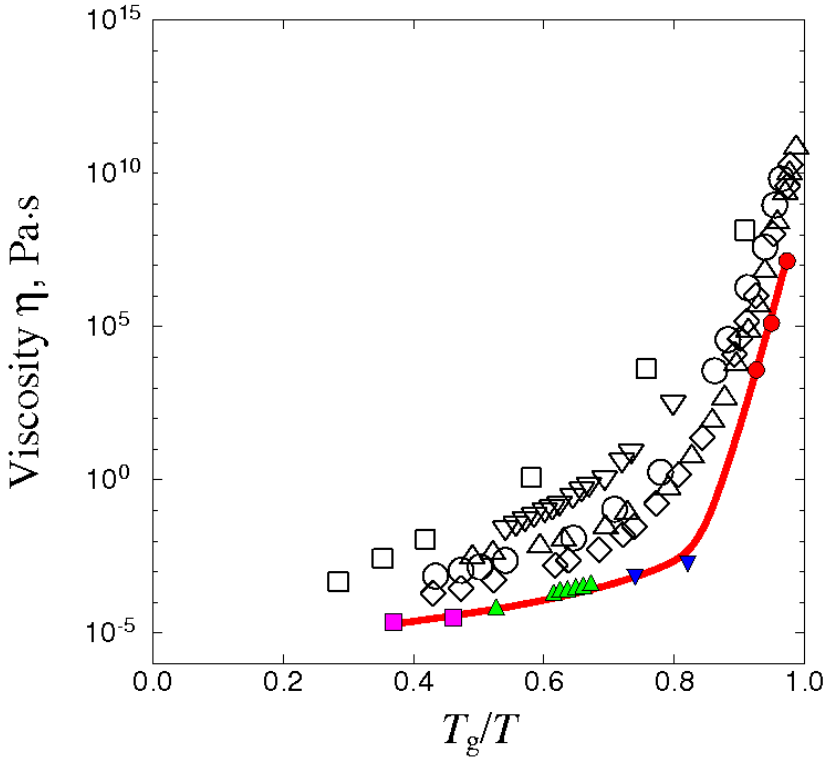
yielding, creep, corrosion, cement

MSS Frontier (bridging the mesoscale gap)

predicting macro behavior using micro input

Fragile behavior of glass formers

(sharp increase in shear viscosity arouns T_x)



molecular-level understanding of macro behavior:

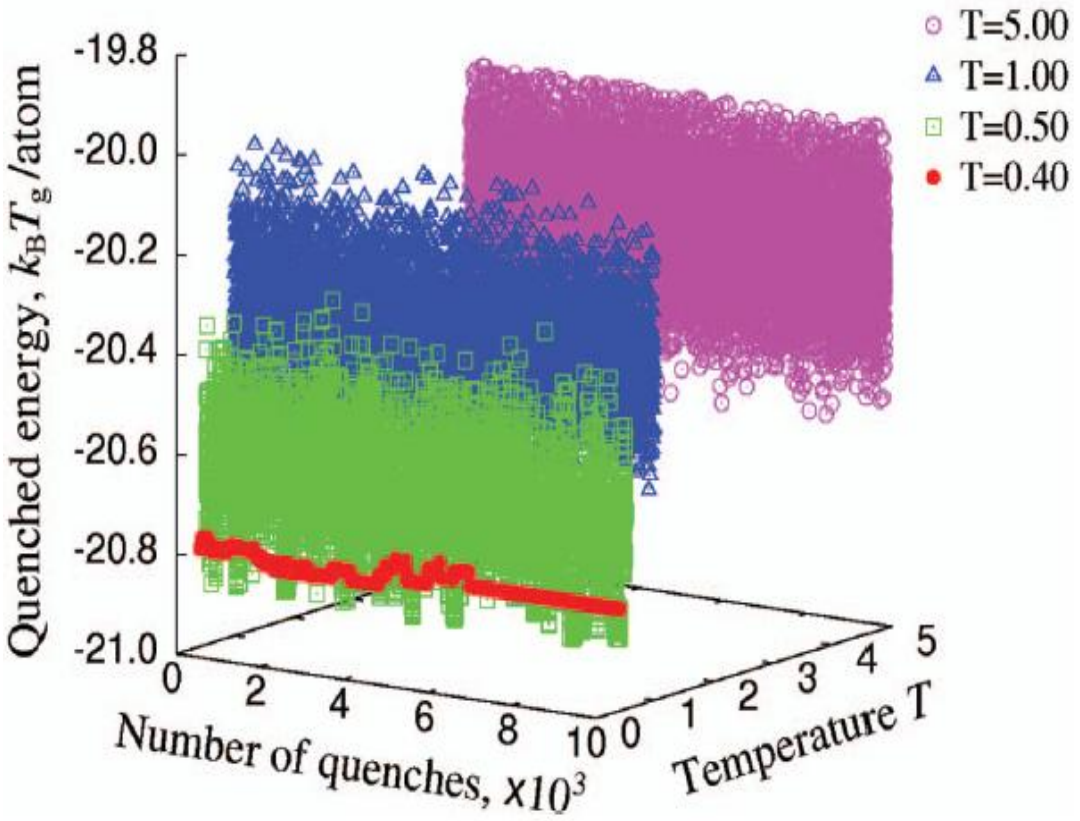
Energetics and atomic configurations of supercooled states (**1**)

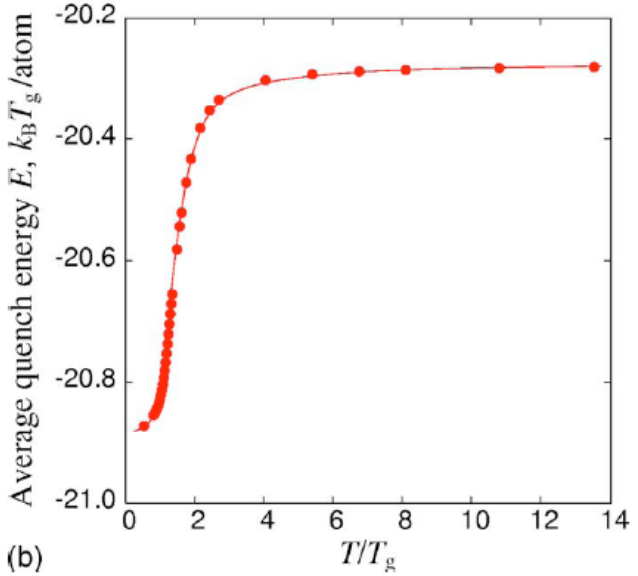
Transition-state (reaction) pathway sampling (**2**)

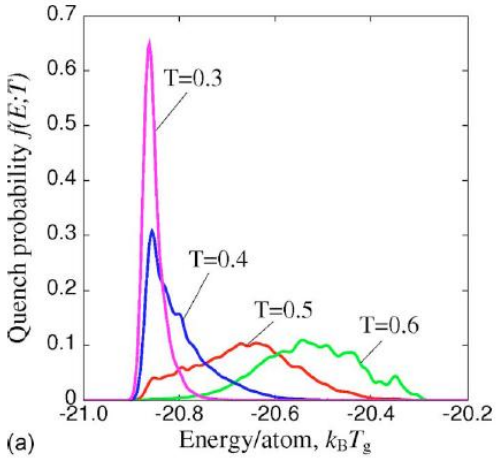
*Linear response theory of transport (**3**)*

1

Inherent Structure of Supercooled Liquids

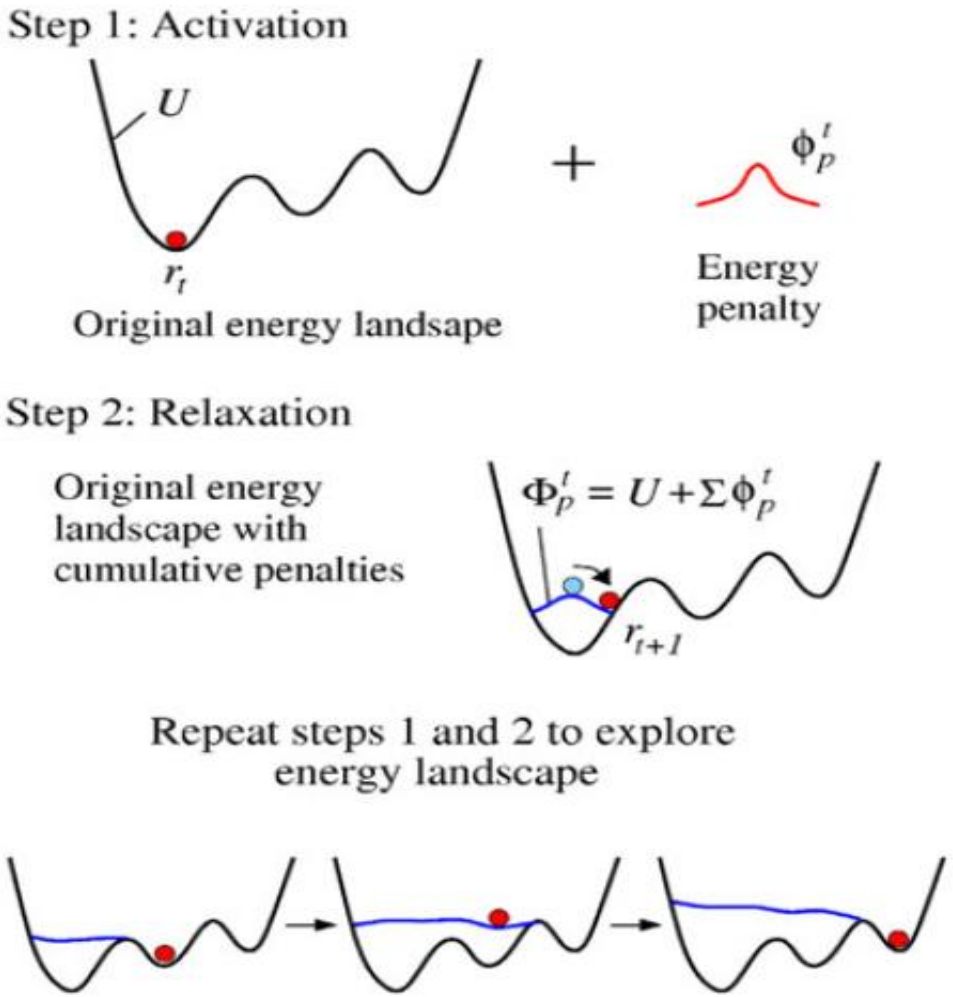






Kushima JCP 2009

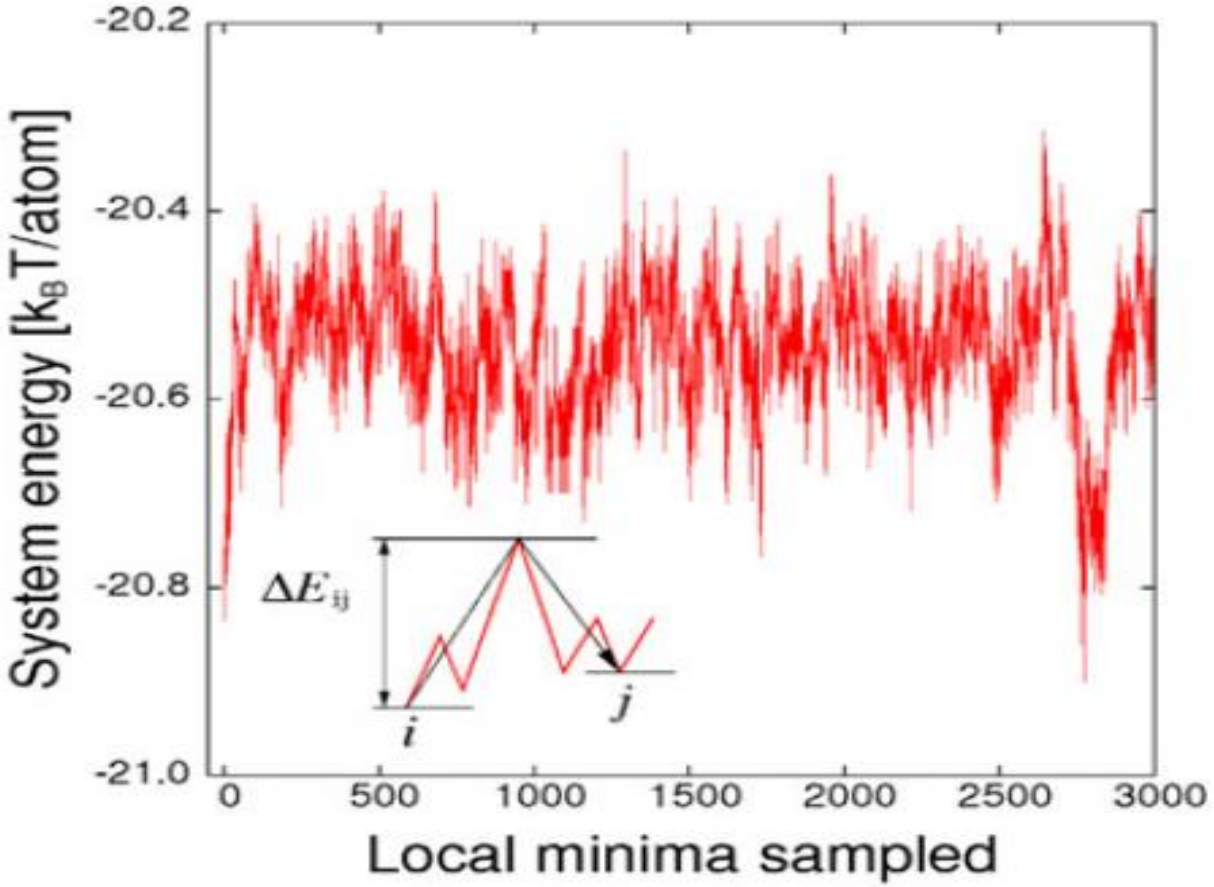
Tansition State Pathway Sampling – metadynamics (ABC)



Kushima JCP 2009

2

Transition State Pathway sampled at T = 1.35 T_g

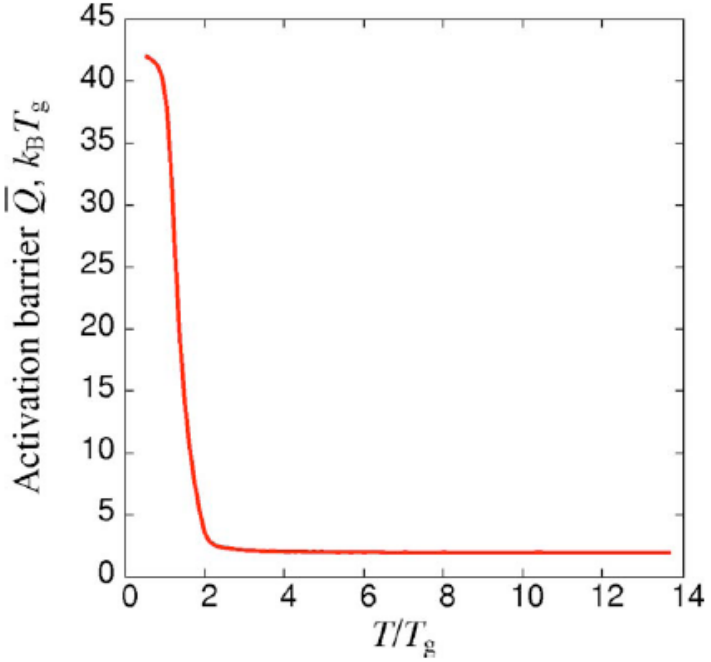


(a) Extract effective activation barrier in the spirit of TST
(b) Direct input into a network model (Green-Kubo calc.

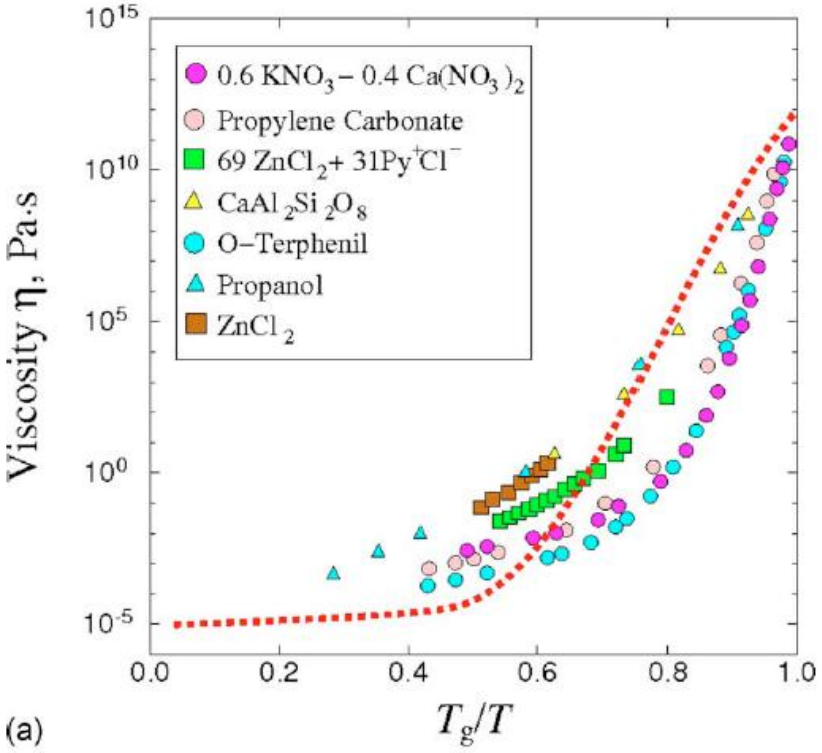
Kushima JCP 2009

3

activation barrier analysis (heuristic model)



$$\eta(T) = \eta_0 \exp[Q(T)/k_B T]$$



Kushima JCP 2009

3 Linear Response (Green-Kubo) theory with network model

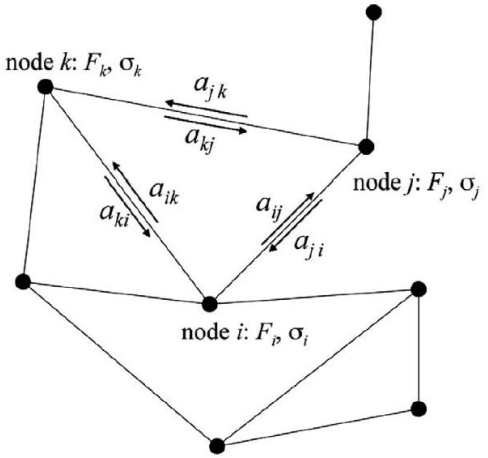
$$\eta(T) = \frac{V}{3k_B T}\int_0^{\infty}\left\langle \sum_{x<y}\tau^{xy}(t)\tau^{xy}(0)\right\rangle dt$$

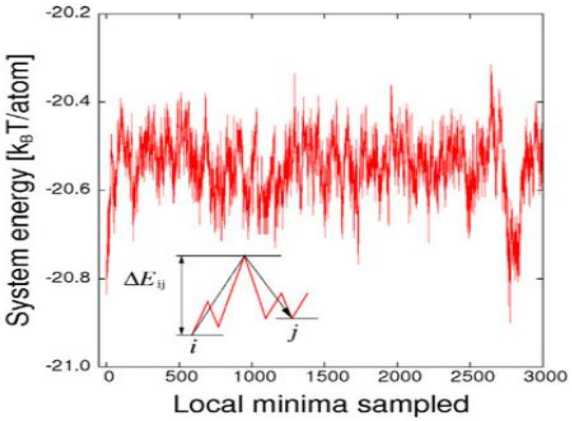
$$\langle \sigma(t)\sigma(t+\tau)\rangle = \sum_i P_i\sigma_i g_i(\tau)$$

$$g_i(\tau) = \sum_j \int_0^{\tau} d\tau' a_{ij} s_i(\tau') g_j(\tau-\tau') + s_i(\tau)\sigma_i$$

$$a_{ij}(T) = v_0 \exp\left(-q_{ij}/k_B T\right)$$

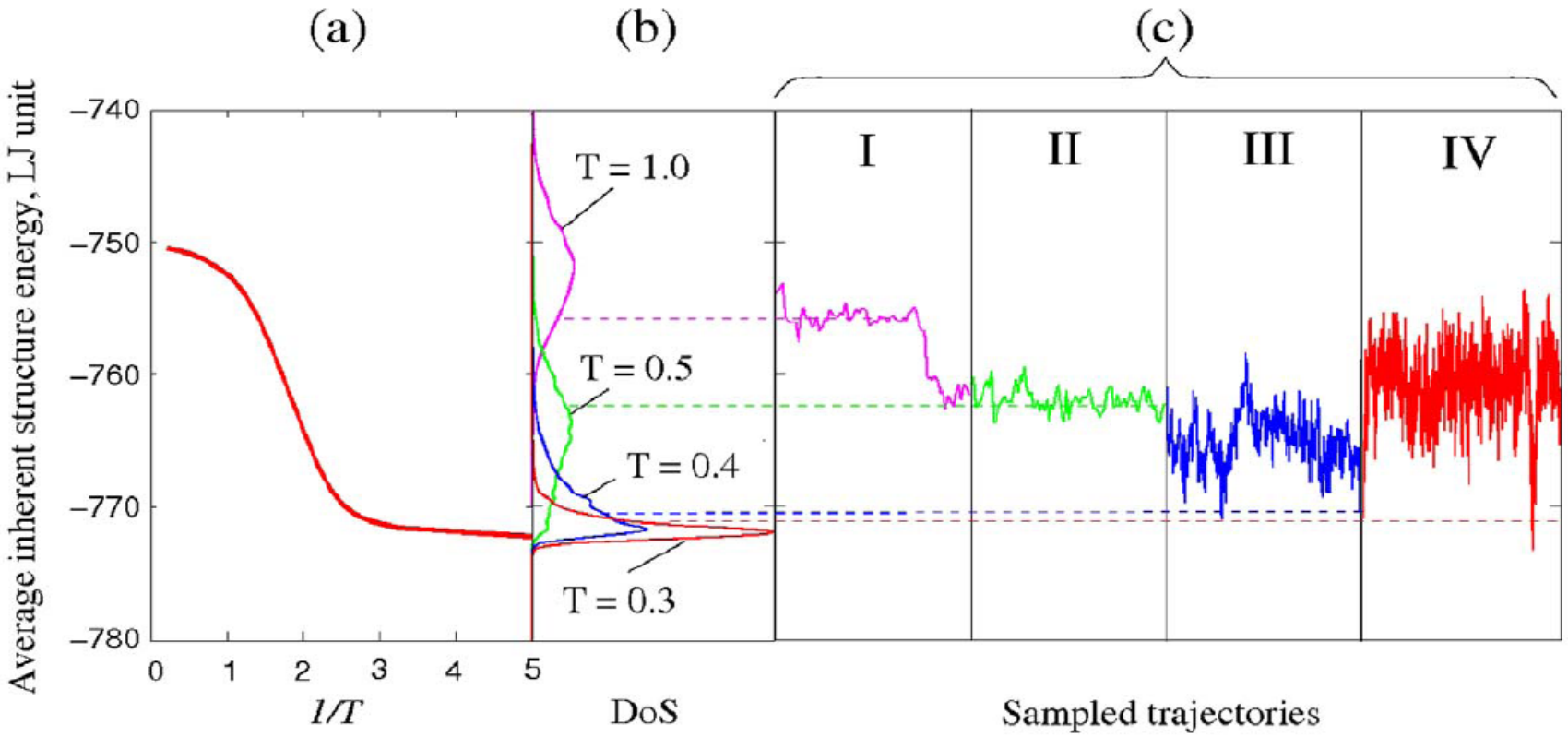
$$s_i(\tau) = \exp(-\tau a_i), \quad a_i \equiv \sum_j a_{ij}, \quad a_{ii} = 0.$$





Li , PLoS ONE 2011

3 Analysis divided into 4 temperature ranges



Li PLoS ONE 2011

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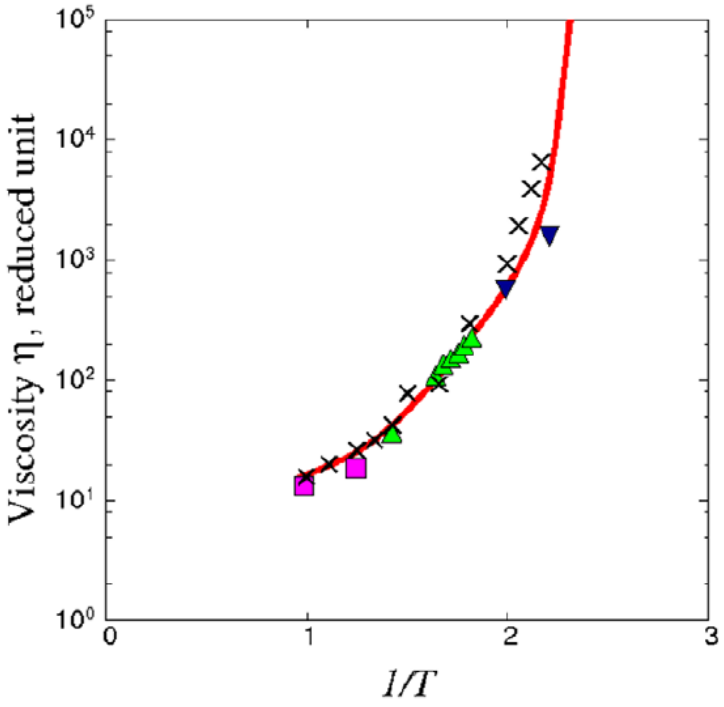
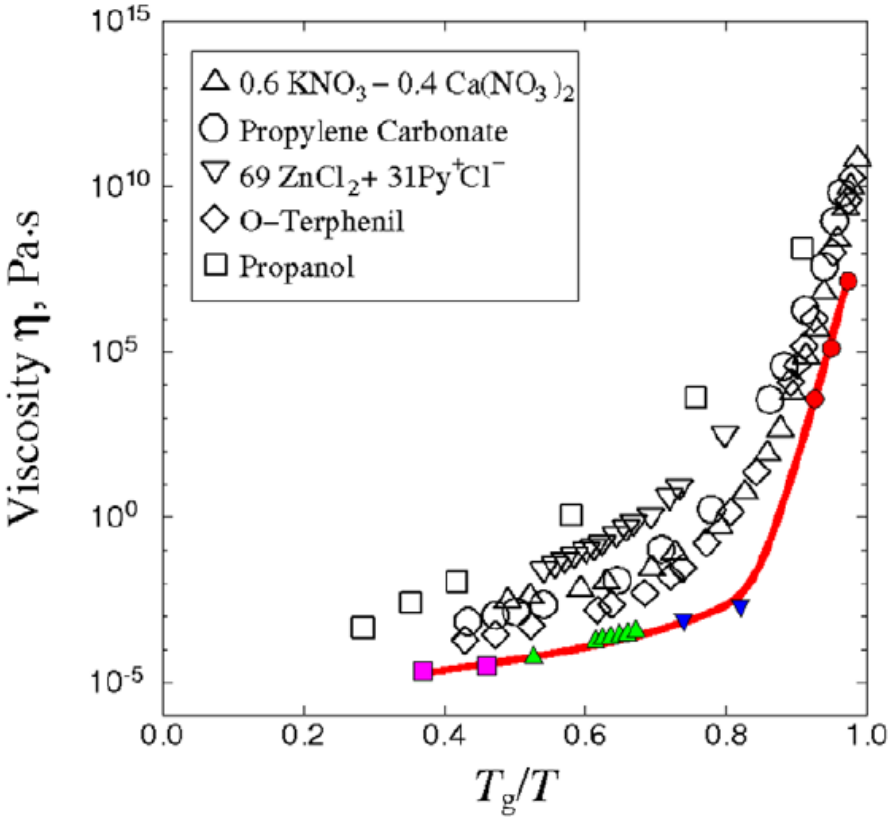
Validation against MD and experiments



MD validation at low-moderate viscosity



Experimental comparison

Kushima EPJ-B 2011

Issues to ponder (connecting a few dots)

“Fragility” as a consequence of energy landscape?

Relevance of TSP (mobility/transport) is essential

Challenge to simulation methodology

Challenge to theoretical approaches

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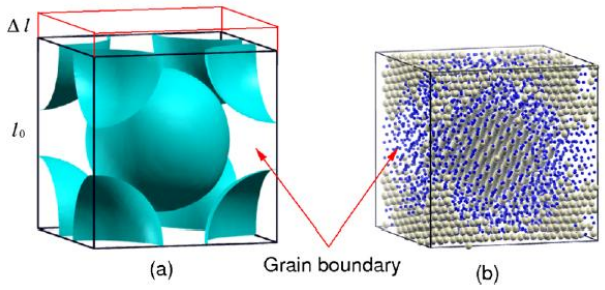
JSL talk on Oct. 16

Applicable to deformation under stress?

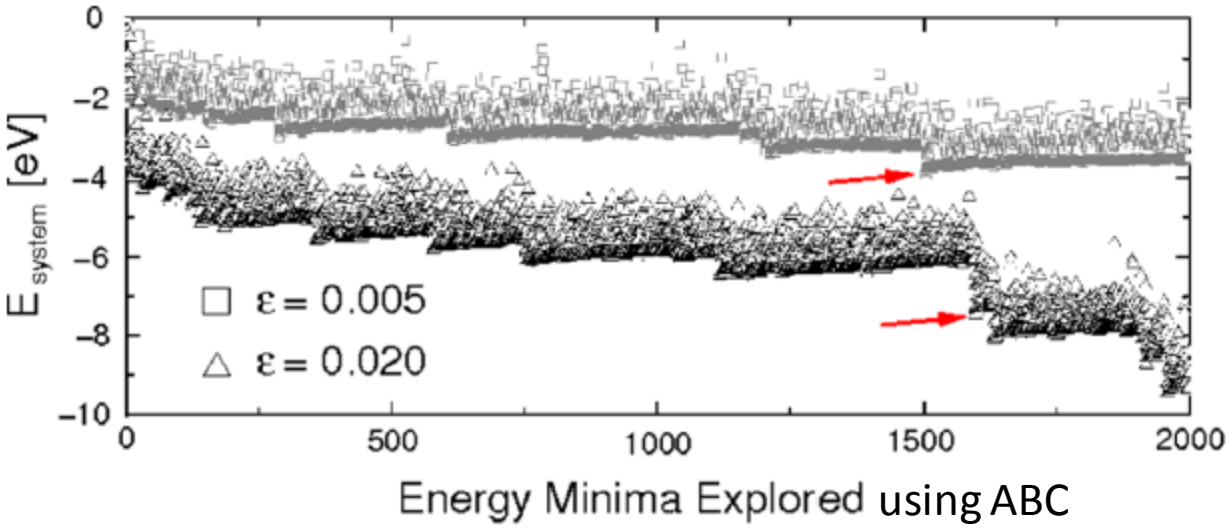
Using TSP sampling (ABC) to study time evolution of a solid under deformation at finite T

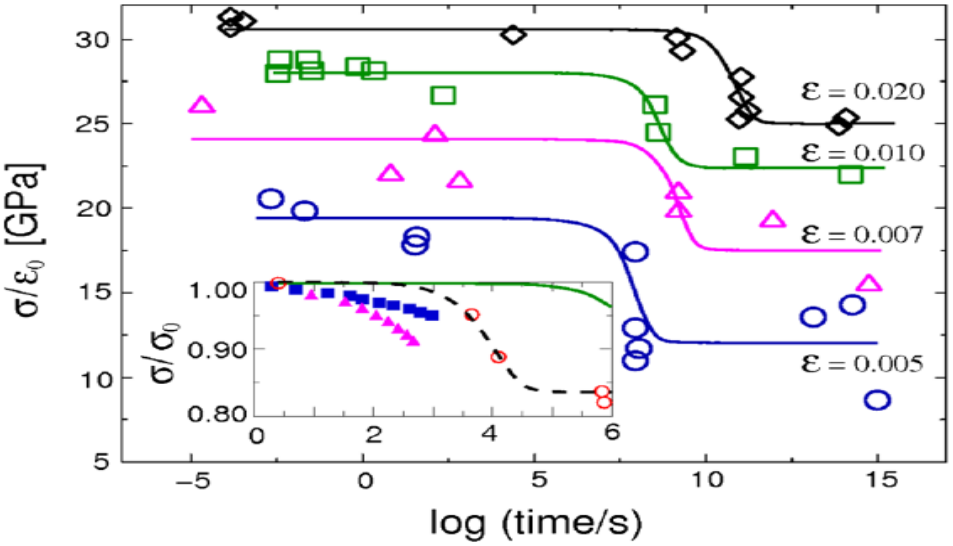
Stress relaxation in uniaxially strained nanocrystal –

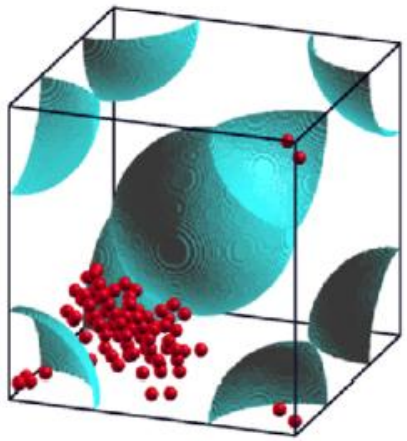
Lau, PRL 2010

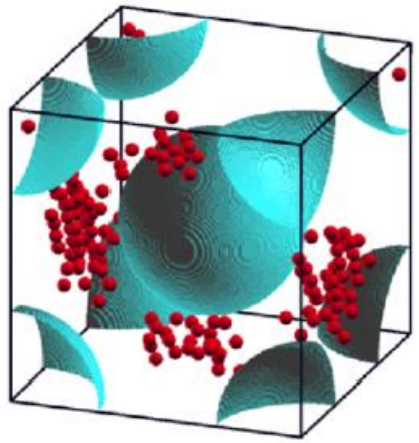


$$\Delta t = \left[\nu_0 \exp\left(-\frac{\Delta U}{k_B T} \right) \right]^{-1}$$

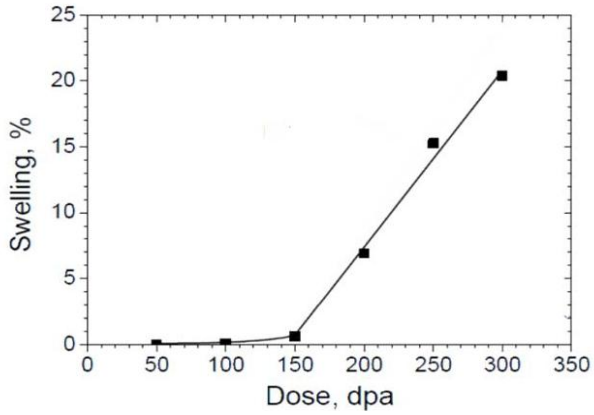


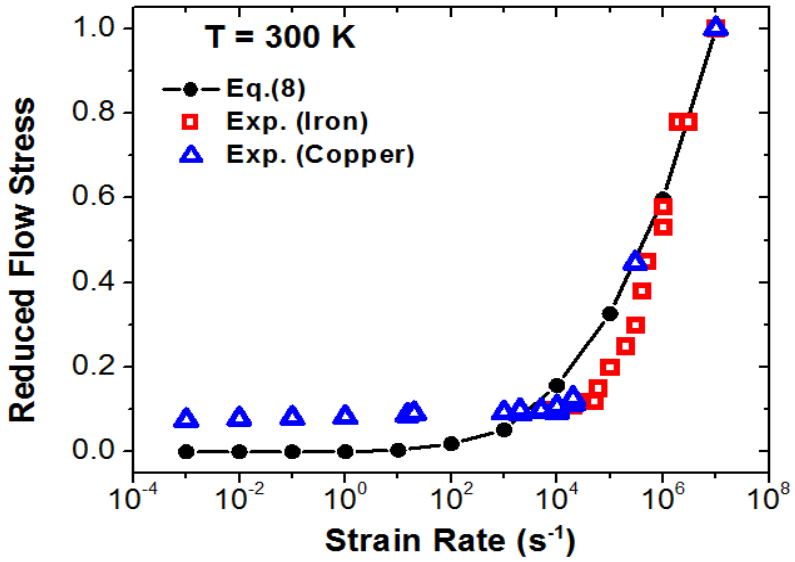


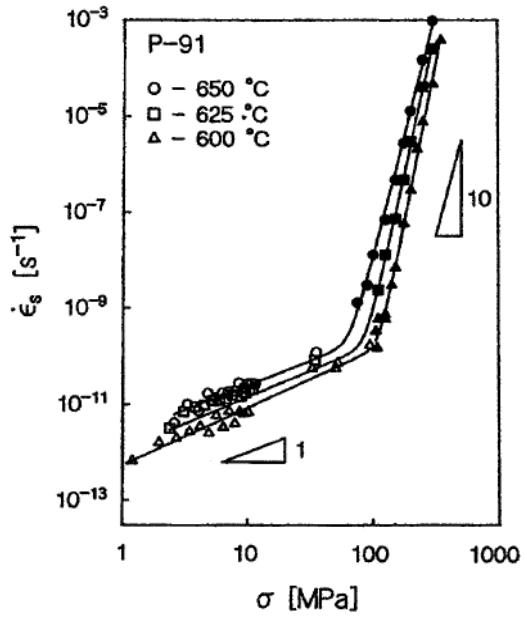


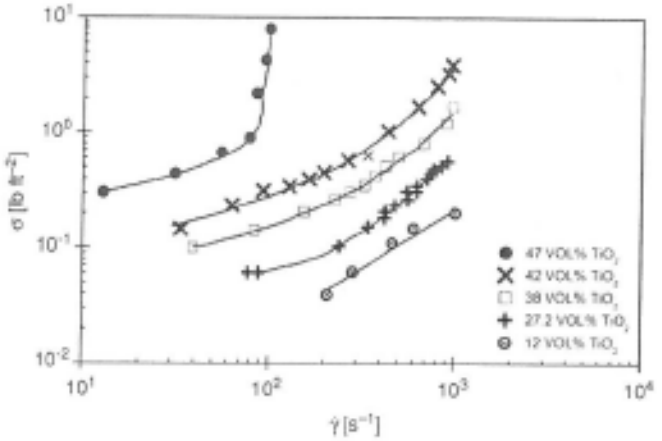


additional phenomena showing upturn/crossover behavior (macroscale)



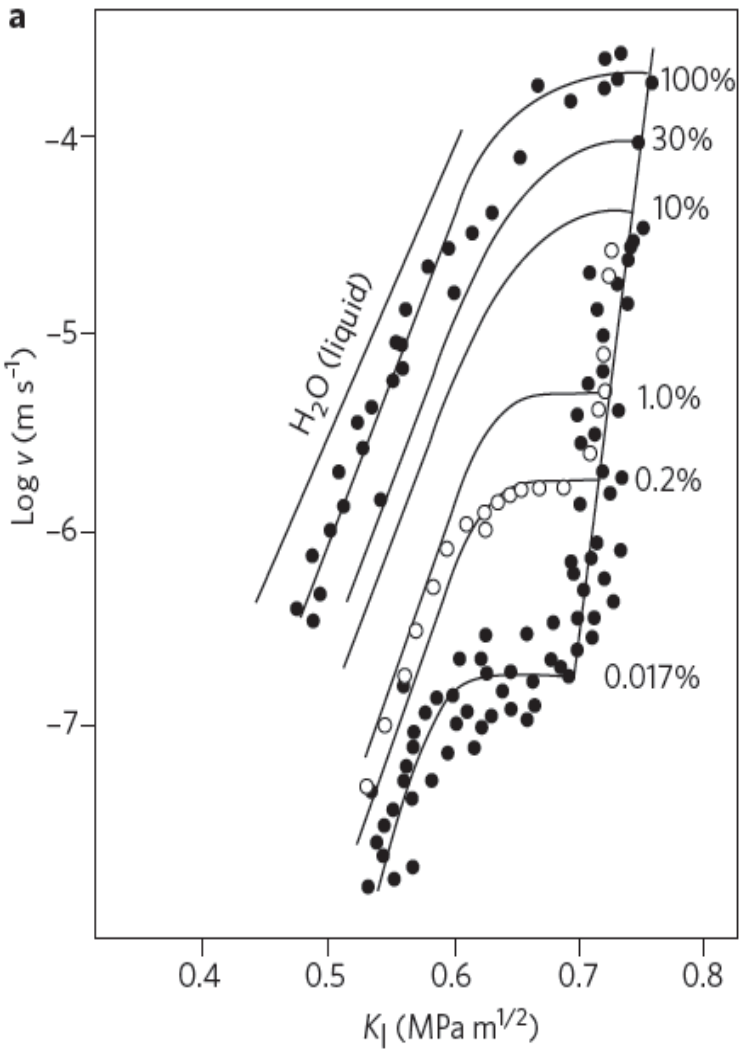


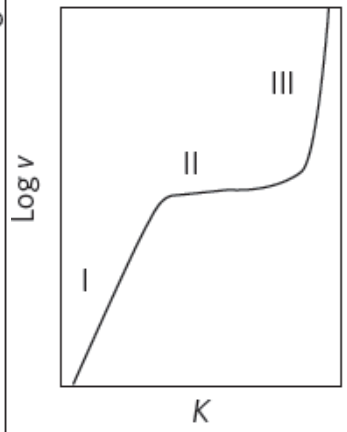


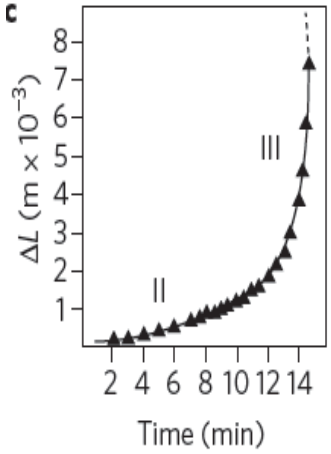


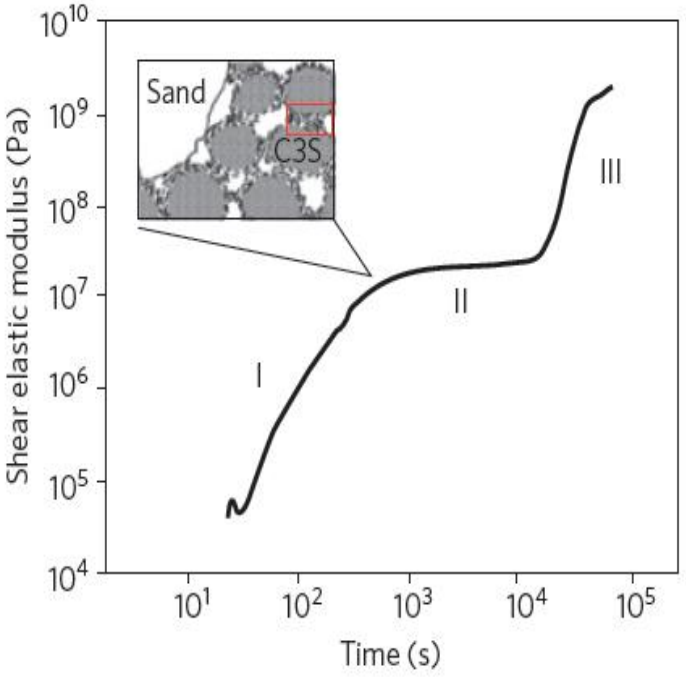
Shear thickening in a dense suspension

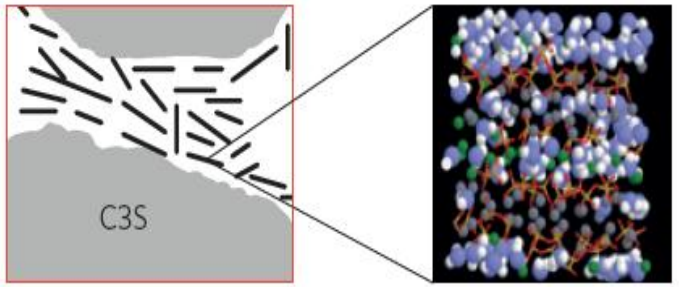
3-stage responses – stress corrosion cracking and cement setting











NMAT 2013

Collaborators

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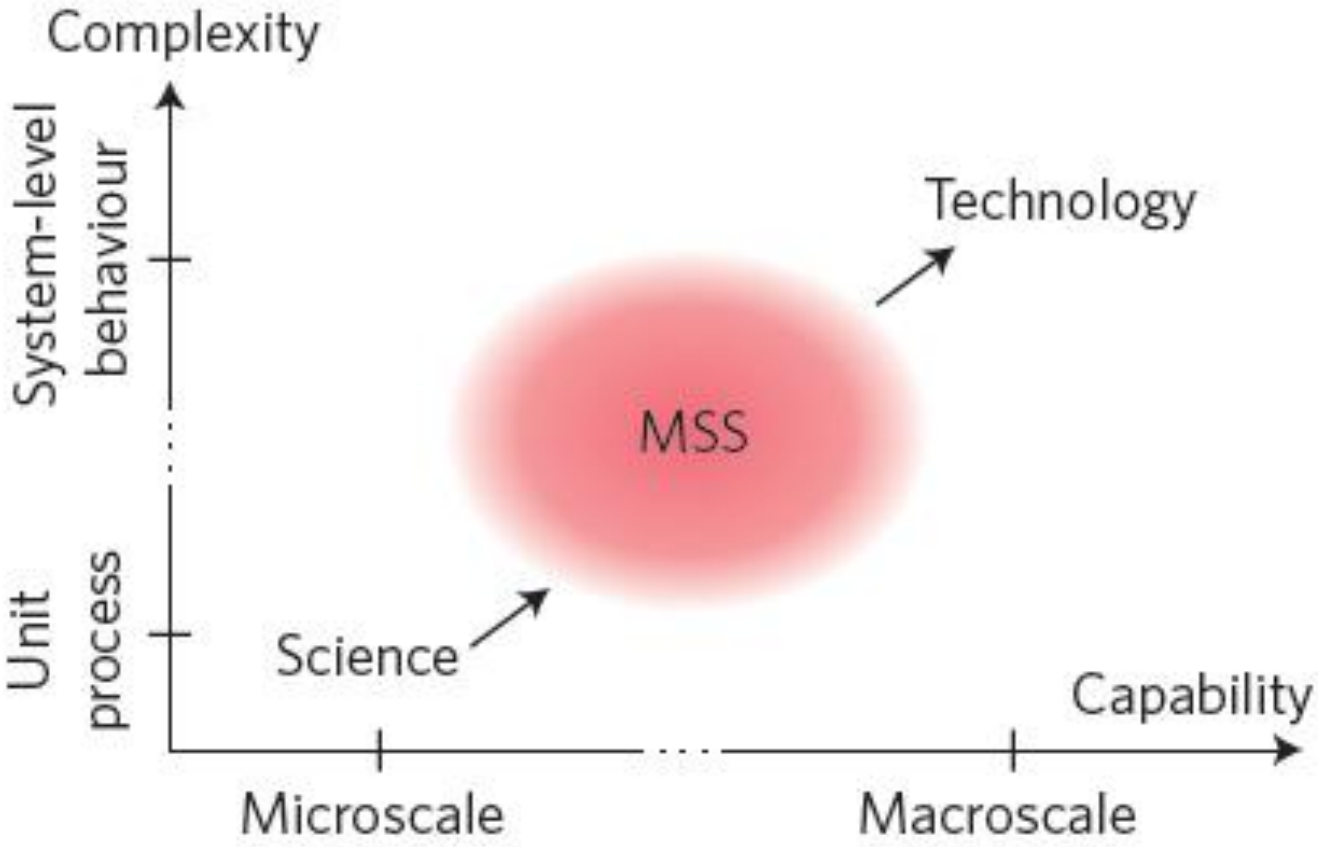
The Mesoscale Science (MSS) Frontier



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Science push w/ technology pull