Glass Simulations: Past & Present

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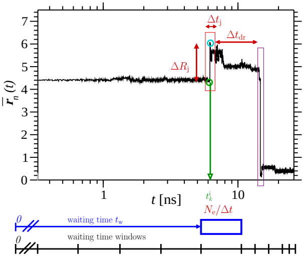
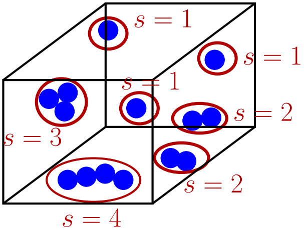
Goettingen University, July 11, 2017



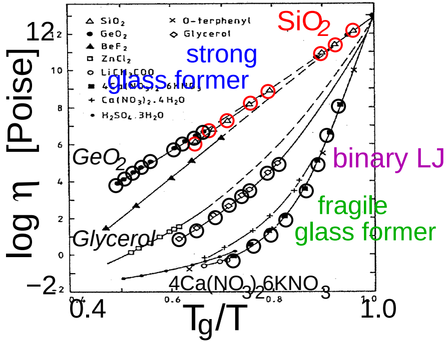


Acknowledgments:

H. E. Castillo, C. H. Gorman, R. Bjorkquist, L. M. Chambers,
A. Zippelius, J. Horbach, J. A. Roman, Chr. Scherer, G. P. Shrivastav,
J. Helfferich, R. Bjorkquist, L. M. Chambers, B. Temelso,
J. Cookmeyer, and Theoretical Physics, Göttingen

Overview

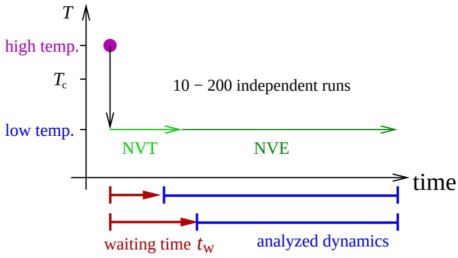
Systems:



[C.A. Angell and W. Sichina, Ann. NY Acad. Sci. 279, 53 (1976)]

- binary Lennard Jones [Kob,Andersen ’94, ’95]
- SiO_2 [BKS, PRL ’90]

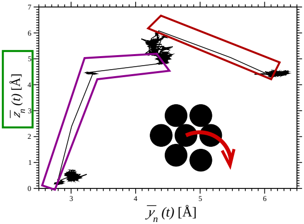
Quench Below T_c:

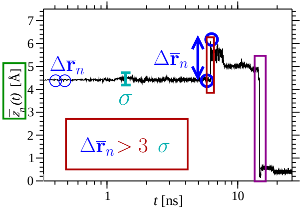


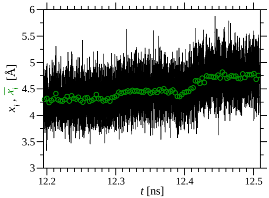
Aging Dynamics:

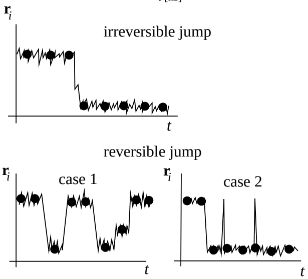
- microscopic
- dynamic heterogeneities

Single Particle Jumps



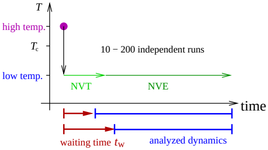


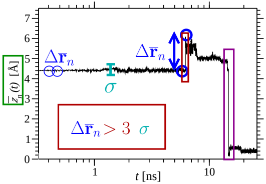




[KVL, JCP 121, 4781 (2004)]

Aging of SiO_2

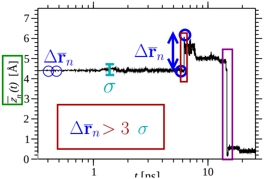


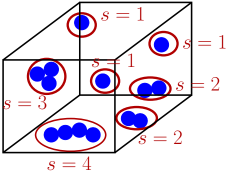


- incoh. interm. scatt. fct. $C(t, t_w, q, \alpha)$ [PRE 2010]
- Jumps:
  - $P(\Delta R)$ and $P(\Delta t_b)$ t_w-independ. [PRL 2013] (CTRW) [Helfferich EPL 2015]
  - $N_{jumps}/\Delta t$ only t_w-depend. [PRL 2013]
  - defects and jumps [KVL, Zippelius, PRE 2013]
- dyn. heterog. χ_4 and $C_{\mathbf{r}}(t, t_w, q, \alpha)$ scale with C and common clock of Si & O [JCP 2016, Editor's Choice]

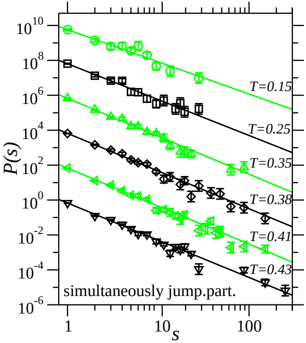
Similar aging dynamics for fragile glass formers
[Kob & Barrat, Warren & Rottler, Helfferich, Castillo]

Clusters of Single Particle Jumps

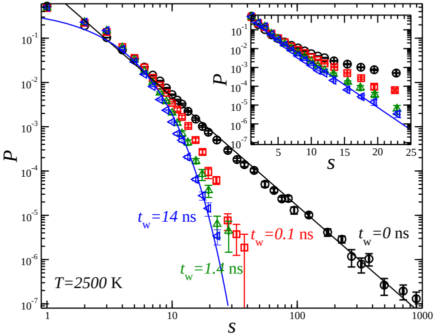




simultaneously jumping particles

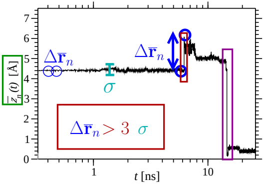


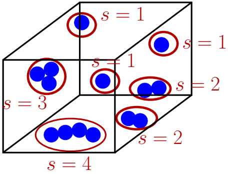
bin. LJ: power law [EPL 2006]
$(N_{\text{tot}} = 1000)$



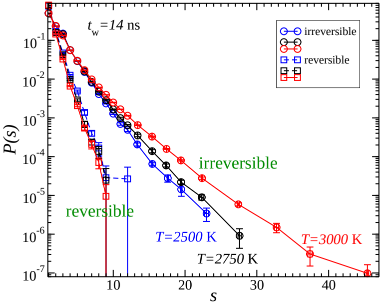
SiO_2: $t_{\text{w}} = 0$ power law; for large t_{w}
exponential $(N_{\text{tot}} = 115248)$

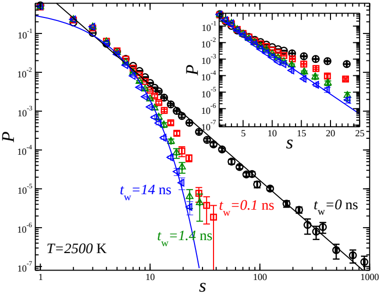
Clusters of Single Particle Jumps





simultaneously jumping particles





SiO_2: temp. & irrev./rev. dep.

SiO_2: $t_{\mathrm{w}} = 0$ power law; for large t_{w} exponential ($N_{\mathrm{tot}} = 115248$)

present: [J.Cookmeyer,KVL]

Thank You

Acknowledgments:

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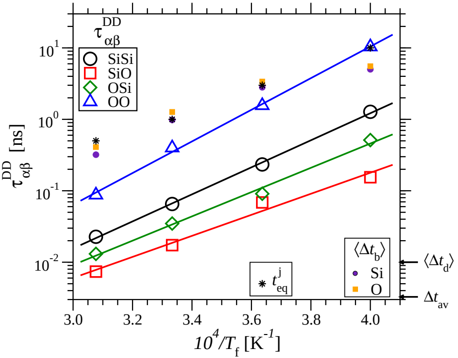
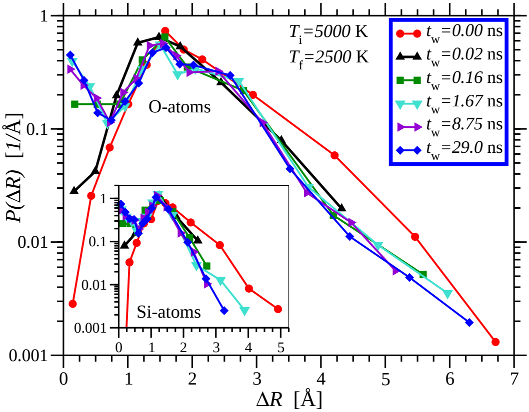
Extra Slide: Time Scales

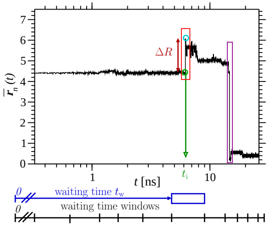


earlier Vs. of Temp.-dep. defect dynamics [KVL,AZ, PRE88 2013]

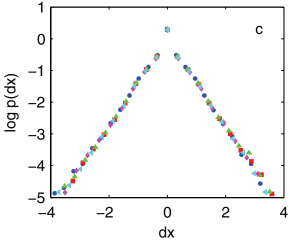
Jump Length Distribution

strong glass former SiO_2:





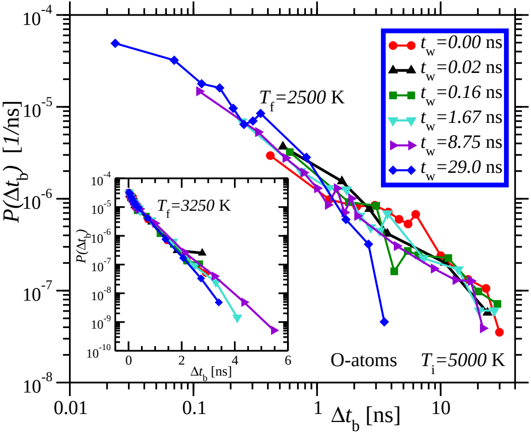
- compare fragile glassformer binary LJ (& polymer) [Warren & Rottler,EPL(2009)]

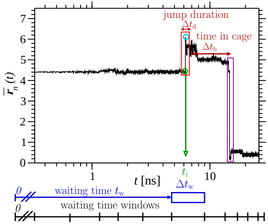


- $P(\Delta R)$ independent of t_w

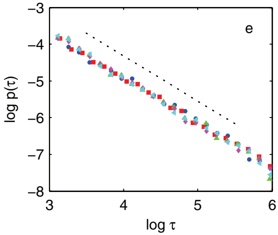
Distribution of Time in Cage $P(\Delta t_\mathrm{b})$: t_w varied

strong glass former SiO_2:



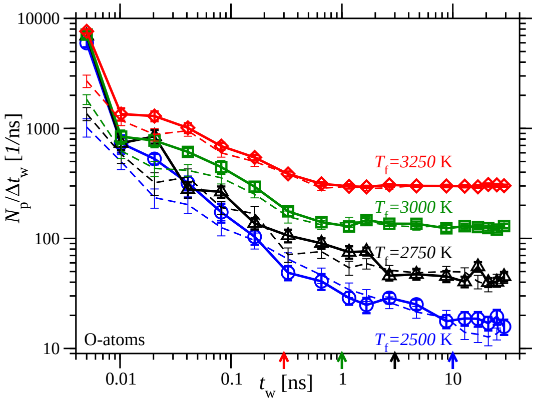


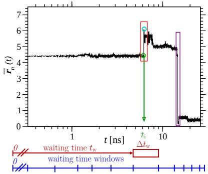
- compare fragile glassformer (binary LJ &) polymer [Warren & Rottler,EPL(2009)]



- $P(\Delta t_\mathrm{b})$ independent of t_w!

Number of Jumping Particles per Time





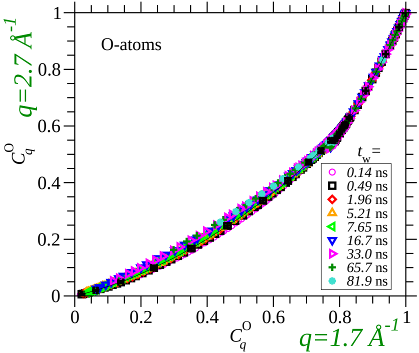
- $N_p/\Delta t_w$ depends strongly on waiting time t_w
  - $N_p/\Delta t_{tw}$ decreasing with increasing t_w
  - compare: soft colloids [Yunker et al.,PRL (2009)]
  - compare fragile glassformer polymer; CTRW [Helfferich et al., EPL 2015]

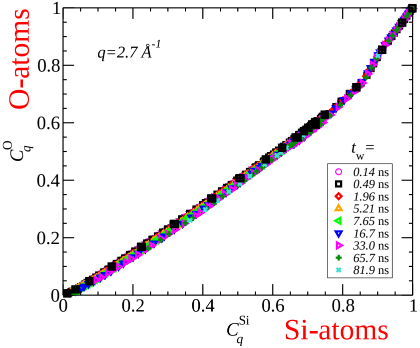
Scaling of Global Incoh. Intermediate Scattering Fct. C

$$f_s^\alpha(t_\mathrm{w}, t_\mathrm{w}+t, \mathbf{q}) = \frac{1}{N_\alpha} \sum_{j=1}^{N_\alpha} \cos\left\{\mathbf{q} \cdot \left(\mathbf{r}_j(t_\mathrm{w}+t) - \mathbf{r}_j(t_\mathrm{w})\right)\right\}$$

$$C^\alpha = \langle f_s^\alpha(t_\mathrm{w}, t_\mathrm{w}+t, \mathbf{q})\rangle$$

$\alpha =$ particle type Si,O



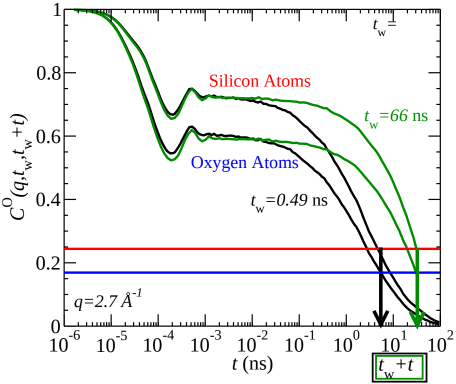


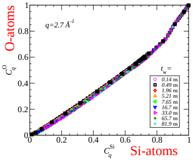
- [Kob,Barrat, EPJB (2000)] for fragile glass former(intermediate t_w)
- for strong glass former SiO_2: $C^\alpha = C^\alpha(z(t_\mathrm{w}, t), q)$

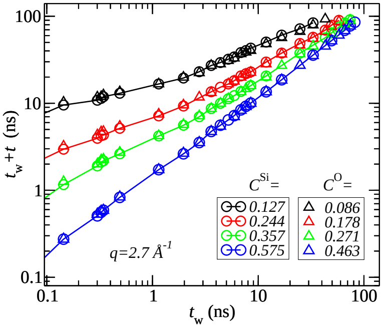
- **directly** particle dependence
- common aging clock
- $C_q = C_q(z(t_\mathrm{w}, t), \alpha)$

$$C = C(z(t_\mathrm{w}, t), q, \alpha)$$

Particle Type: Common Aging Clock





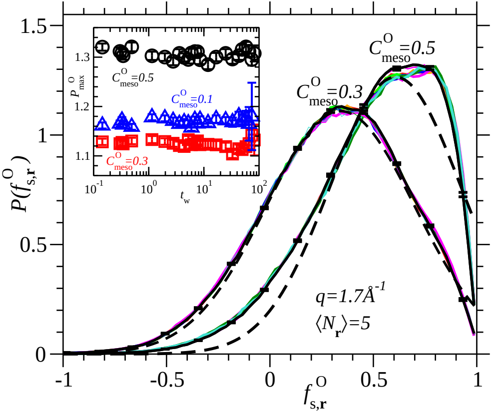


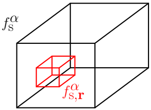
$\longrightarrow$ faster O-atoms and slower Si-atoms have

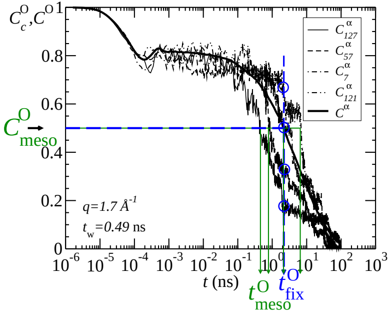
common aging clock

Improved Scaling of Local Incoh. Intermed. Scattering Fct.

$$f^{\alpha}_{s,\mathbf{r}}(t_{\mathrm{w}}, t_{\mathrm{w}}+t, \mathbf{q})) = \frac{1}{N^{\alpha}_{\mathbf{r}}} \sum_{\mathbf{r}_j(t_{\mathrm{w}})\in B_{\mathbf{r}}} \cos\left(\mathbf{q}\cdot[\mathbf{r}_j(t_{\mathrm{w}}+t)-\mathbf{r}_j(t_{\mathrm{w}})]\right)$$







$\longrightarrow$ $P(f^{\alpha}_{s,\mathbf{r}}(t_{\mathrm{w}}, t))$ scales with $C^{\alpha}_{\mathrm{meso}}(t_{\mathrm{w}}, t)$

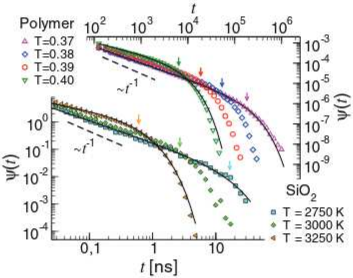


Fig. 1: (Colour on-line) Waiting time distribution $\psi(t)$ for the polymer model (open symbols, top right) and the amorphous silica (filled symbols, bottom left). The WTD for the polymer is given at four different temperatures: $T = 0.37$ (△), 0.38 (◊), 0.39 (◯) and 0.40 (▽). The WTD for the oxygen atoms in SiO_2 is given for the quench from $T_i = 5000$ to $T_f = 2750$ K (■), 3000 K (♦), and 3250 K (◄). The dashed lines are power laws with exponent −1, the solid lines are fits of eq. (1) to the data. The fit results are listed in table 1. The arrows indicate the values of λ^{-1}.

[Helfferich et al., EPL 109, 36004, 2015]