

UCSB - KITP
Physics of Glasses (Glass 10)
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Atomistic Models of Slow Dynamics: Calculating Viscosity, Fragility and Creep

Sidney Yip

Nuclear Science and Engineering
and Materials Science and Engineering
MIT

Well-known temperature variation of viscosity of supercooled liquids in need of theoretical understanding - calculate $\eta(T)$ using interatomic potentials

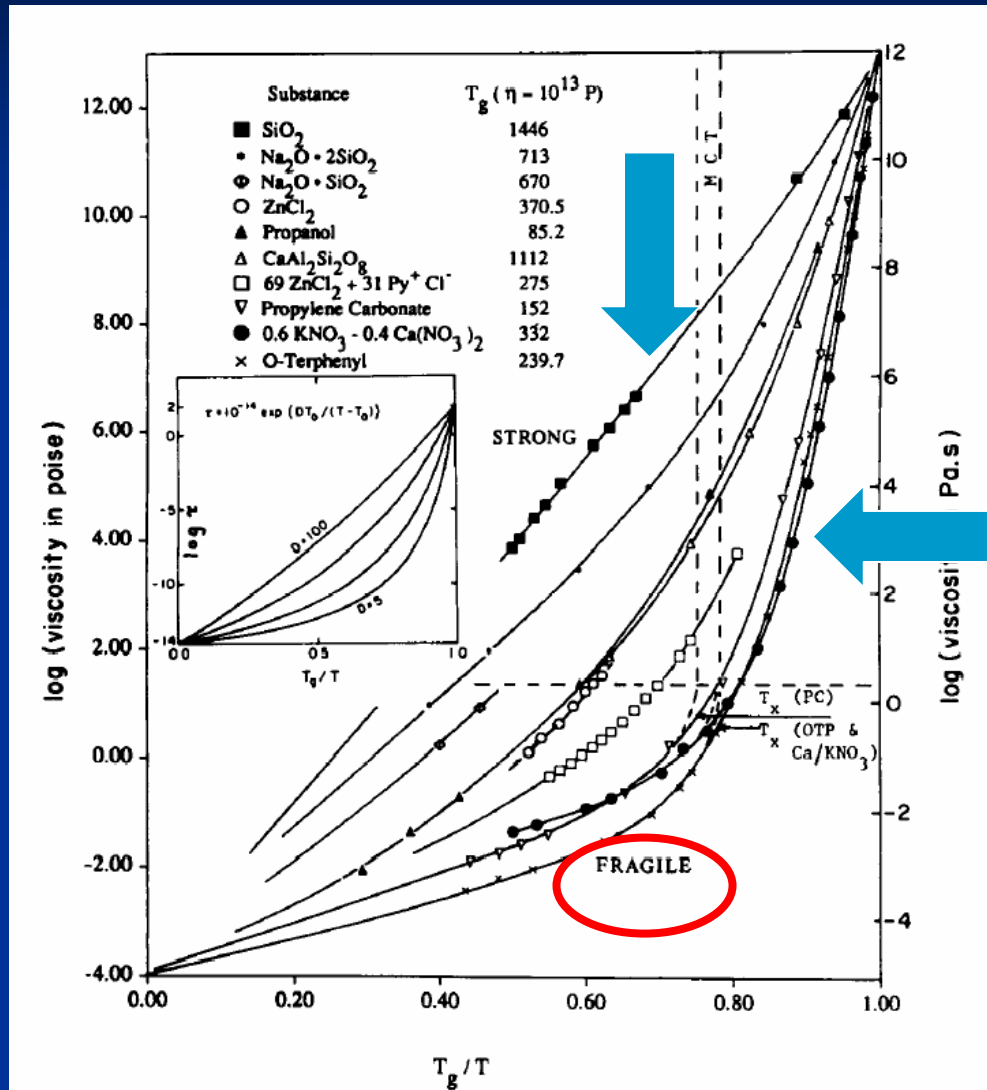
An approach, applied to BL-J and silica models, suggested in 2009

Fragility is universal to viscous liquids (dynamical crossover)

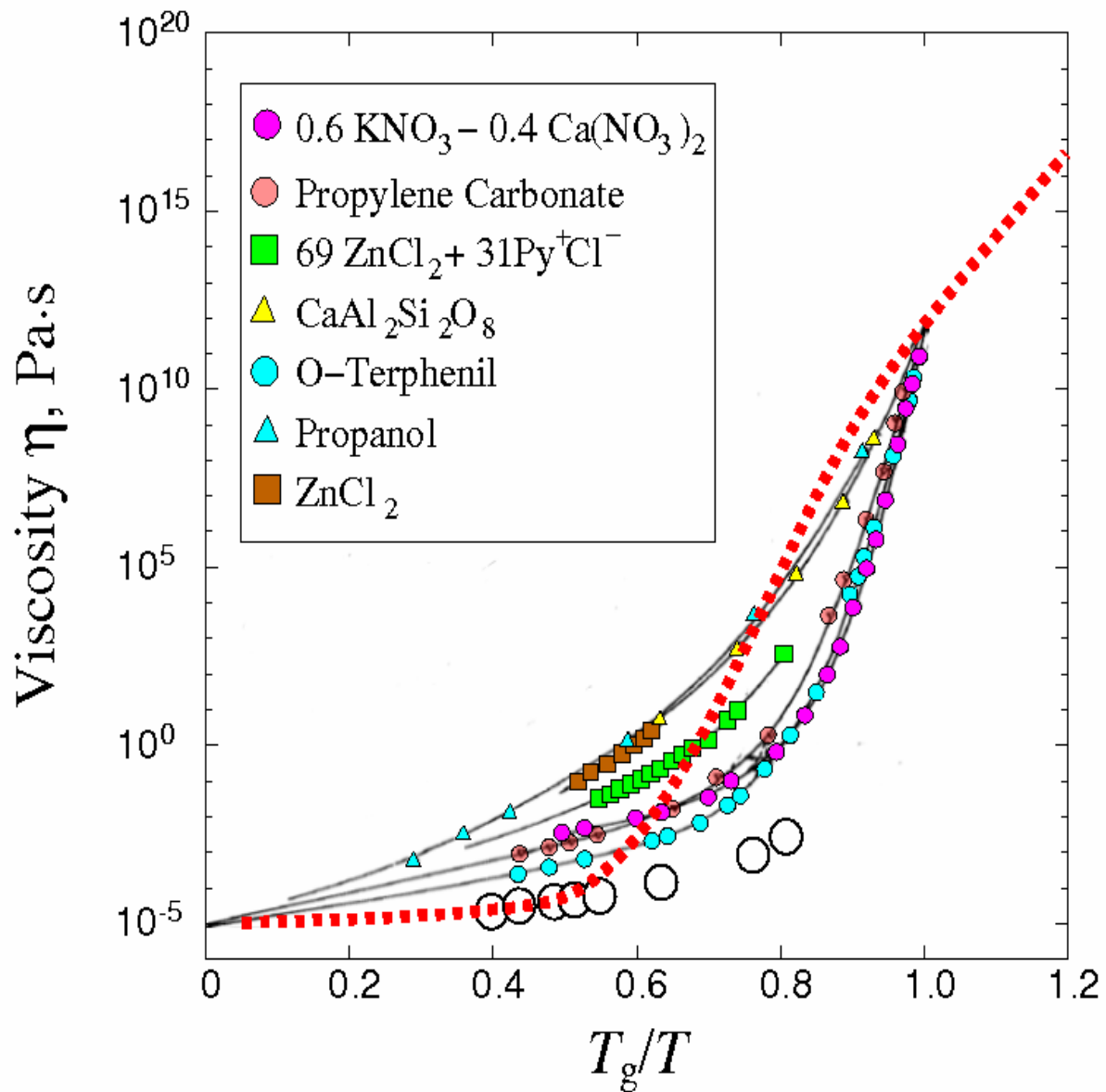
A way to unify studies of transport (viscosity) and deformation (creep) through energy-landscape perspective and TSP sampling

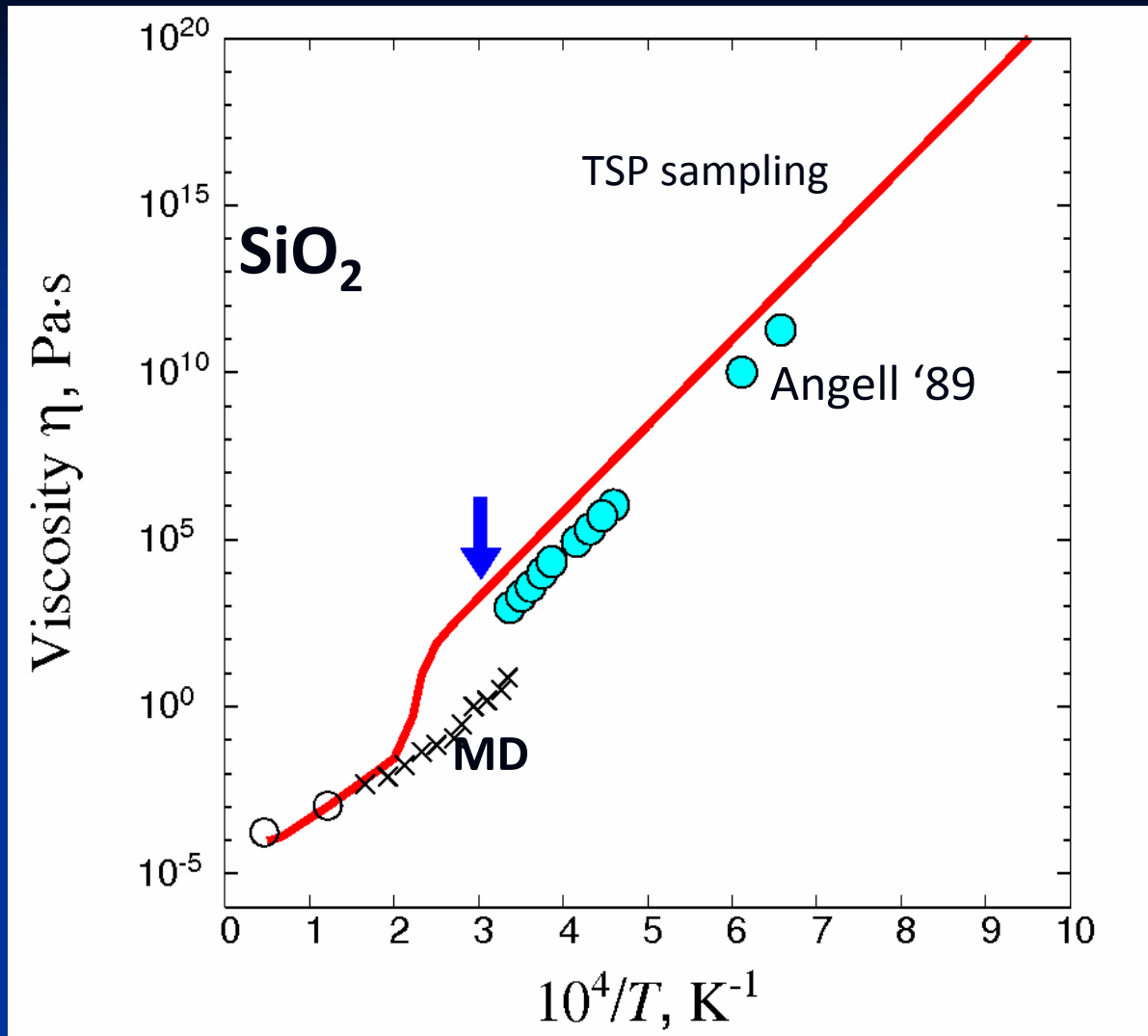
Viscosity of vitrified liquids

no theoretical explanation, challenge to atomistic simulation

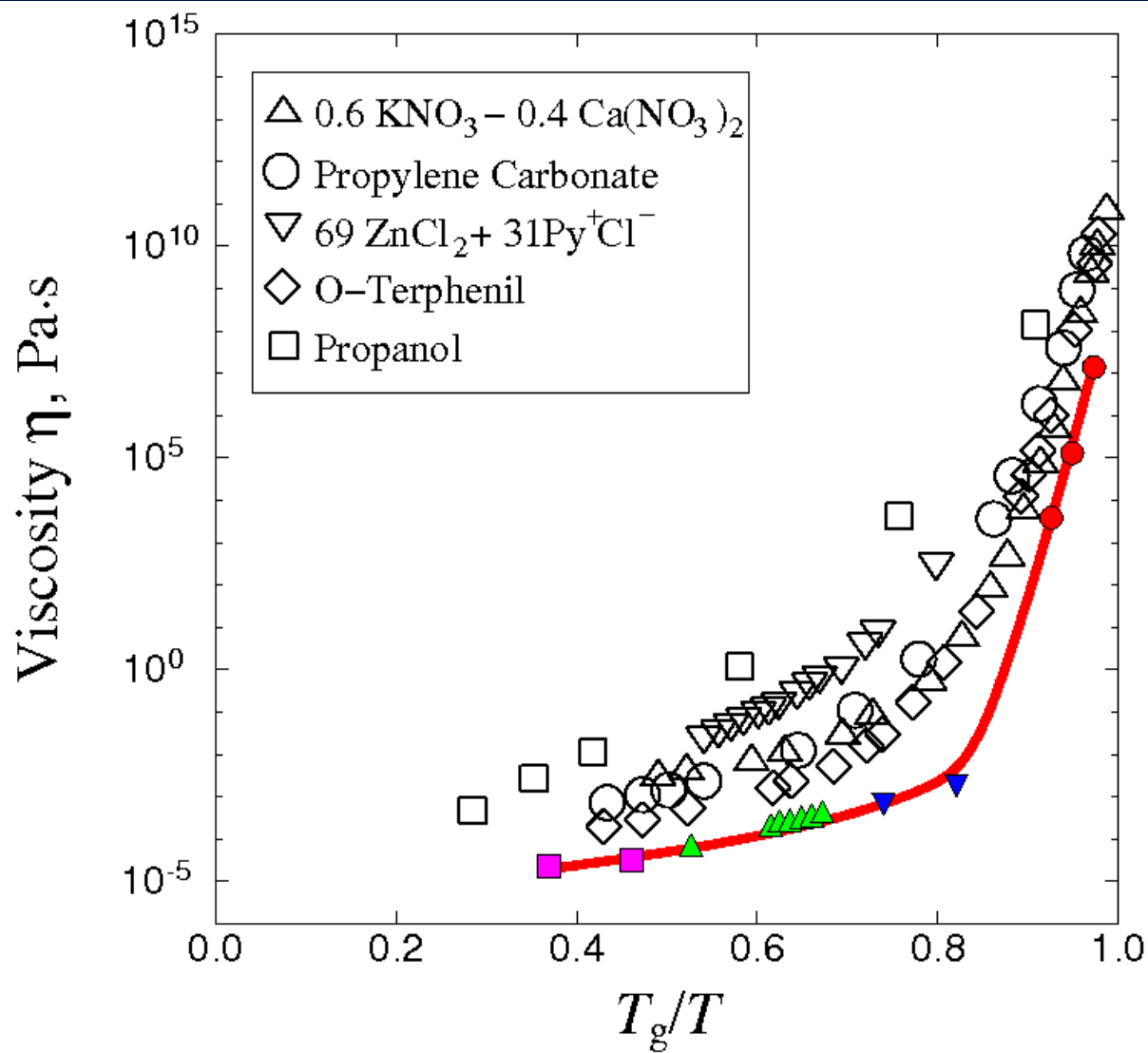


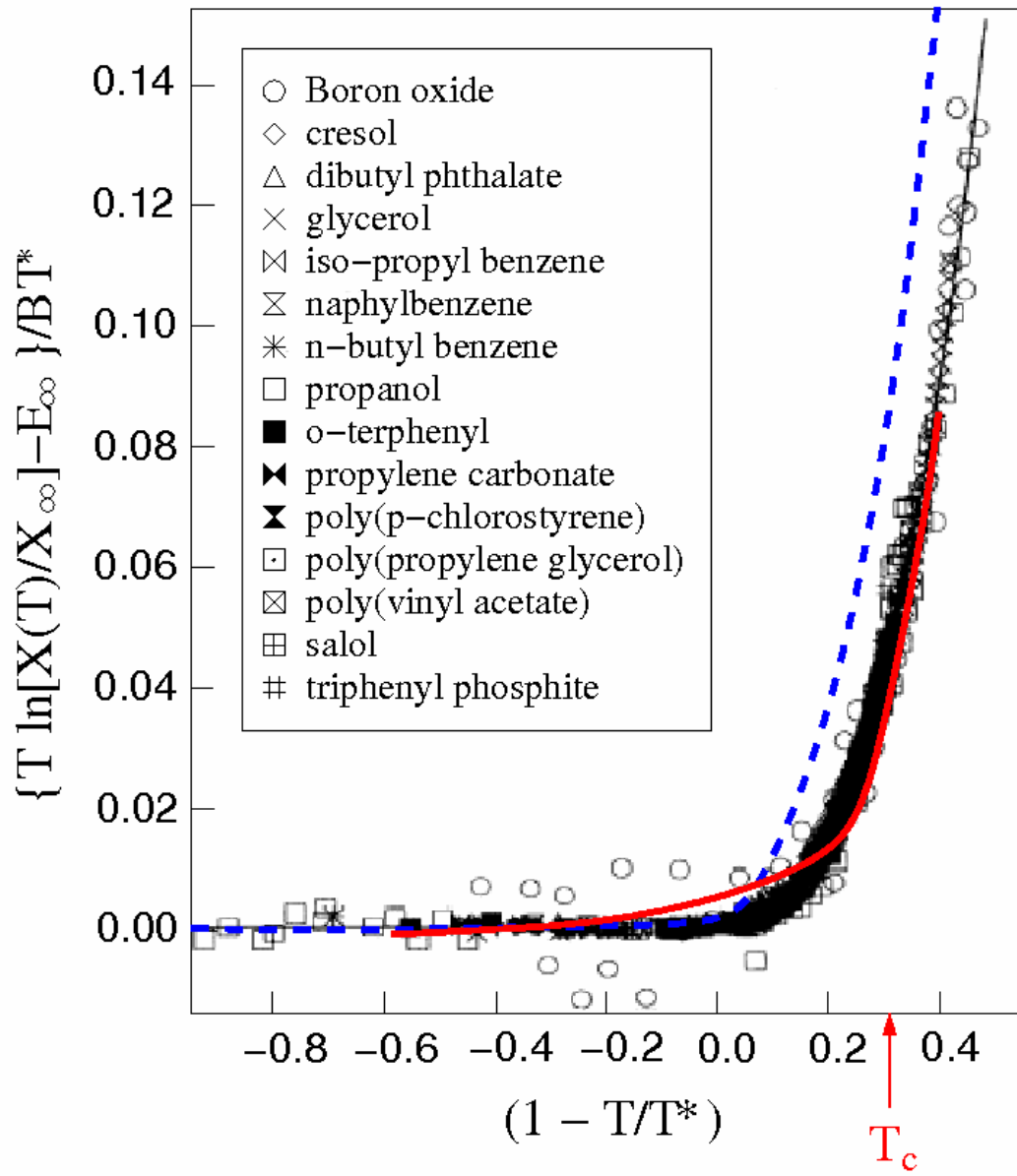
C. A. Angell, 1989

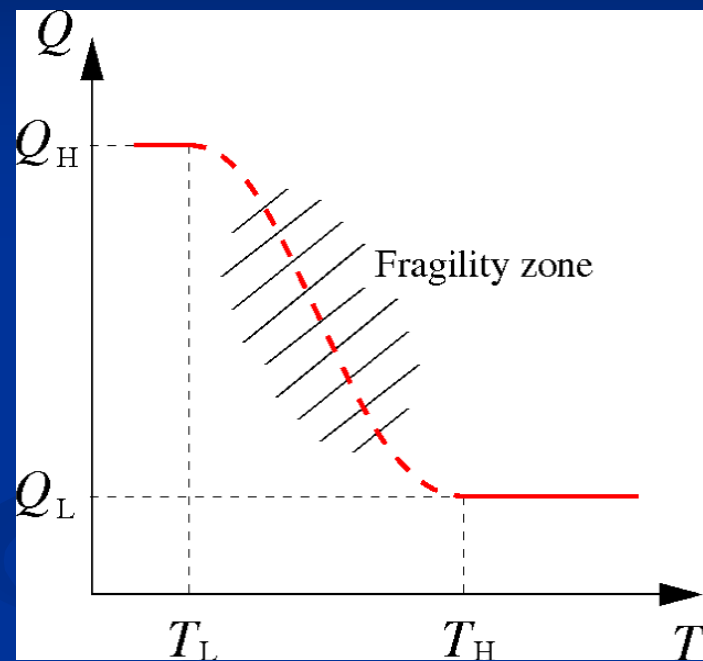
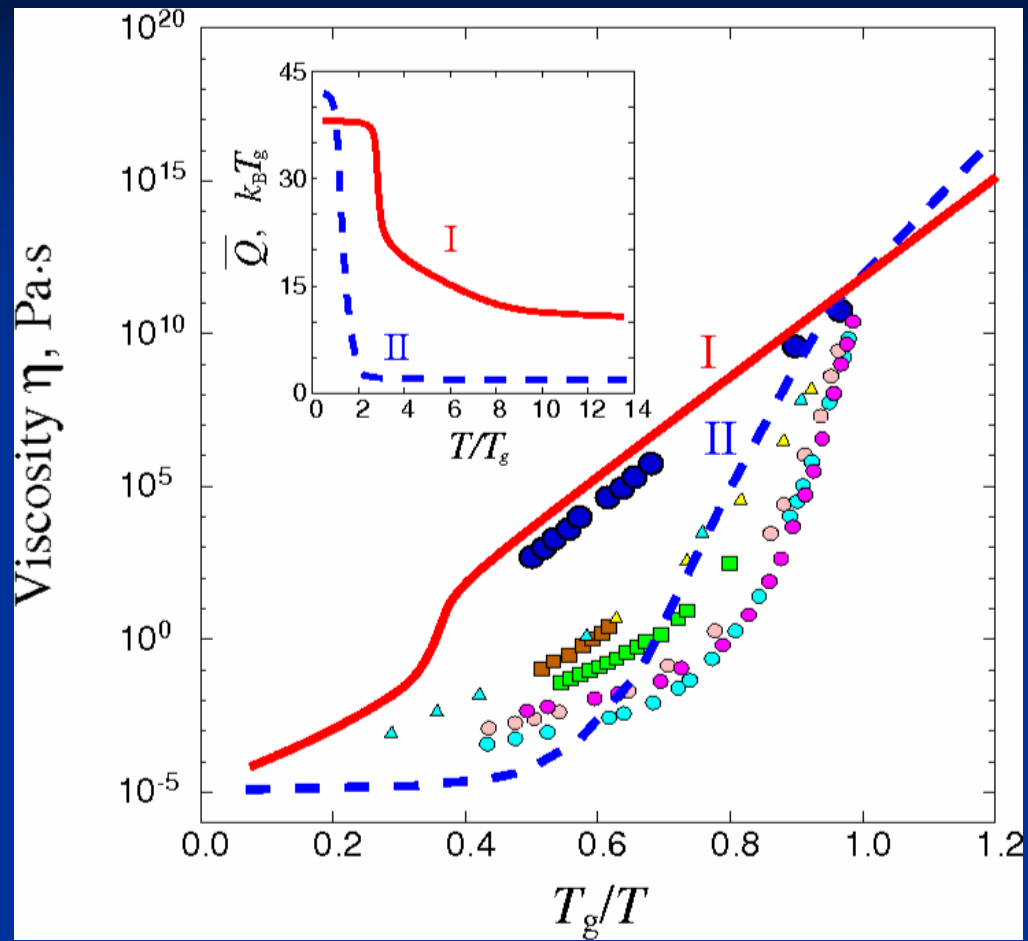




Kushima et al., JCP, 131, '09

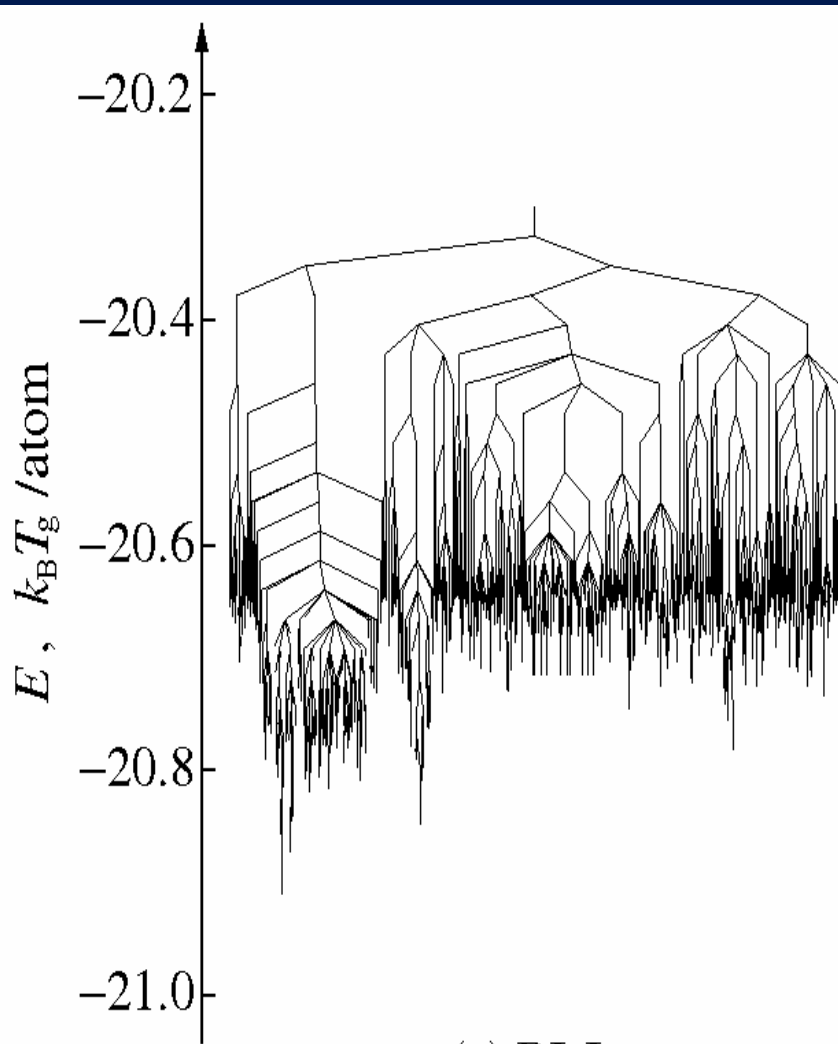




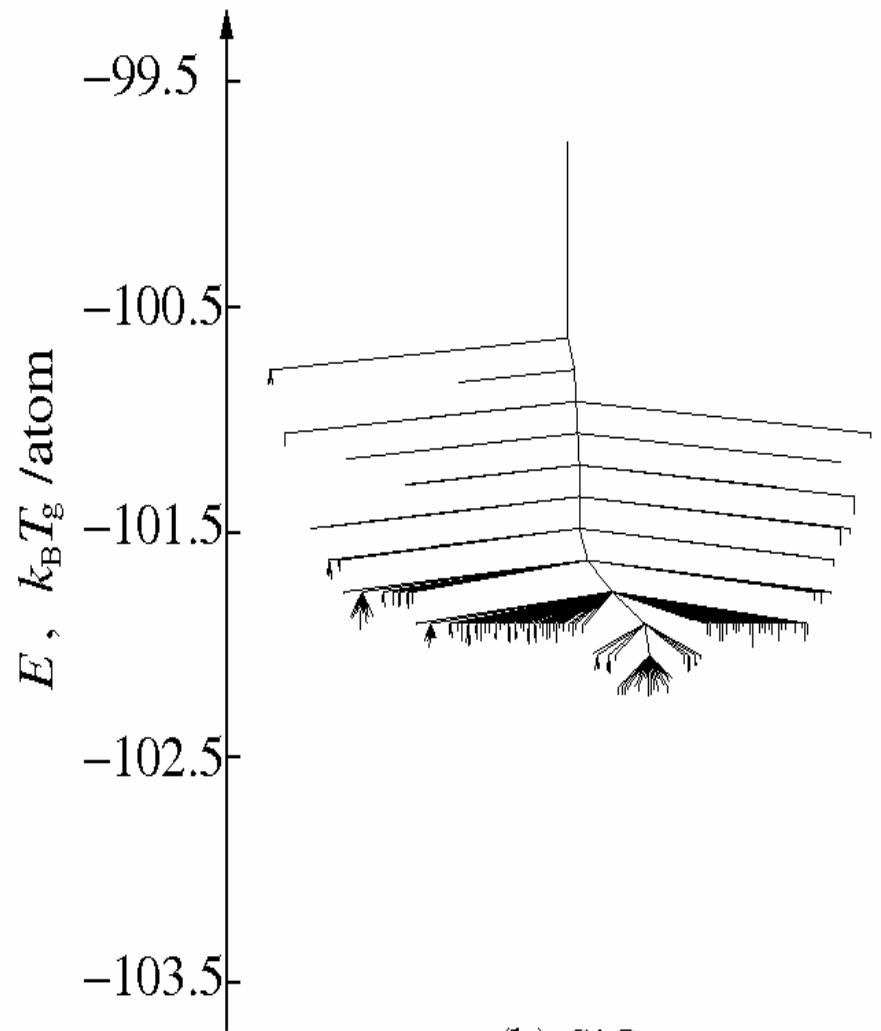


Kushima et al., JPCM, 21, '09

Disconnectivity graphs derived from TSP trajectories

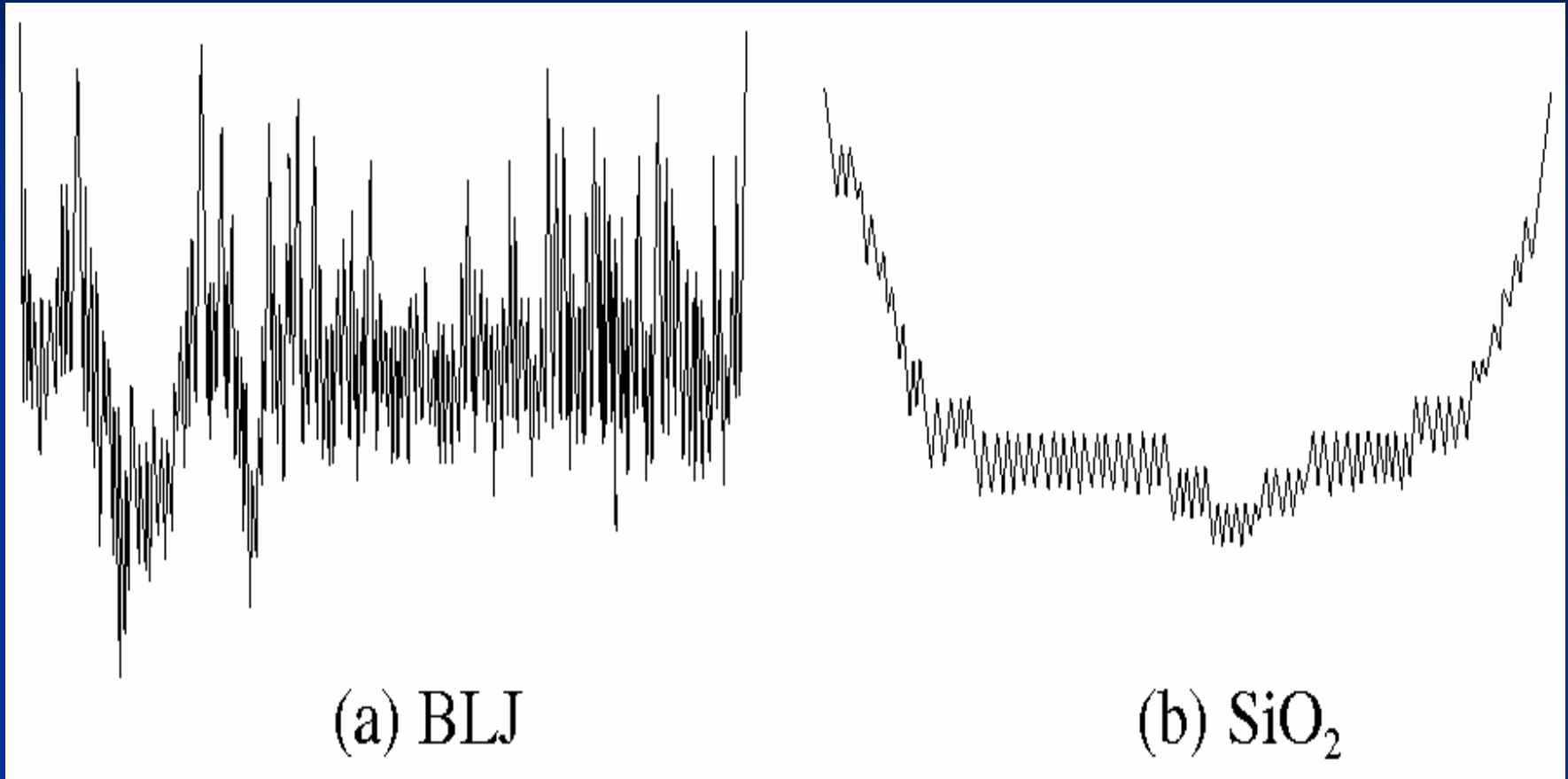


(a) BLJ



(b) SiO₂

Potential energy profiles of binary L-J and silica models



ABC is a method for slowly relaxing processes involving many steps of activation-relaxation

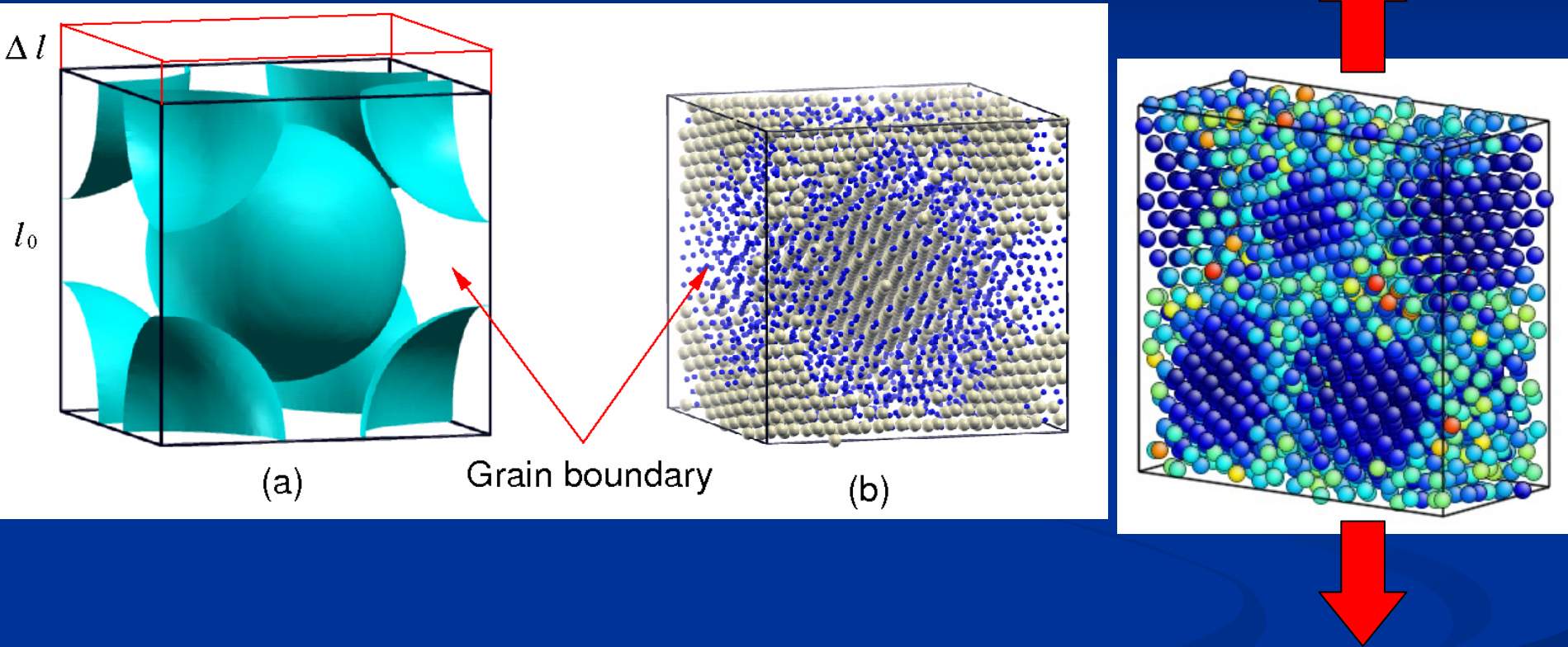
$$\eta = G \tau$$

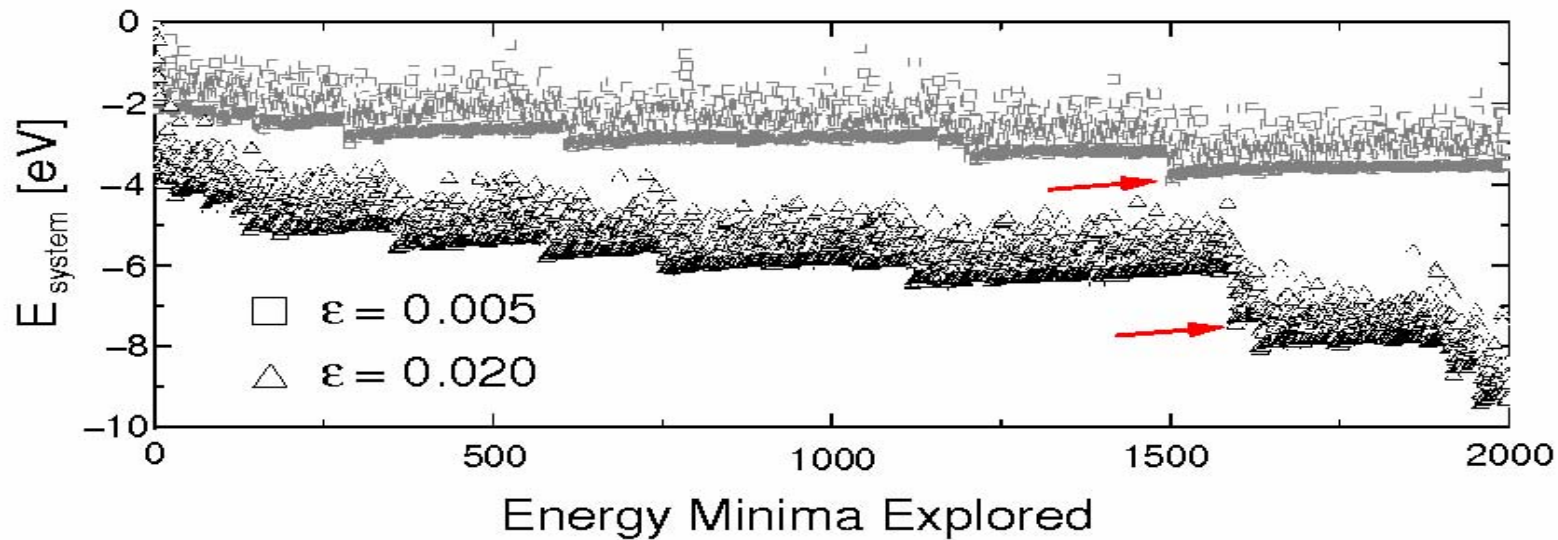
Isomorphism between shear relaxation (thermally activated) and structural deformation (stress-induced)

$$Q(T) \rightarrow Q(\sigma)$$

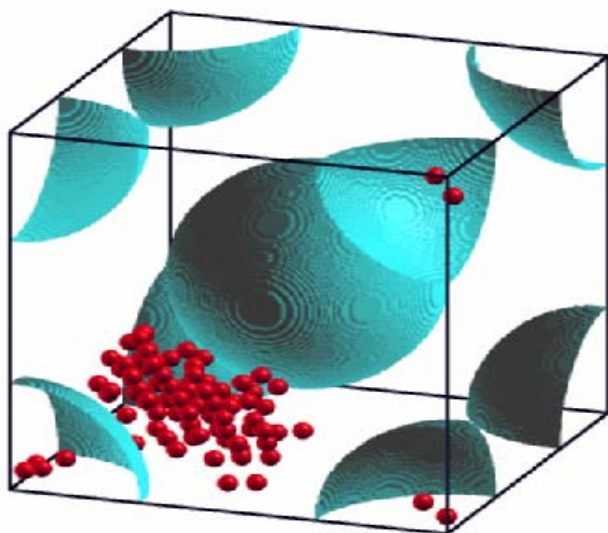
Apply this approach to creep (stress-dependent activation barrier)

Stress relaxation under constant strain

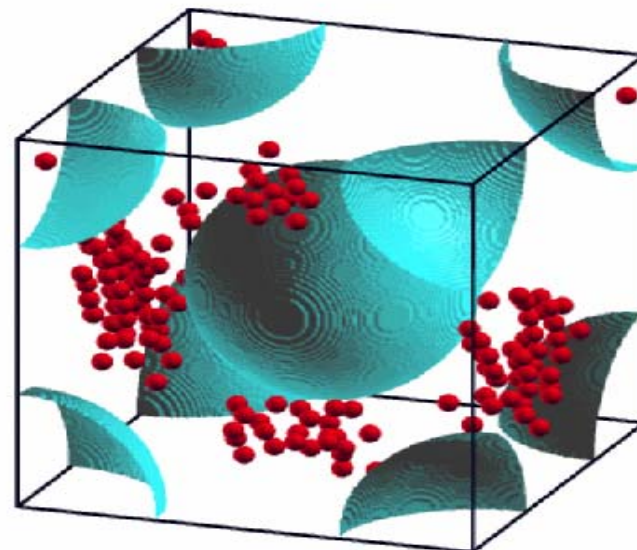




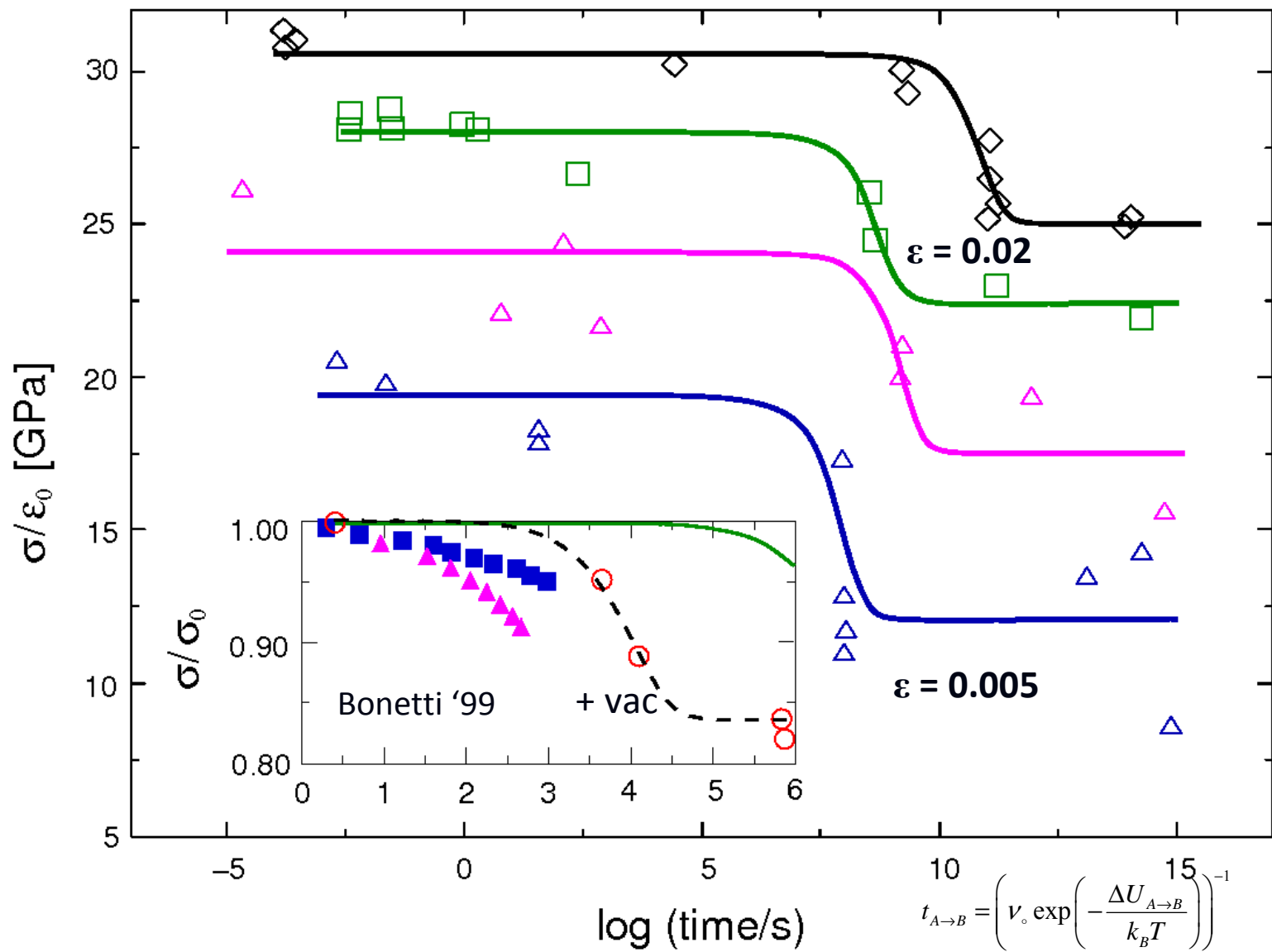
(a)

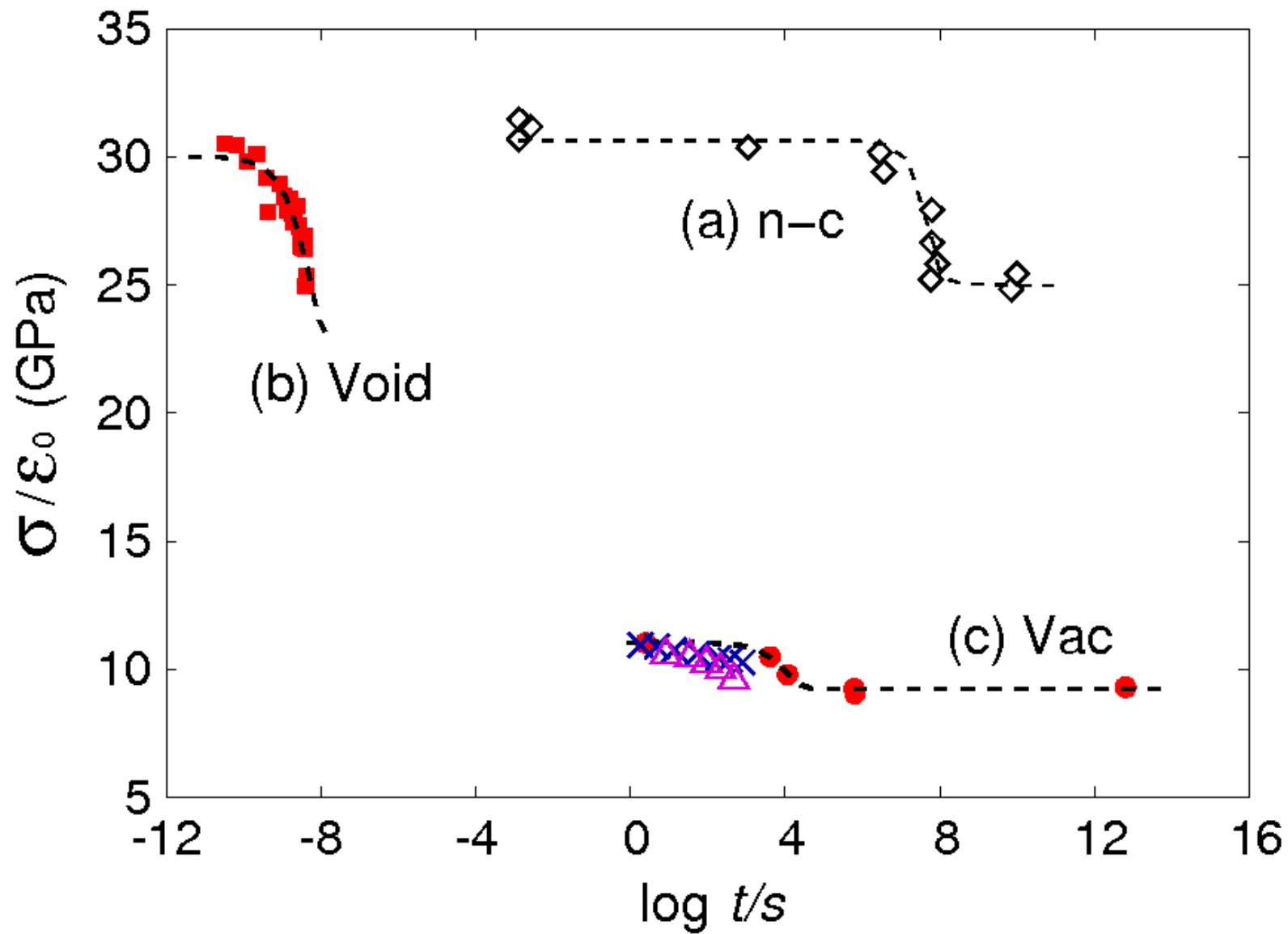


(b) $\epsilon = 0.005$



(c) $\epsilon = 0.020$



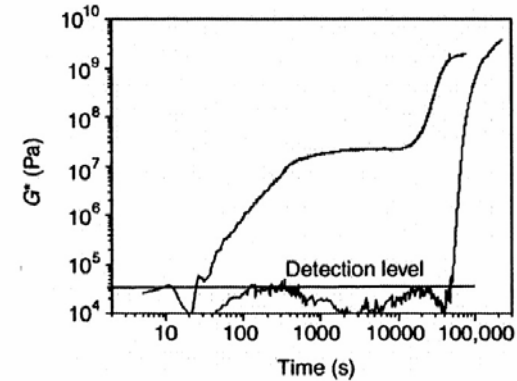
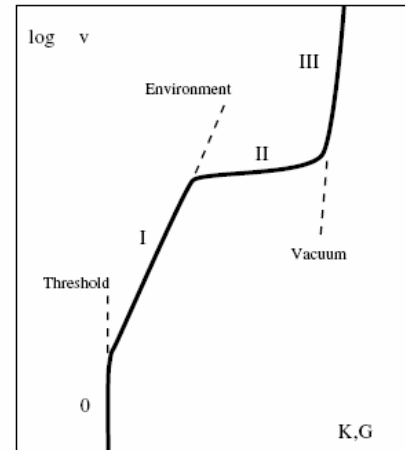
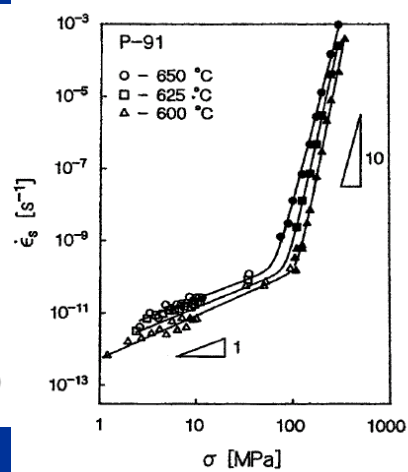
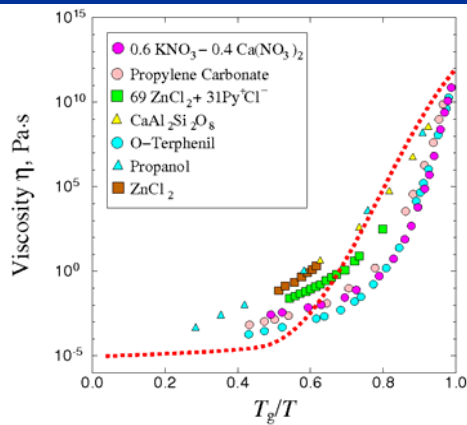


Reaching long time scales is
a current challenge in atomistic simulations

Special design of experimental tests will be required

Other problems of slow dynamics ...

radiation damage, stress corrosion cracking, cement setting



Collaborators

Akihiro Kushima (MIT)

Xi Lin (Boston U)

Jacob Eapen (N. Carolina State U)

Timothy Lau (MIT)

Ju Li (U Penn)

Xiaofeng Qian (MIT)

John Mauro and Phong Diep (Corning)