Mechanical and Transport Properties in **Disordered Materials**

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Modeling Nanomaterials of Energy Transport and Storage

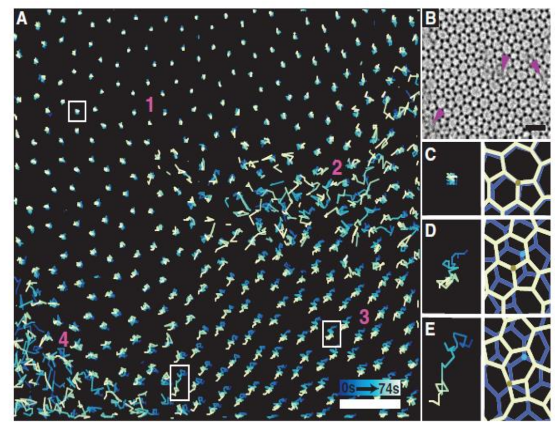
Monacoste Summer School
(8-13 may 2022)

Role of **structural disorder** on the **mechanical properties** of amorphous materials?

Copyr. Entre Terre & Talents

Imaging Atomic Rearrangements in Two-Dimensional Silica Glass: Watching Silica's Dance

Pinshane Y. Huang,[1] Simon Kurasch,[2*] Jonathan S. Alden,[1*] Ashivni Shekhawat,[3] Alexander A. Alemi,[3] Paul L. McEuen,[3,4] James P. Sethna,[3] Ute Kaiser,[2] David A. Muller[1,4]†

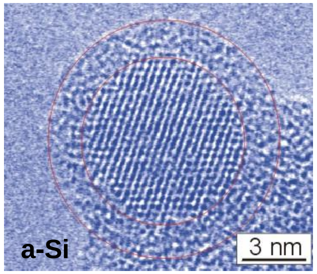


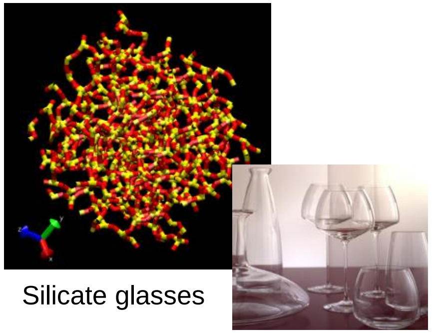
P.Y. Huang et al. Science (2013)

Heterogeneous and non-periodic material

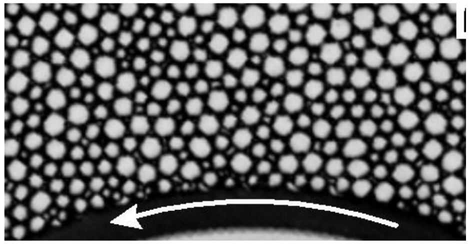
Examples of **Amorphous** Materials:

Metallic glasses, Vitreloy

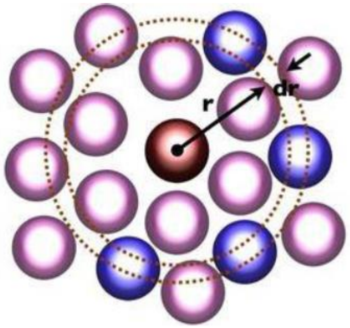


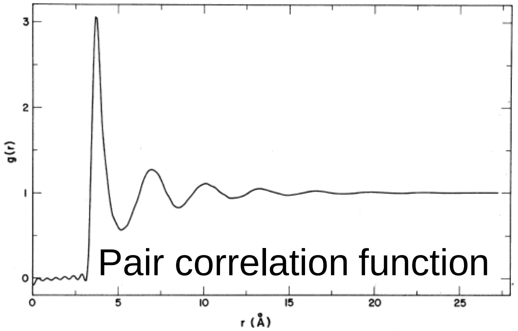


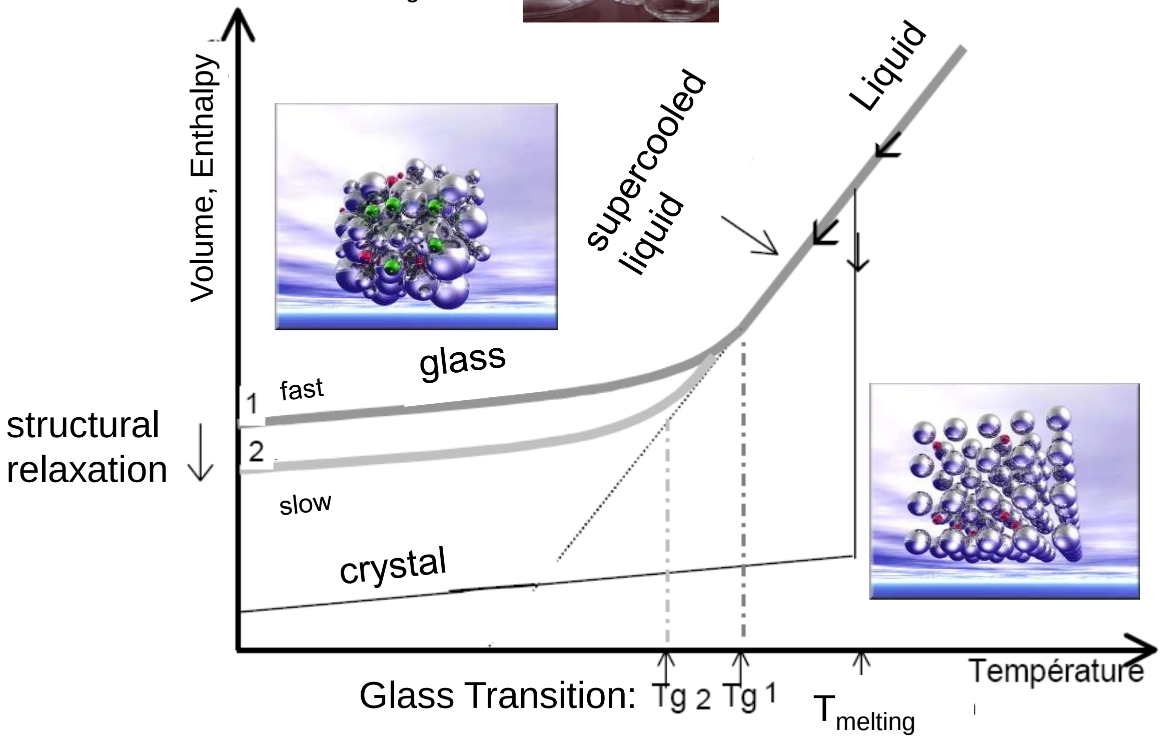
Silicate glasses



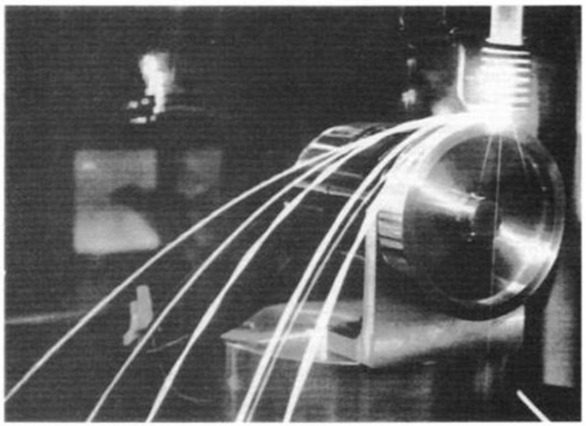
Foams





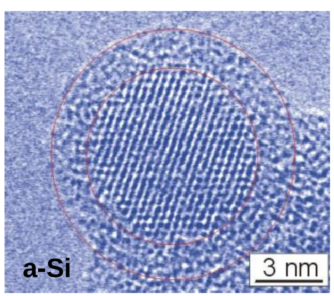


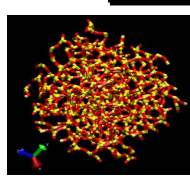
Processing **Amorphous** Materials:

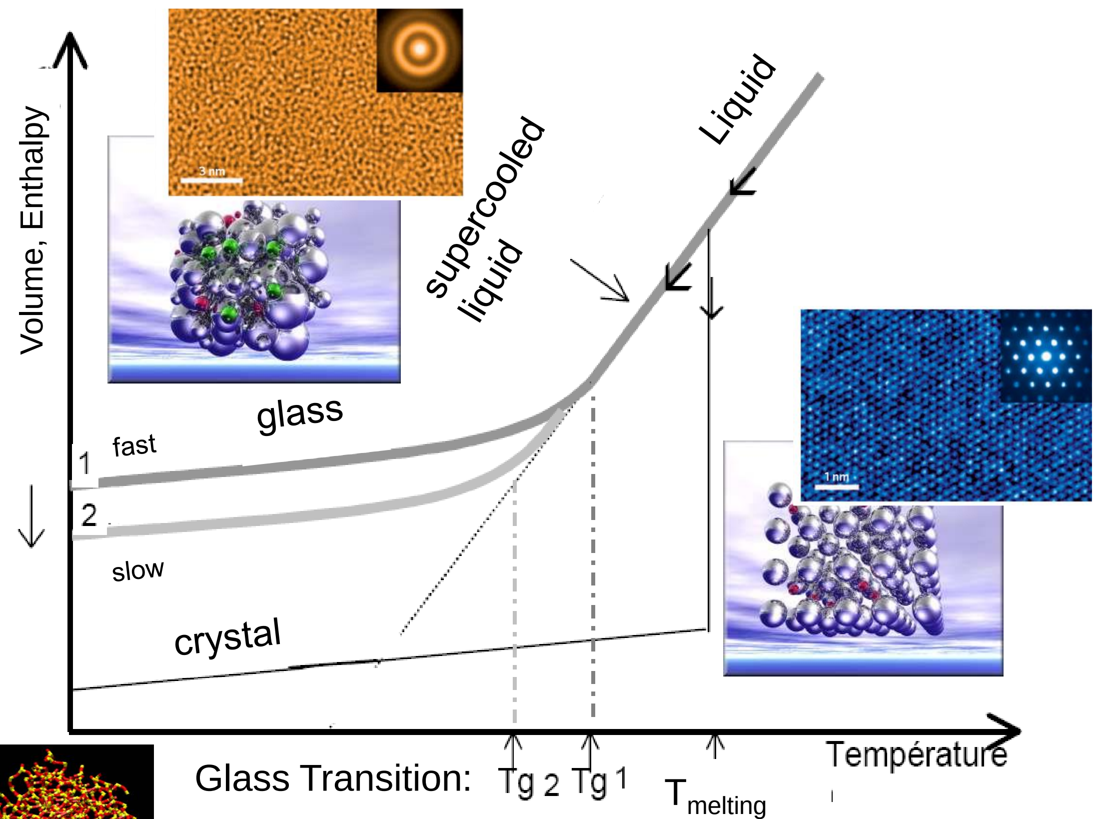


J.-L. Soubeyroux

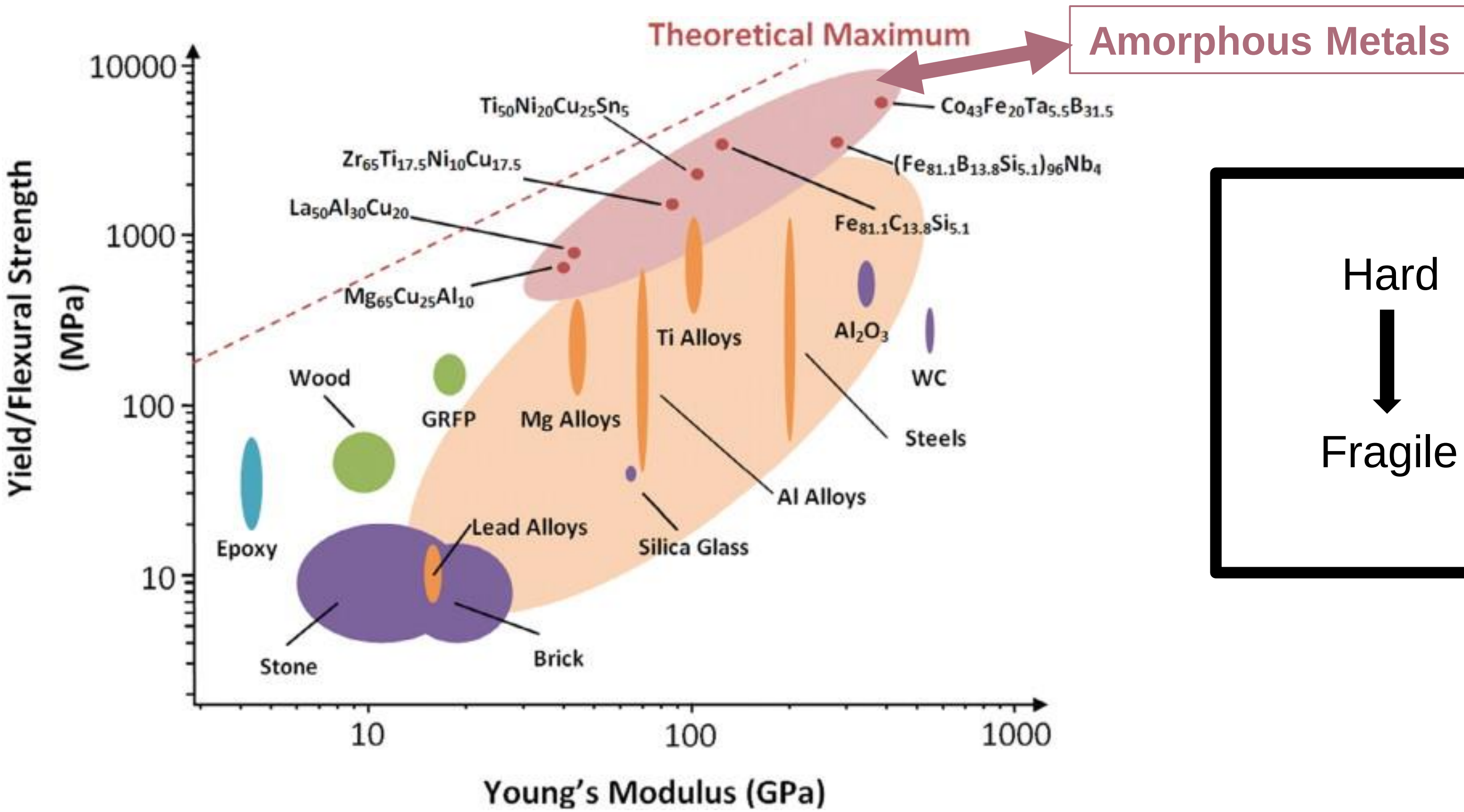
structural relaxation







Very **hard** materials

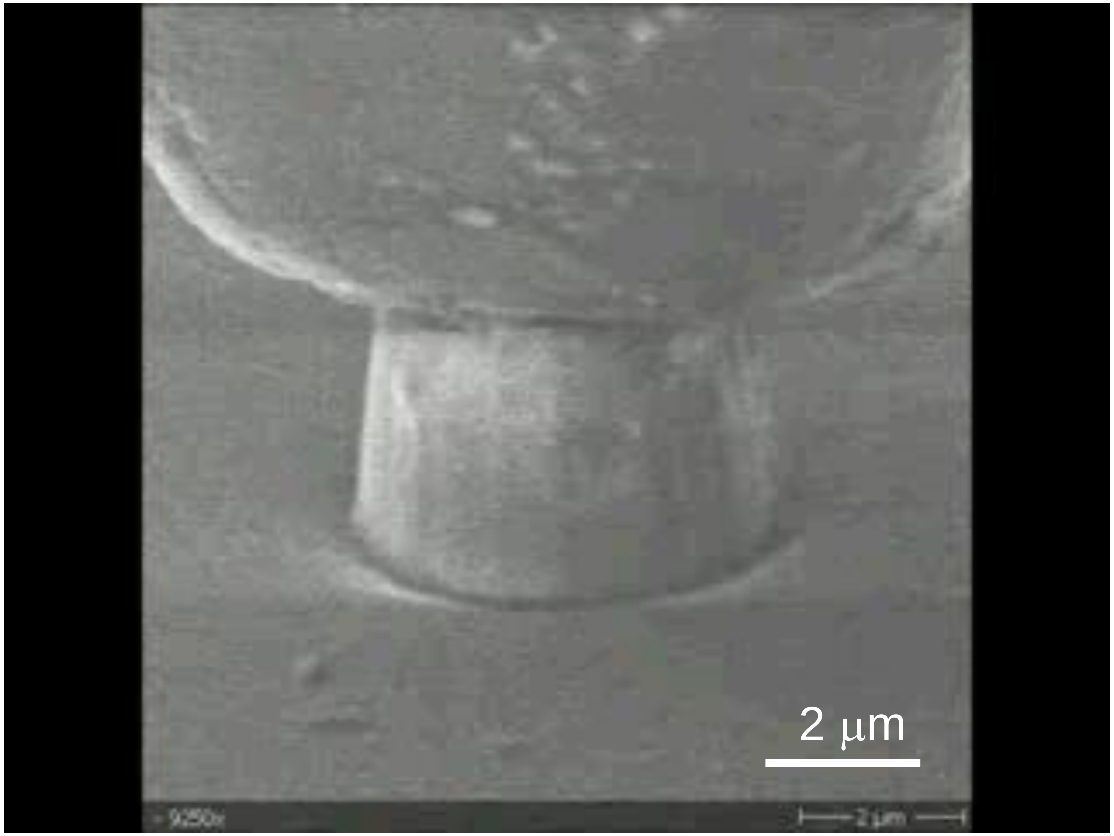


Hard

↓

Fragile ?

Ductile at **small** scale

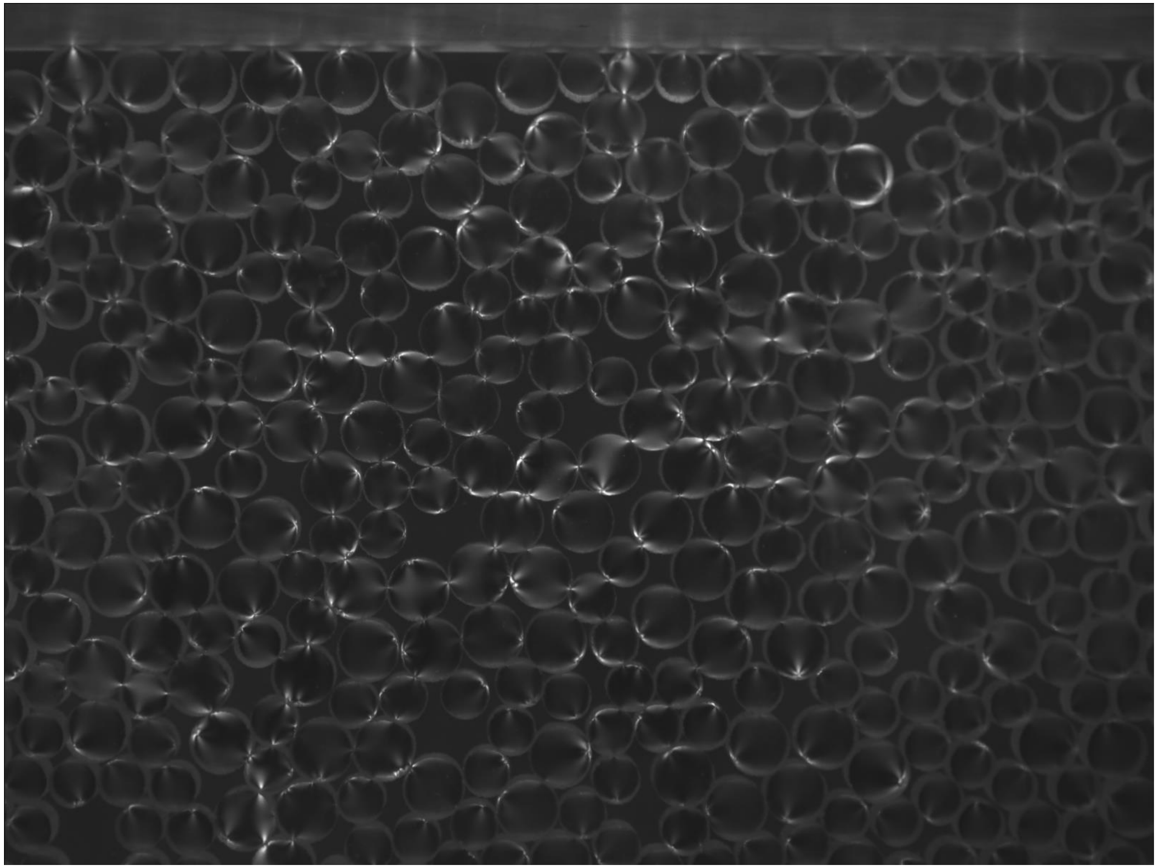


G. Kermouche, E. Barthel (2015)

Micropillar in pure silica glass

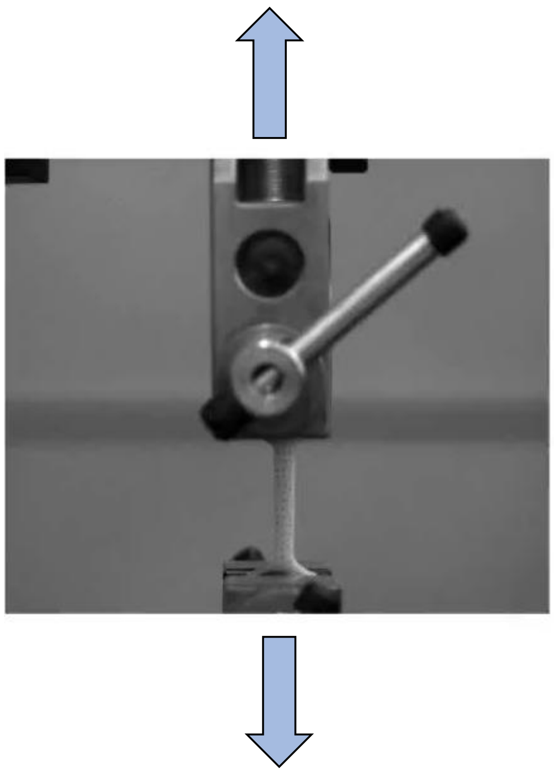
What happens **inside** a **disordered material** ?

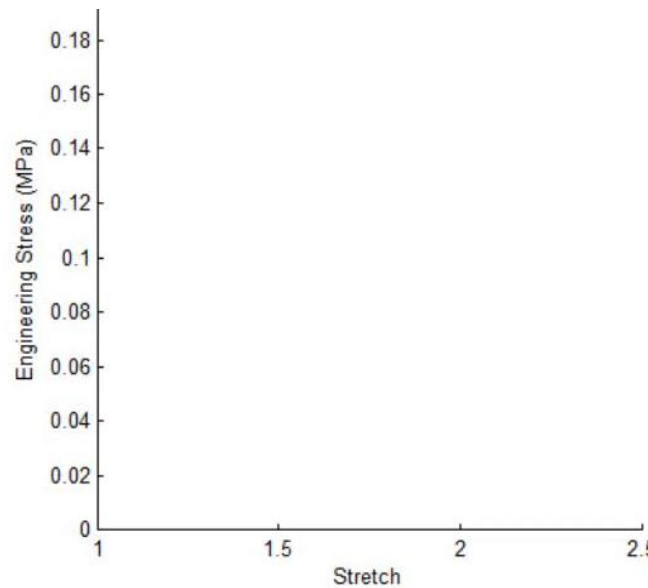
Heterogeneous response & Localization



E. Kolb et al. (2008)

Heterogeneities and force chains allow supporting **strong loads**





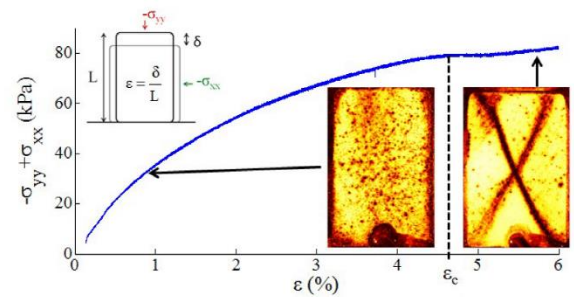
Example of amorphous polymer

P. Reis et al. (2019)

Local rearrangements may organize progressively along **shear bands**

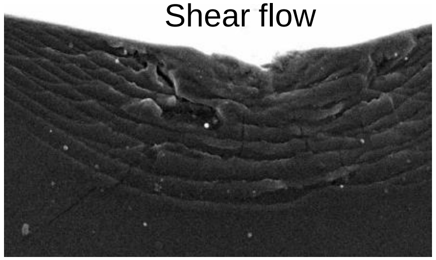
$\varepsilon = 0.14\ \%$

A. Amon et J. Crassous (2008)



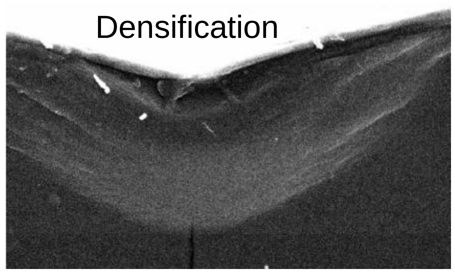
This behaviour is **composition** and **loading** dependent

Shear flow

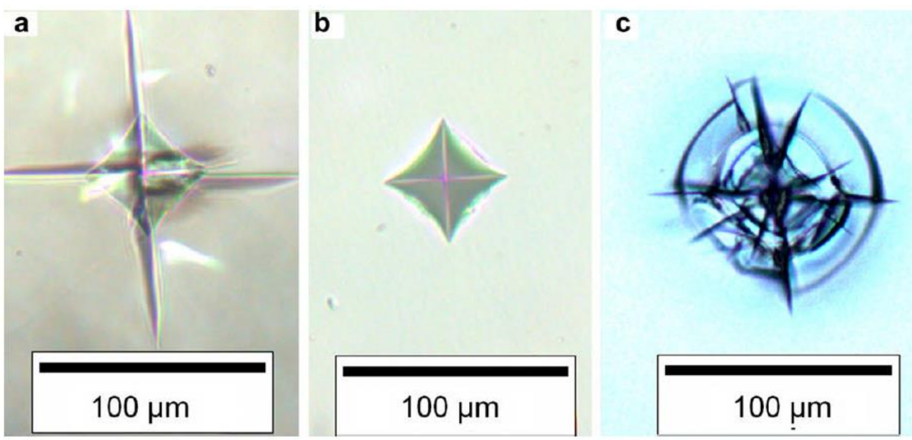


Soda-lime glass

Densification



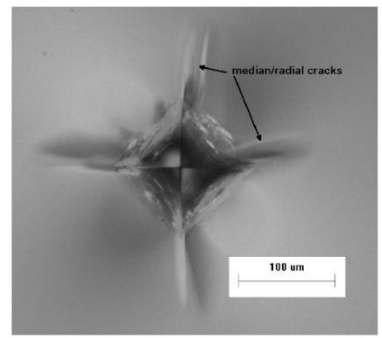
Anomalous glass



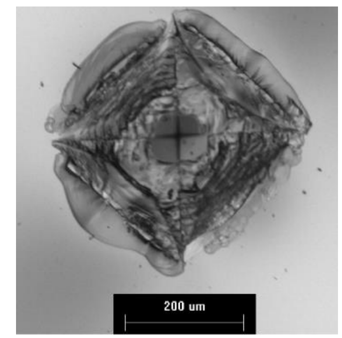
(a) 60% SiO_2 20% Al_2O_3 20% CaO; (b) 80% SiO_2 10% Al_2O_3 10% CaO; (c) 100% SiO_2

T.M. Gross et al. (2008, 2009)

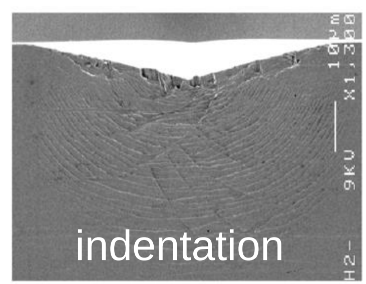
Quasi-static indentation (0.2 mm/mn, 69N)



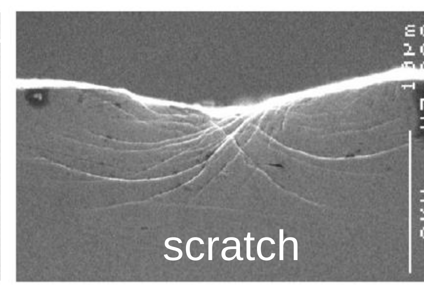
Impact velocity (410 mm/s, 562N)



T.M. Gross et al. (2013)

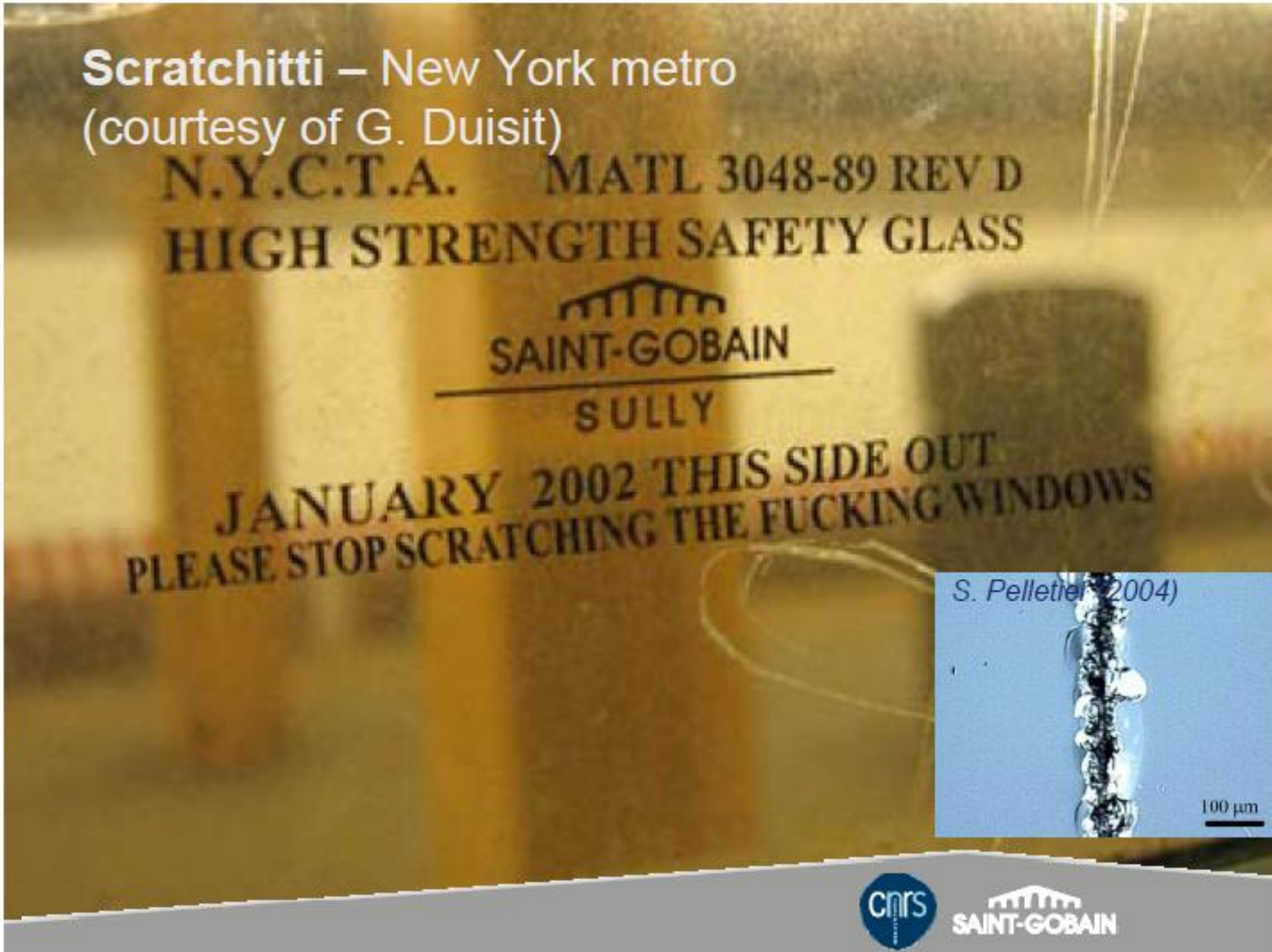


Bulk Metallic Glass

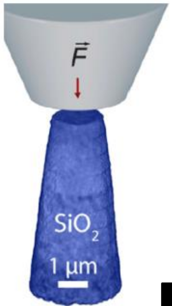


V. Keryvin et al. (2008)

Scratchitti – New York metro (courtesy of G. Duisit)



S. Pelletier (2004)

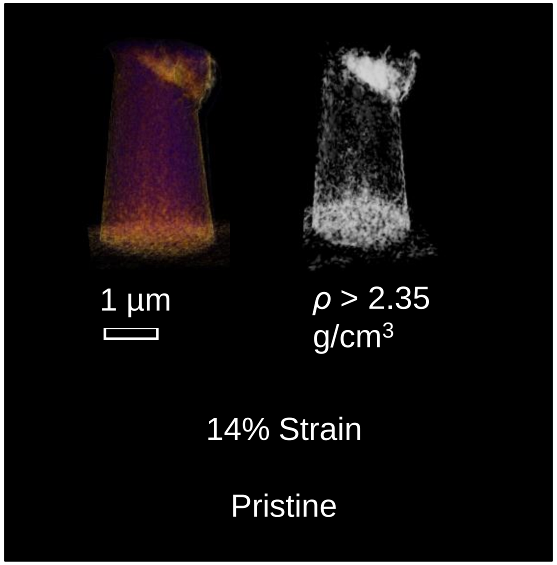


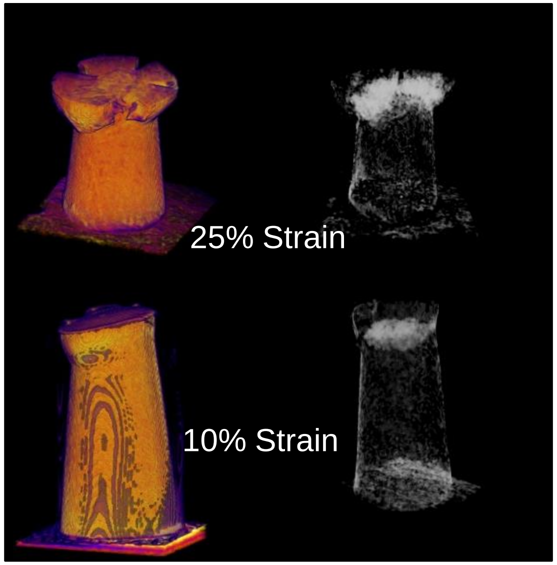
This behaviour is **composition** and **loading** dependent

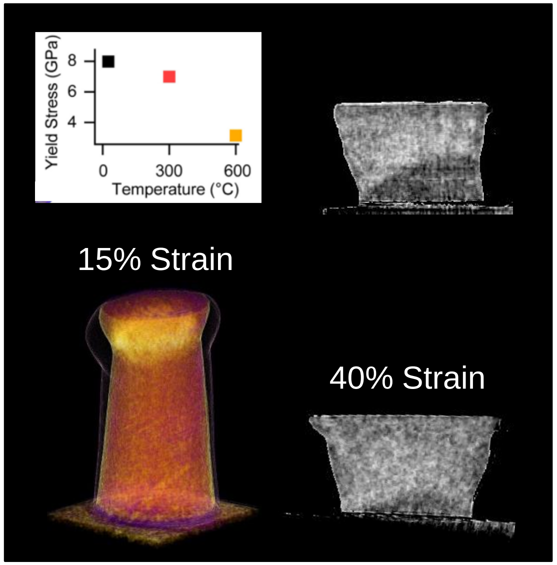
T=25°C | T=300°C | T=600°C

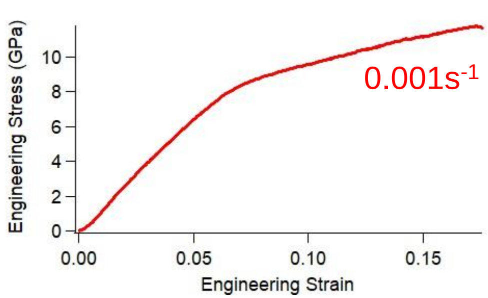
$0.001\ s^{-1}$

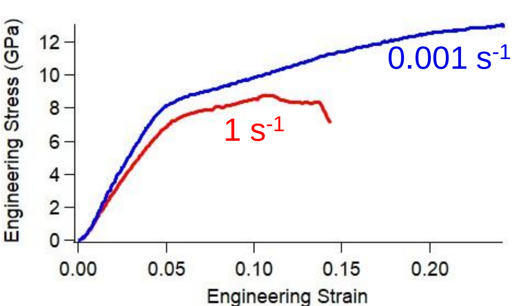
$1\ s^{-1}$

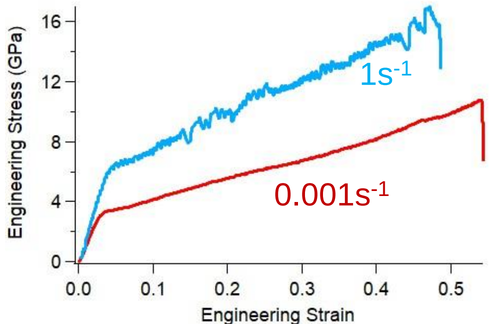


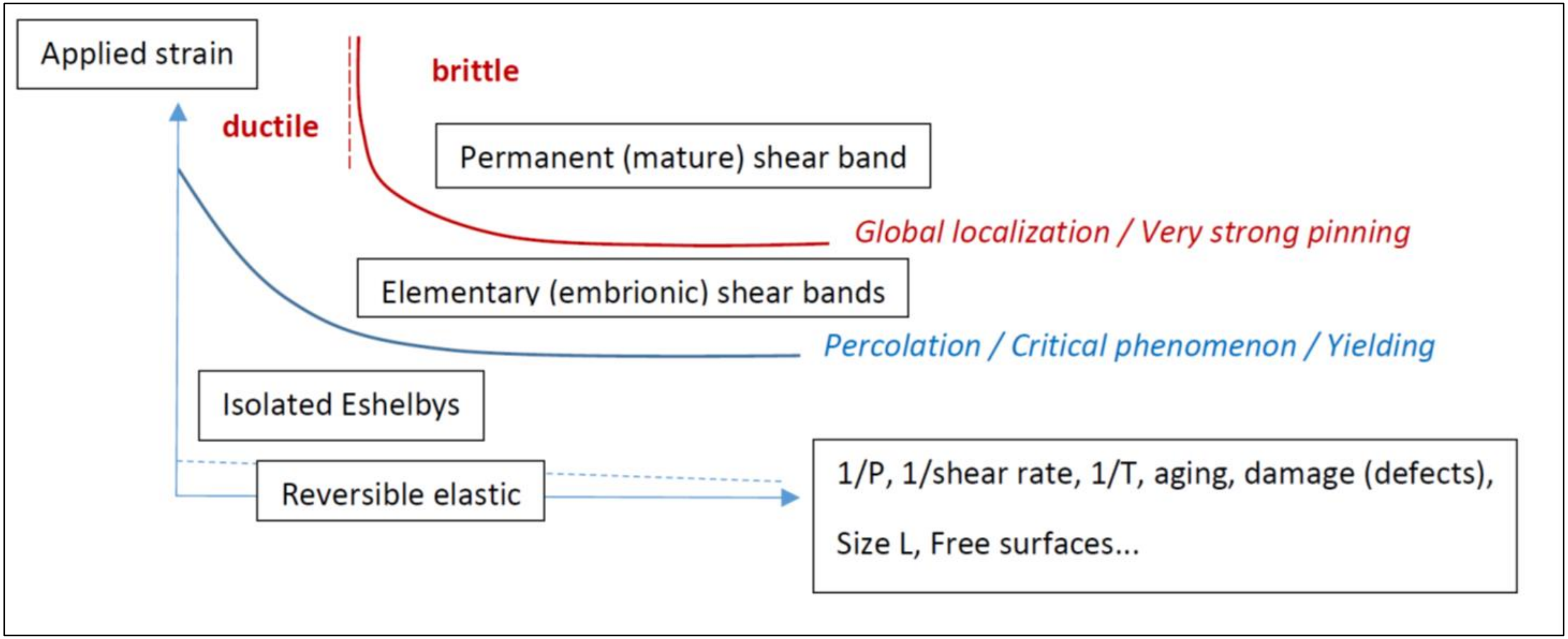












A. Tanguy (2021)

In **Amorphous Materials**

- What are the **microscopic sources** of **mechanical deformation** ?
- Is it possible to define **Phonons** ?
- Is it possible to quantify **Thermal transport** ?

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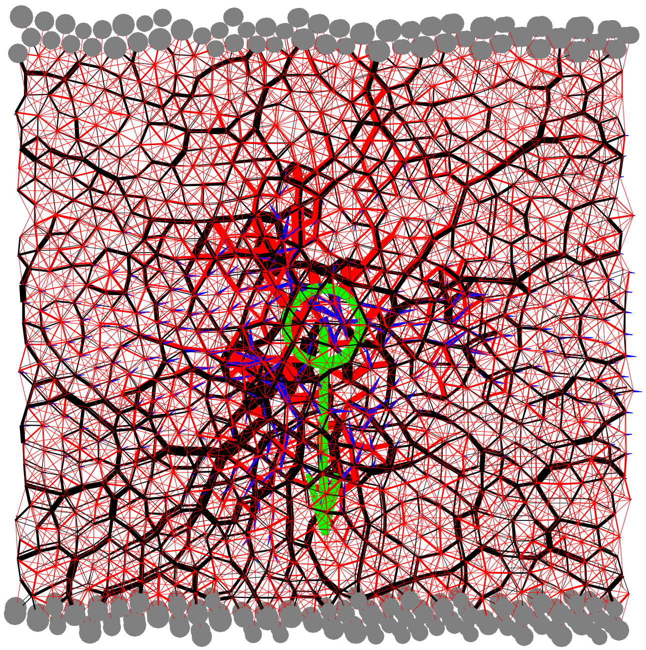
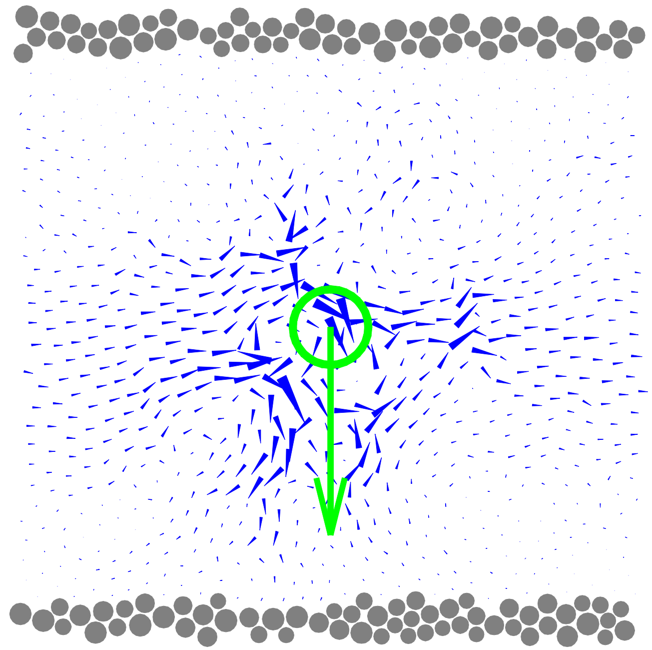
1. Elasticity of **Heterogeneous** Materials

F. Léonforte et al. (2004)



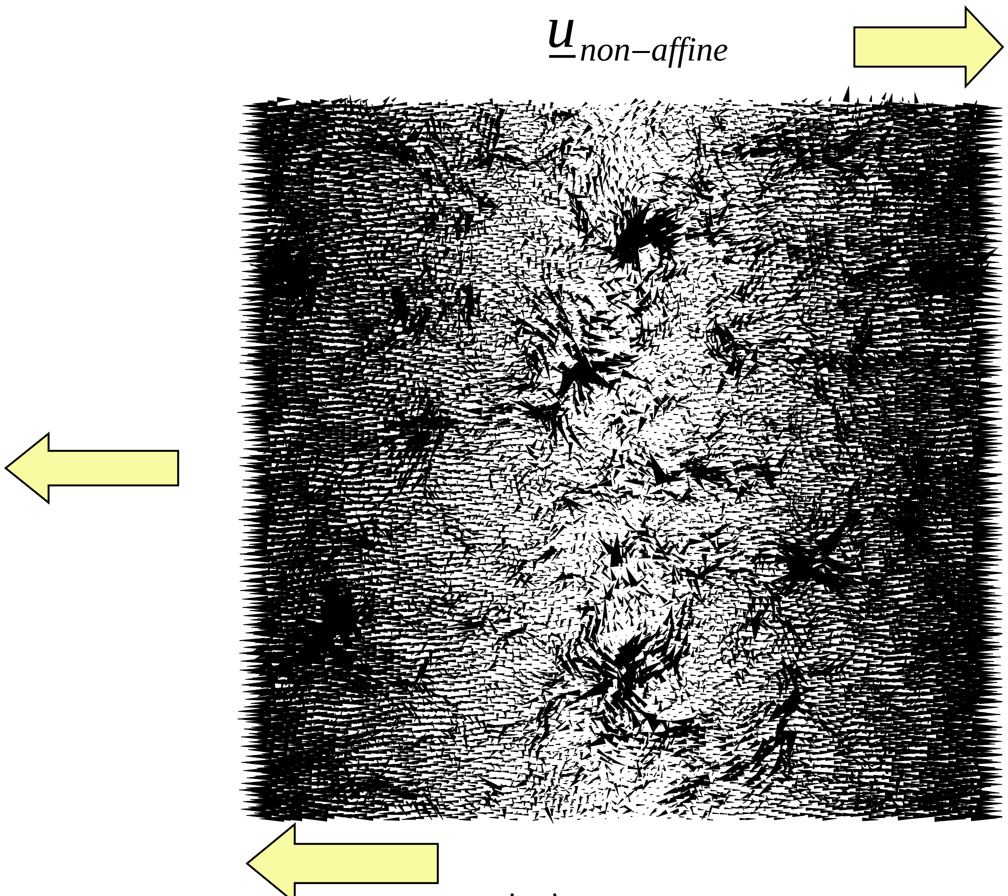
Response to a Point source force
(inverse Green Function)

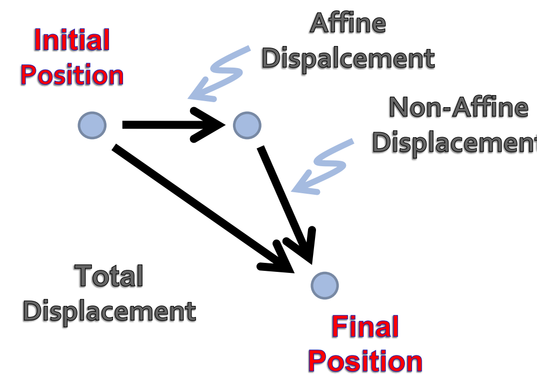


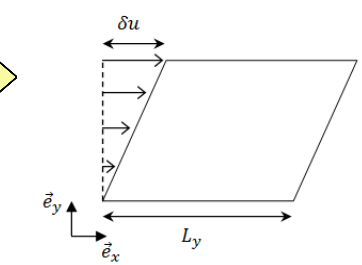
Force chains
Heterogeneous deformations
Rotational Motion

Atomistic Modeling of a 2D Lennard-Jones Glass

Non-affine displacement **field**







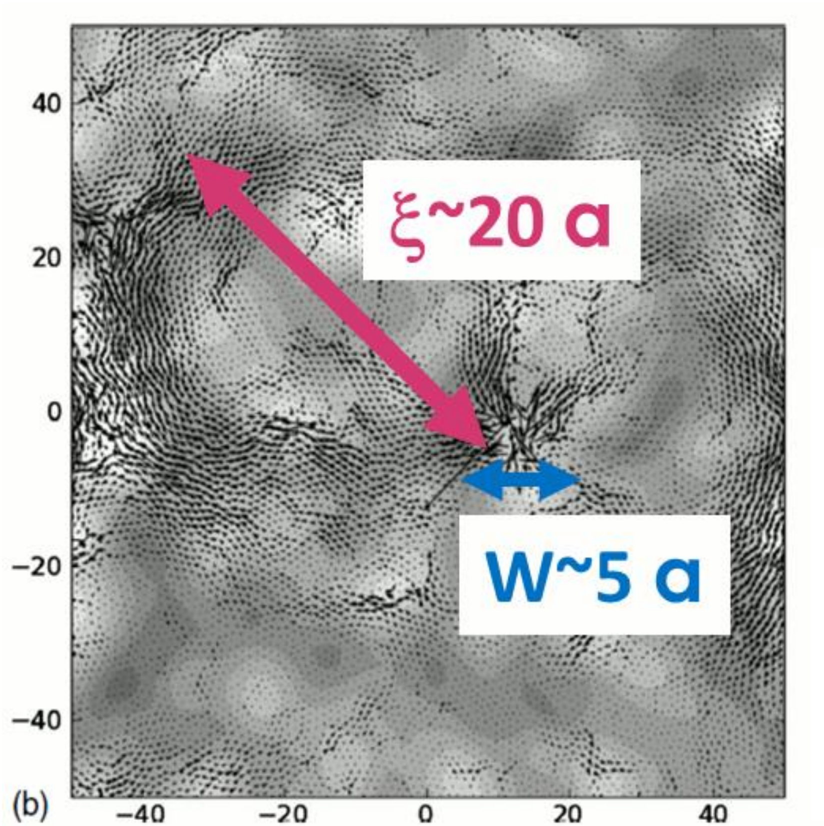
$$\underline{u} = \langle \underline{\underline{\varepsilon}} \rangle . \underline{r} + \underline{u}_{non-affine}$$

J.R. Williams et at. (1997)
G. Debrégeas et al. (2001)
A. Tanguy et al. (2002)
B. Doliwa et al. (2003)
E. Kolb et al. (2003)
A. Lemaître et al. (2004)
E.R. Weeks et al. (2006)

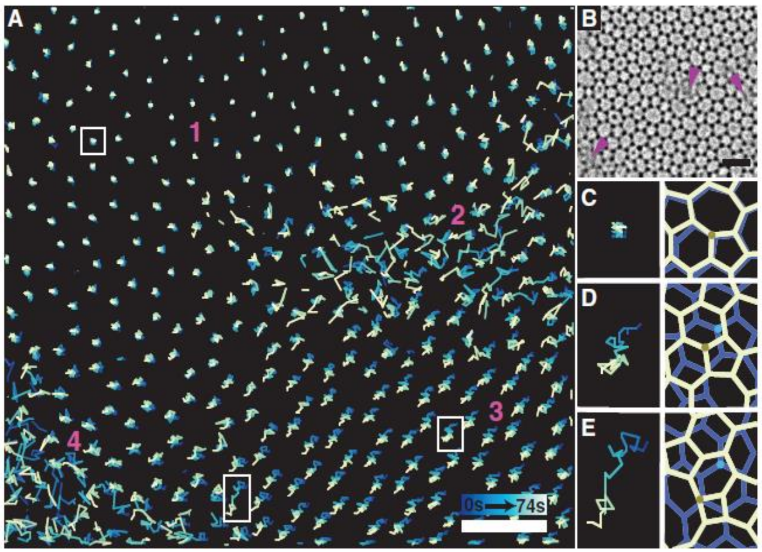
LaMCoS Unité Mixte de Recherche 5259 · CNRS · INSA Institut National des Sciences Appliquées Lyon · Université de Lyon

Laboratoire de Mécanique des Contacts et des Structures

Characteristic lengths in amorphous solids:



A. Tanguy et al. (2002)
M. Tsamados et al. (2009)



Imaging Atomic Rearrangements in Two-Dimensional Silica Glass: Watching Silica's Dance

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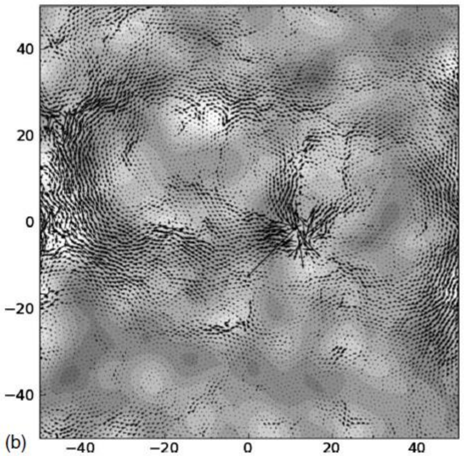
P.Y. Huang et al. Science (2013)

Heterogeneous displacements

Voigt calculation (1889): $\left\langle \underline{\underline{\varepsilon}} \right\rangle : \underline{\underline{\underline{\underline{C_{eff}}}}} : \left\langle \underline{\underline{\varepsilon}} \right\rangle \leq \left\langle \underline{\underline{\varepsilon}} \right\rangle : \left\langle \underline{\underline{\underline{\underline{C}}}} \right\rangle : \left\langle \underline{\underline{\varepsilon}} \right\rangle$

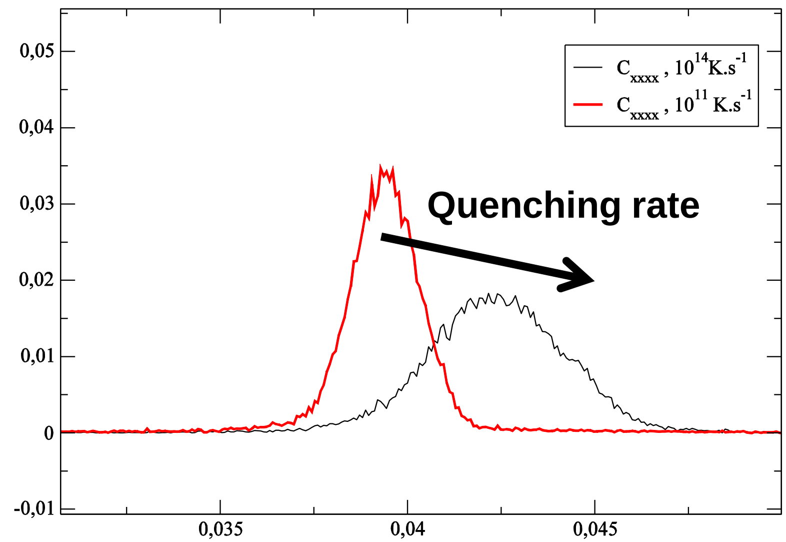
with equality only if $\underline{\underline{\varepsilon}}(\underline{r}) = \left\langle \underline{\underline{\varepsilon}} \right\rangle$



(b)

TABLE II. Comparison of structural properties for A-Si for different quenching rates with λ=21.

Property	10^{11} K/s	10^{12} K/s	10^{13} K/s	10^{14} K/s
Average coord.	4.08	4.12	4.19	4.39
Average angle	108.81	108.50	108.1	106.96
Angle Dev.	11.92	13.69	15.52	19.46
C44 (GPa)	34.24	32.04	29.98	27.66
B0 (GPa)	100.59	105.19	108.71	118.57
ν	0.347	0.362	0.374	0.392
Density (g/cm^3)	2.30277	2.32238	2.32238	2.32238
Pressure (GPa)	0.638	1.34	1.019	−0.8787



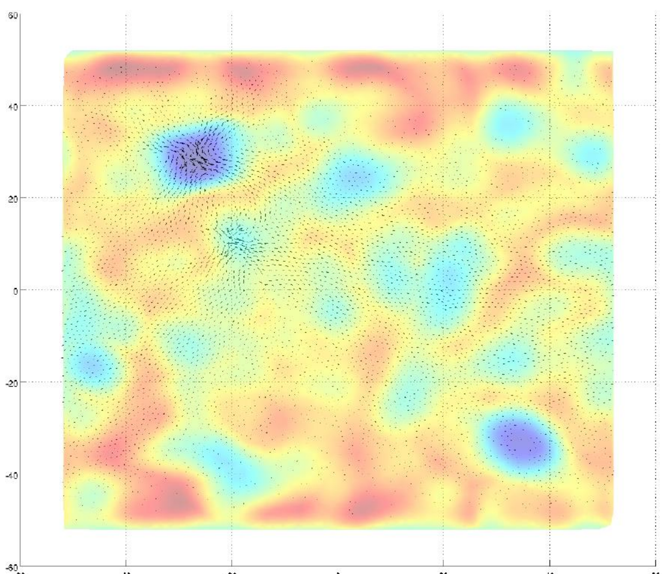
Low Effective Elastic Modulus (Reuss, 1929) when large dispersion of local elasticity

Local **Elastic Moduli**

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1131} & C_{1112}\\ C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2231} & C_{2212}\\ C_{3311} & C_{3322} & C_{3333} & C_{3323} & C_{3331} & C_{3312}\\ C_{2311} & C_{2322} & C_{2333} & C_{2323} & C_{2331} & C_{2312}\\ C_{3111} & C_{3122} & C_{3133} & C_{3123} & C_{3131} & C_{3112}\\ C_{1211} & C_{1222} & C_{1233} & C_{1223} & C_{1231} & C_{1212}\end{bmatrix} \cdot \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ 2\,\varepsilon_{23}\\ 2\,\varepsilon_{31}\\ 2\,\varepsilon_{12}\end{bmatrix}$$

Linear Hooke's Law
21 unknown parameters

Best reliability
between local stresses and local strains.
Local optimization with 6 different deformations



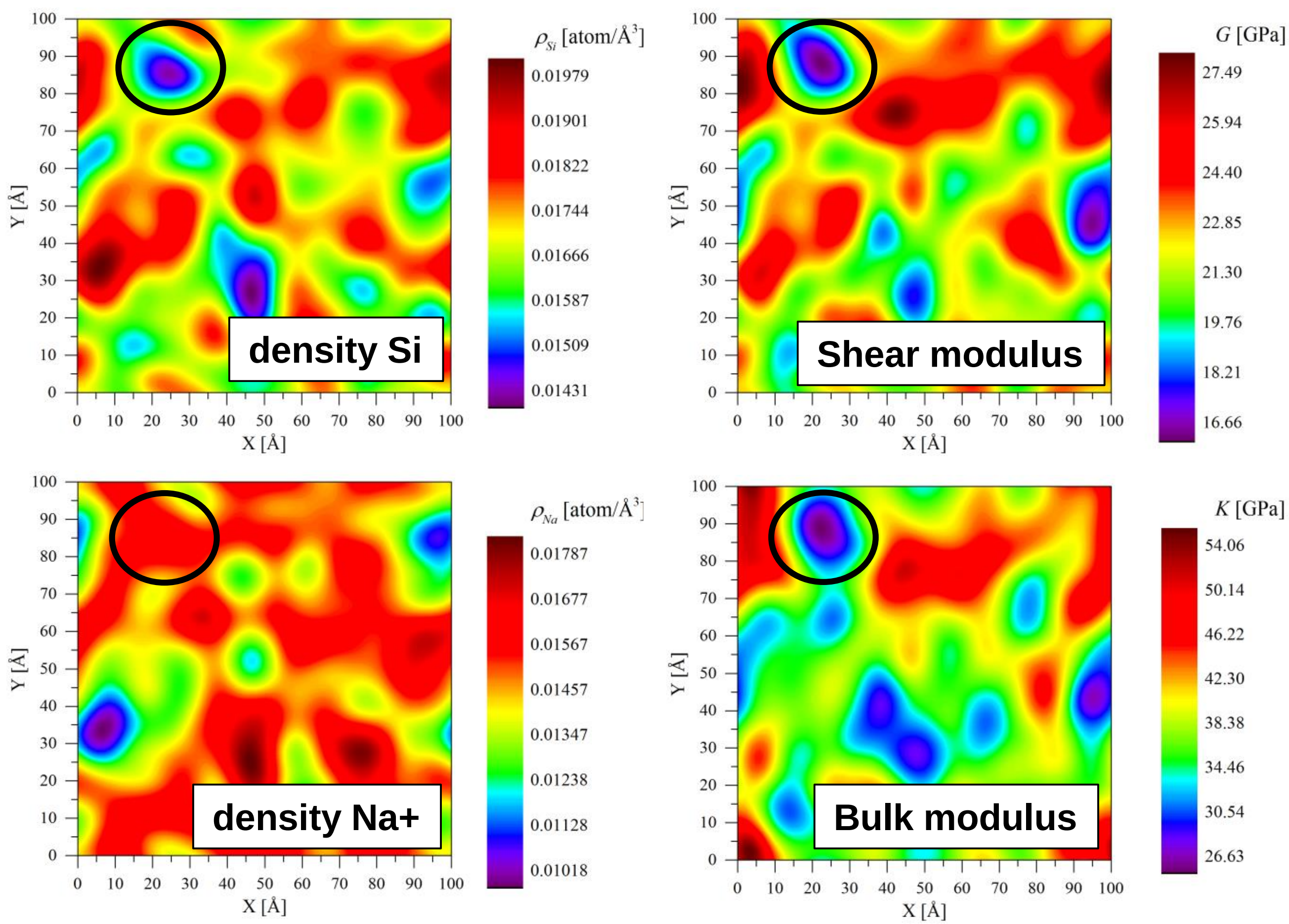
Linear Elasticity

Coarse Graining Length ω	0	5	10	15	20 a
Hooke's law	NO	YES	YES	YES	YES
Homogeneity $\frac{<c>(W)-2\mu}{2\mu}<10\%$	NO	NO	YES	YES	YES
$\frac{\Delta C}{<c>}<10\%$	NO	NO	NO	YES	YES
Isotropy $\frac{c_2-c_1}{2\mu}<10\%$	NO	NO	NO	NO	YES

Isotropic Elasticity

M. Tsamados et al. (2009)

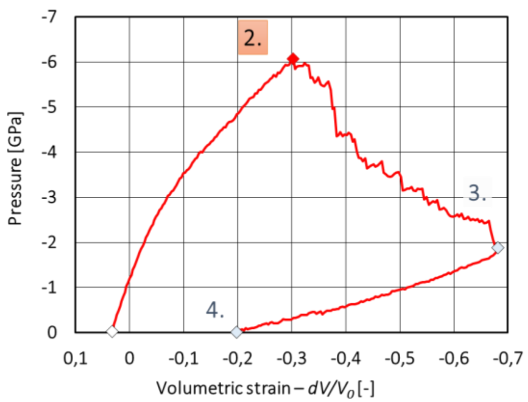
Elastic Moduli in a sodo-silicate glass $(1-x)SiO_2 + xNa_2O$:

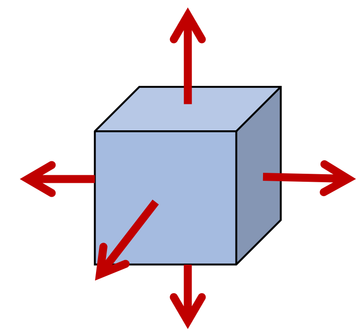


High loca Na+ density↔ Low Elastic Modulus

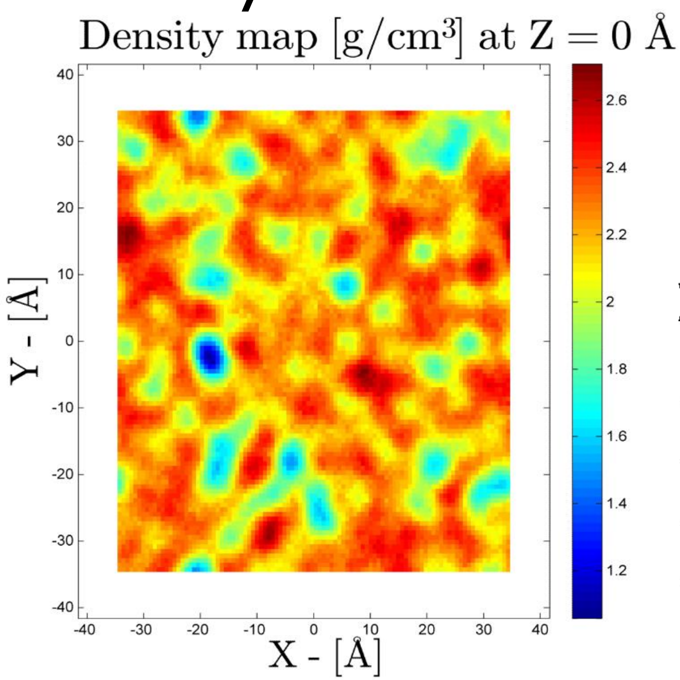
G. Molnar et al. (2016)

Crack Initiation in a sodo-silicate glass $(1\text{-}x)SiO_2 + xNa_2O$:

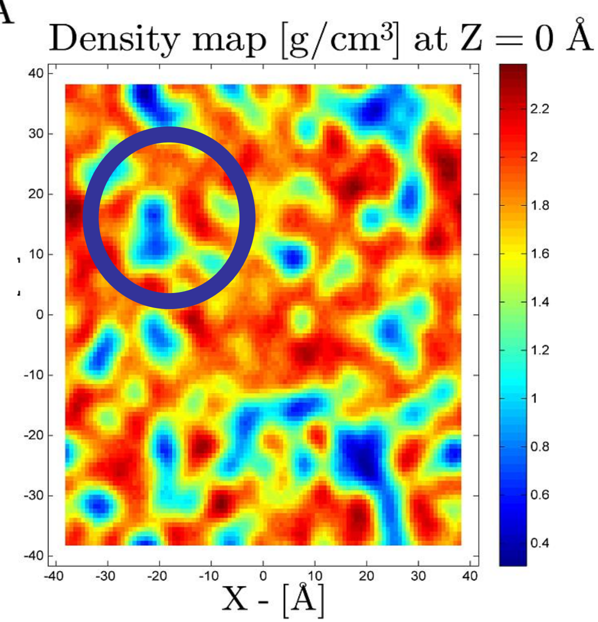




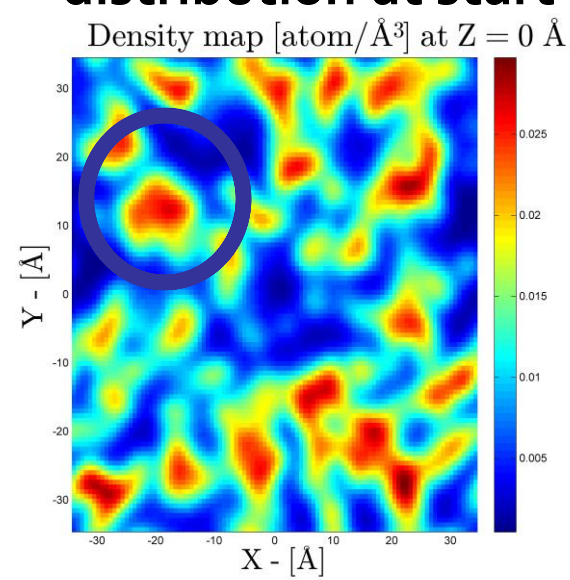
density at start



loosened density (initial cracks)

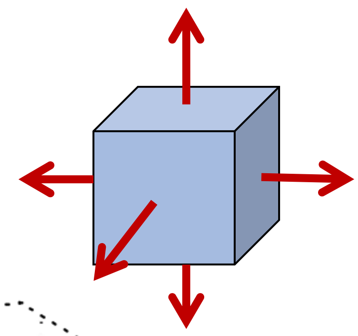


Na density distribution at start

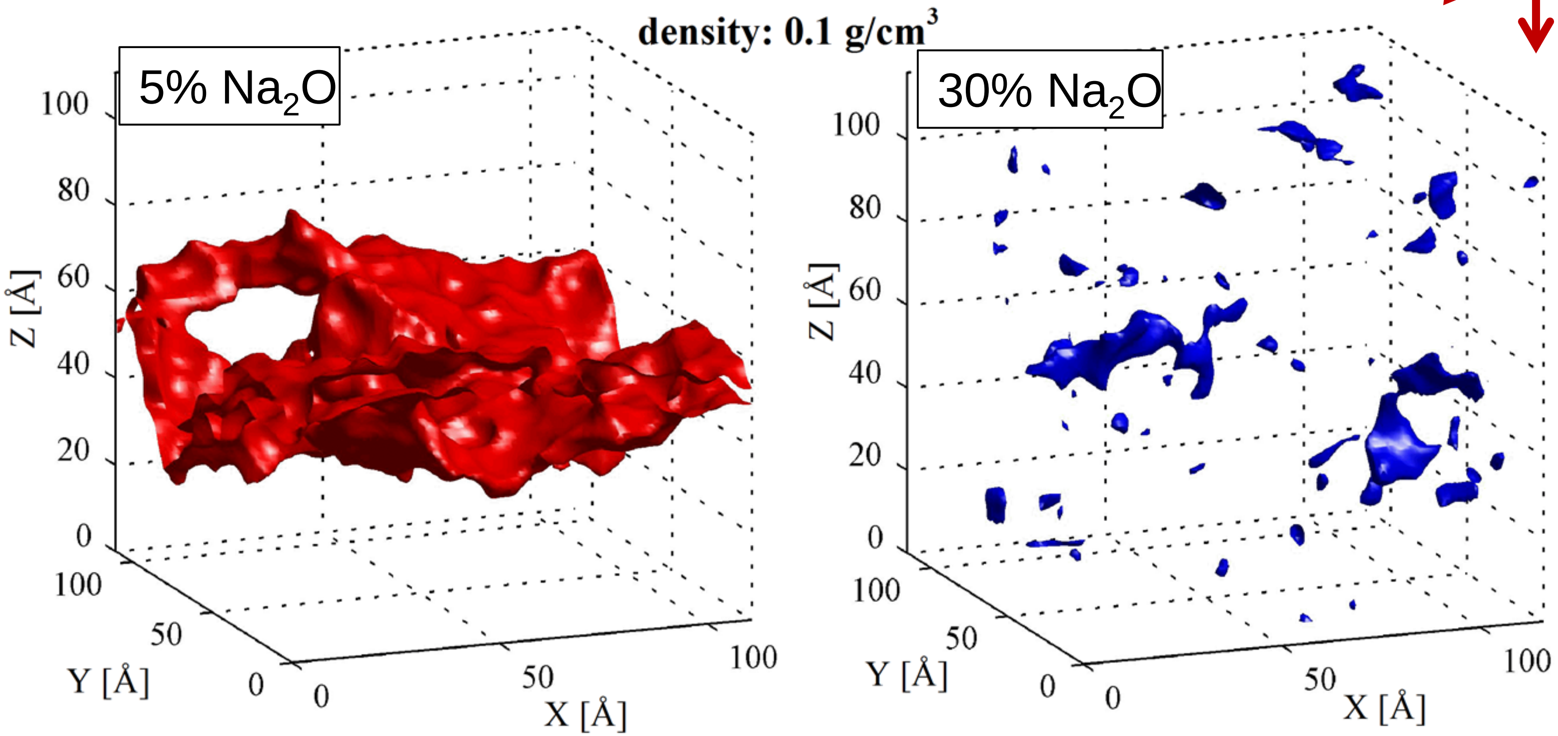


G. Molnar et al. (2016)

Crack Initiation in a
sodo-silicate glass
$(1\text{-}x)SiO_2 + xNa_2O$:



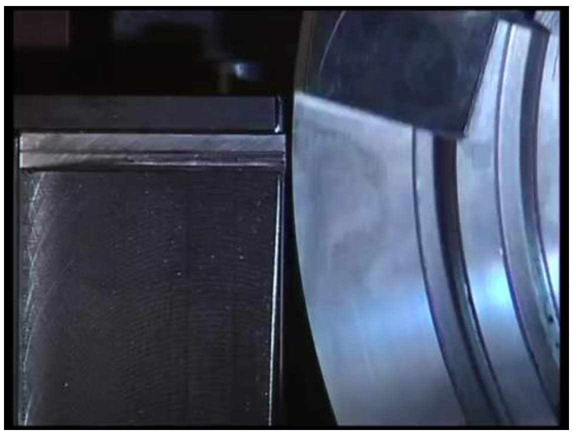
Effect of composition: density profile at max. tractions

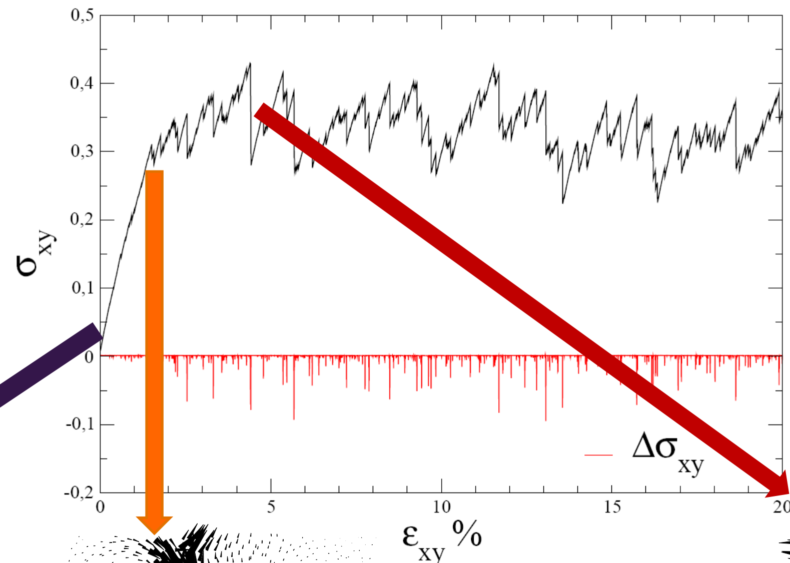


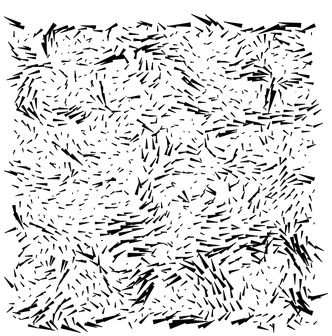
G. Molnar et al. (2016)

2. Irreversible **Plastic** deformation

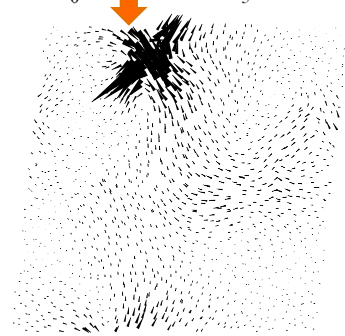
Plastic Deformation



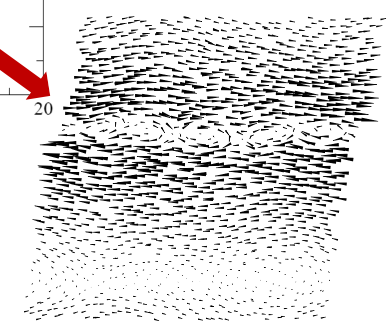




Non-affine **reversible** displacements (x10³)



Local shear **ir**reversible (x40) quadrupolar event



Elementary Shear band (x0.4)

Reminder: Hill's Criterion for Crystals Stability (1962) : Continuous Media

Helmholtz Free Energy $$F(Y) \equiv F(X) + \Omega(X)\left\{ \tau_{ij}(X)\,\eta_{ij} + \frac{1}{2} C_{ijkl}(X)\,\eta_{ij}\,\eta_{kl} + \cdots \right\}$$

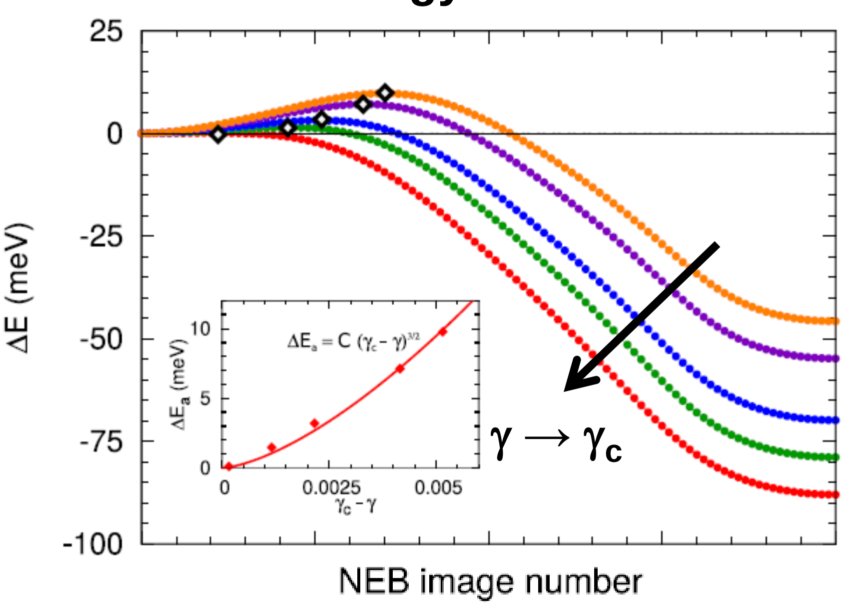
Stability Criterion $$\boxed{\min_{\{\underline{w},\underline{k}\}} \left(C_{ijkl} w_i w_k k_j k_l \right) \geq 0}$$

$\eta_{ij} \propto w_i k_j$

Slip Plane

Burgers Vector

Energy Barriers



A. Lemaitre and C. Maloney (2004)
T. Albaret and D. Rodney (2018)

In **Amorphous materials**: Atomistic description

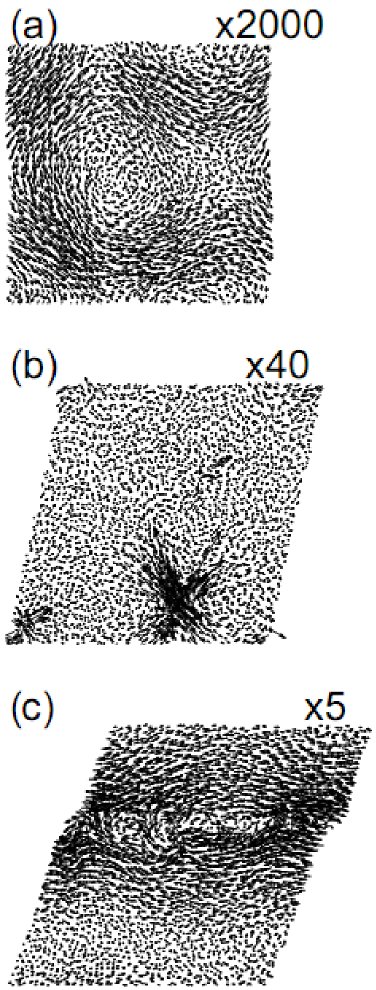
$$m_i \frac{\partial^2 u_\alpha}{\partial t^2}(\underline{r_i}, t) = -\sum_{j,\beta} M_{ij}^{\alpha\beta} . u_\beta(\underline{r_j}, t)$$

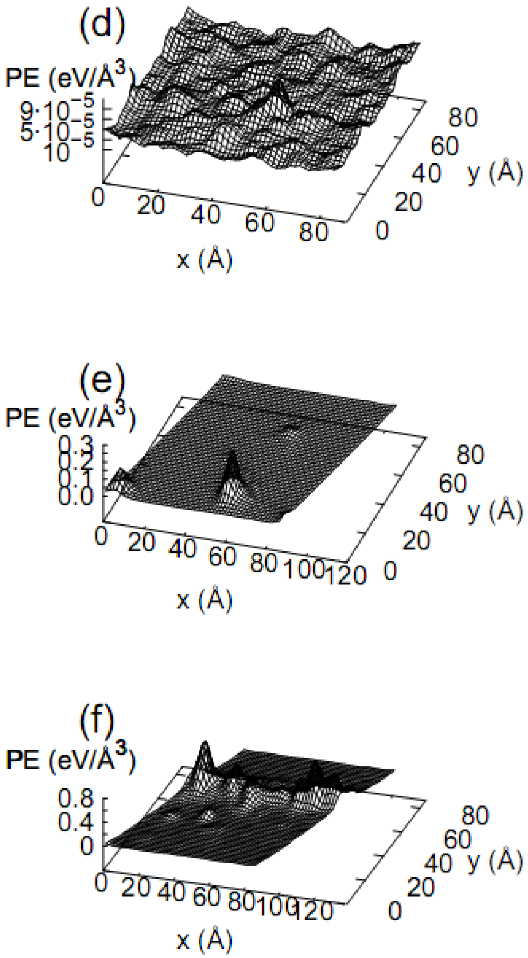
with $M_{ij}^{\alpha\beta} = -\dfrac{\partial^2 E_{total}}{\partial r_{i\alpha} \partial r_{j\beta}}$ including external forces

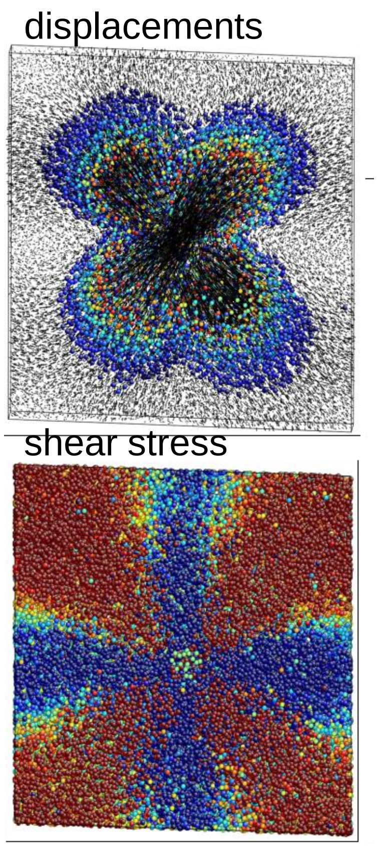
$$\underline{V}(\underline{r_i}) e^{i\omega t} = \sqrt{m_i}\, \underline{u}(\underline{r_i}, t) \,,\; D_{ij}^{\alpha\beta} = \frac{M_{ij}^{\alpha\beta}}{\sqrt{m_i m_j}}$$

$\boxed{\omega^2 \underline{V} = \overline{\overline{D}} . \underline{V}}$ $\omega \rightarrow 0$ **Instability**

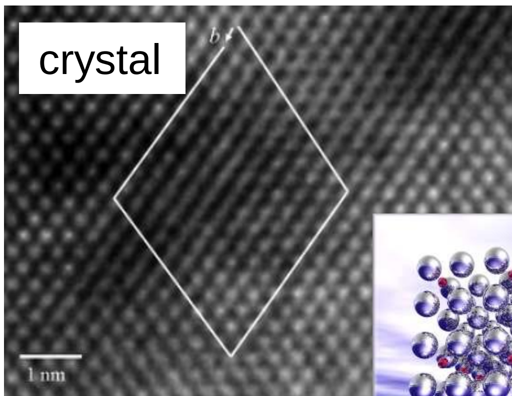
Local Irreversible **Plastic** deformation

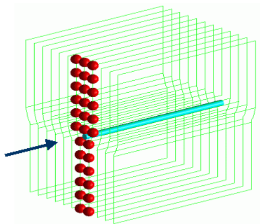


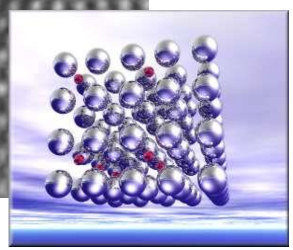




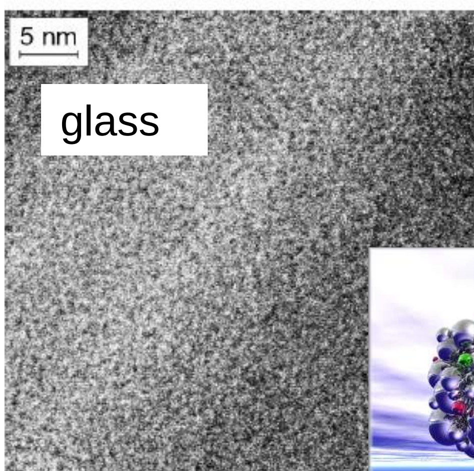
Glasses vs. Crystals

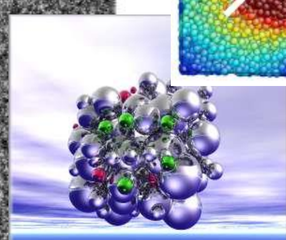


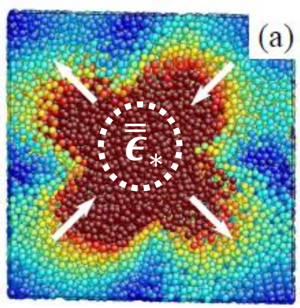




Dislocations

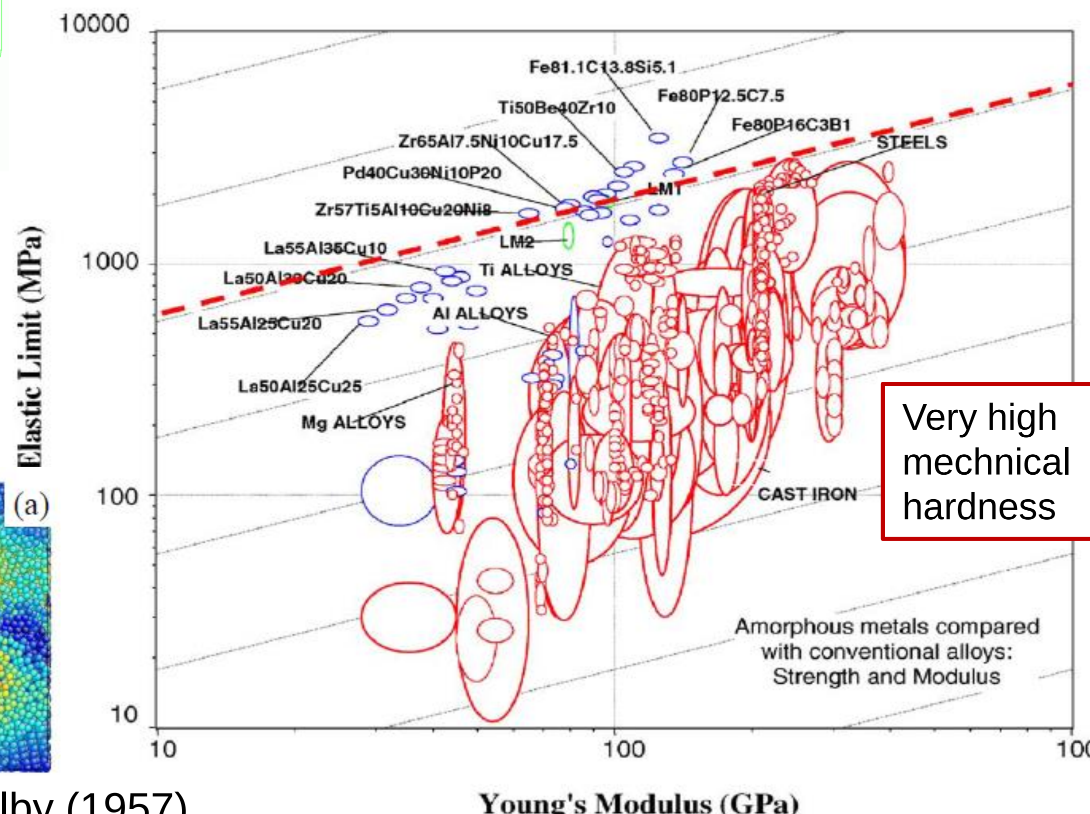






Local Eshelby inclusions

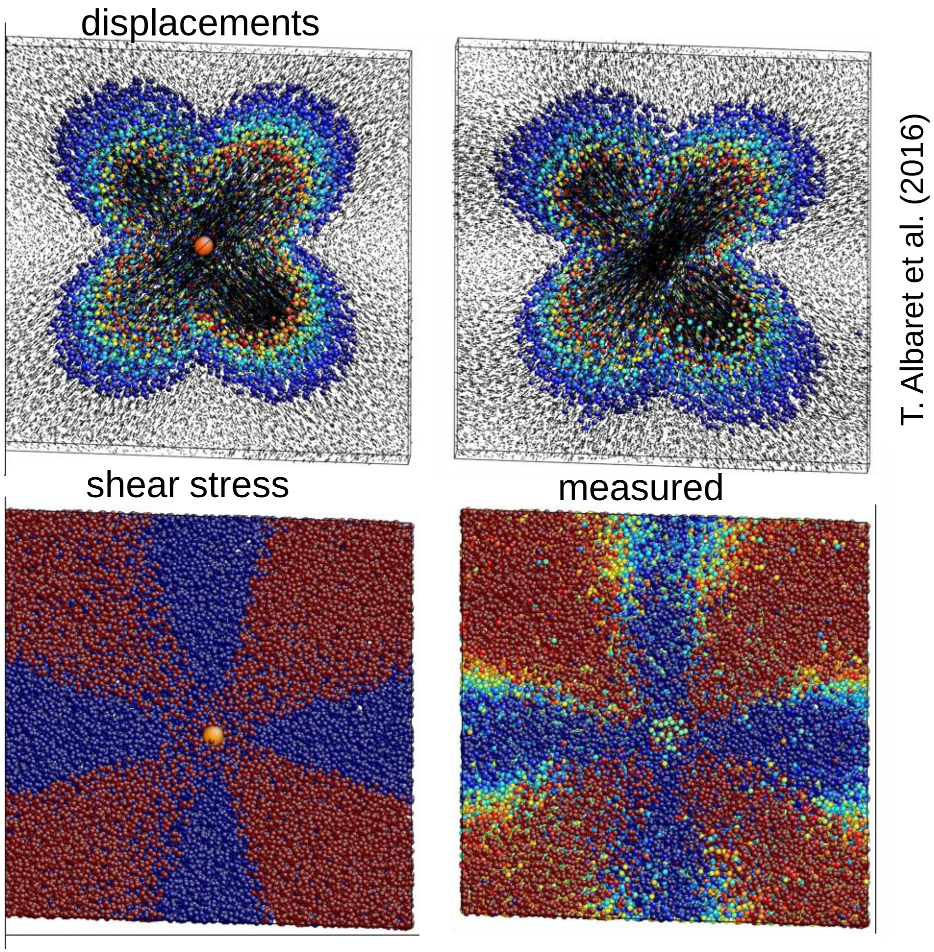
Eshelby (1957)
Lemaitre (2004)
Albaret (2016)

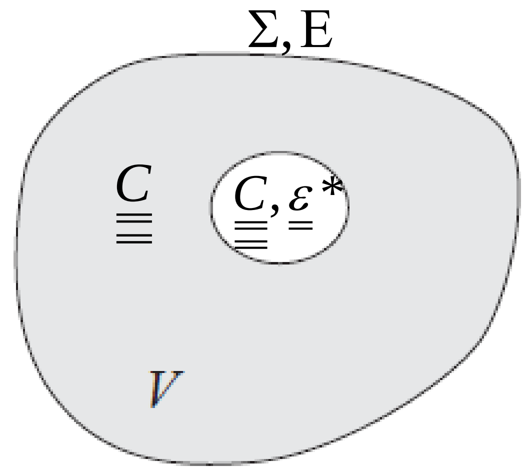


Very high mechnical hardness

M.F. Ashby (2006)

Local Irreversible **Plastic** deformation



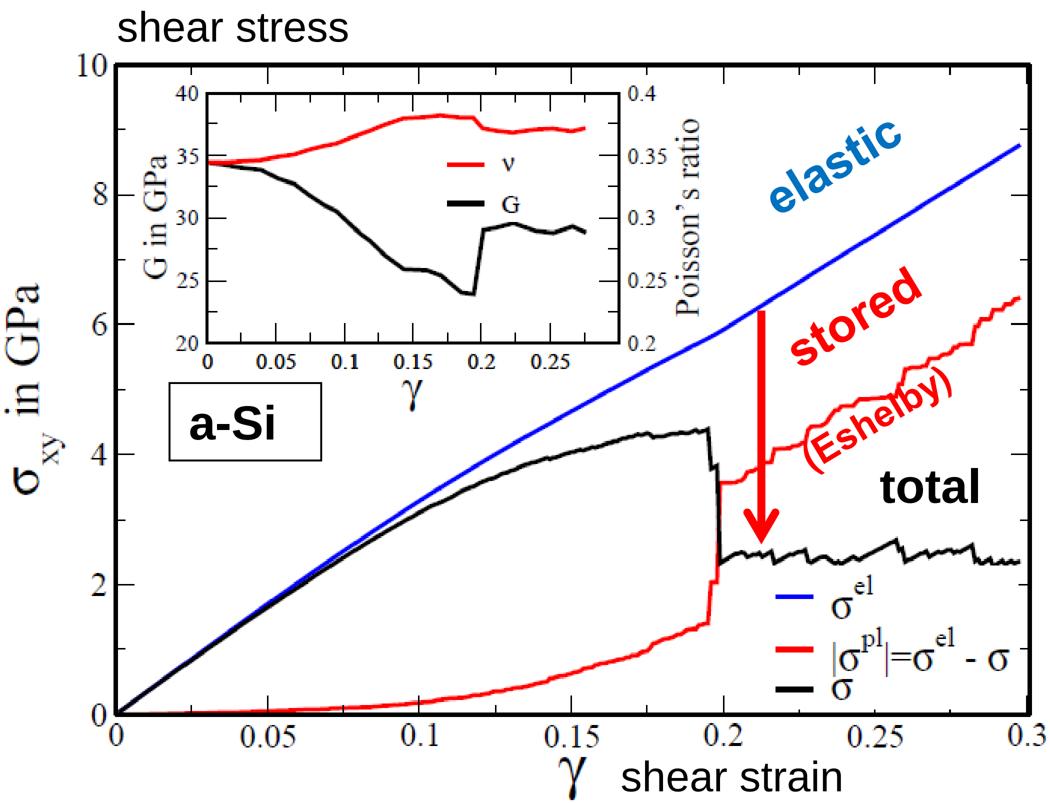


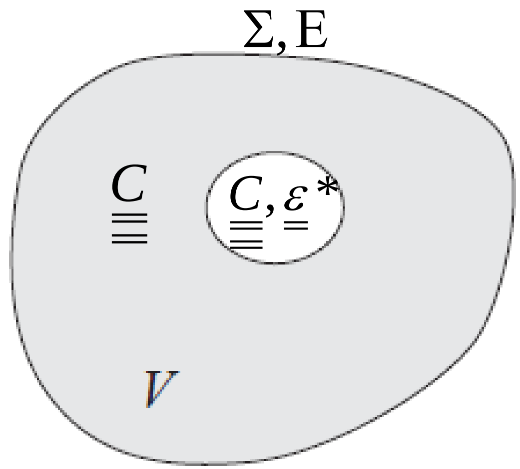
Eshelby-like Inclusion

$$\mathrm{div}\,\underline{\underline{\sigma}}^I = 0 \Leftrightarrow \mathrm{div}\left(\underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}\right) + f\left(\underline{\underline{\varepsilon}}^*\right) = 0$$

$$f\left(\underline{\underline{\varepsilon}}^*\right) = \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}^* . \underline{n}\,\delta\left(S^I\right) \Rightarrow \underline{\underline{\varepsilon}} = \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^*$$

Local Irreversible **Plastic** deformation





Eshelby-like Inclusion

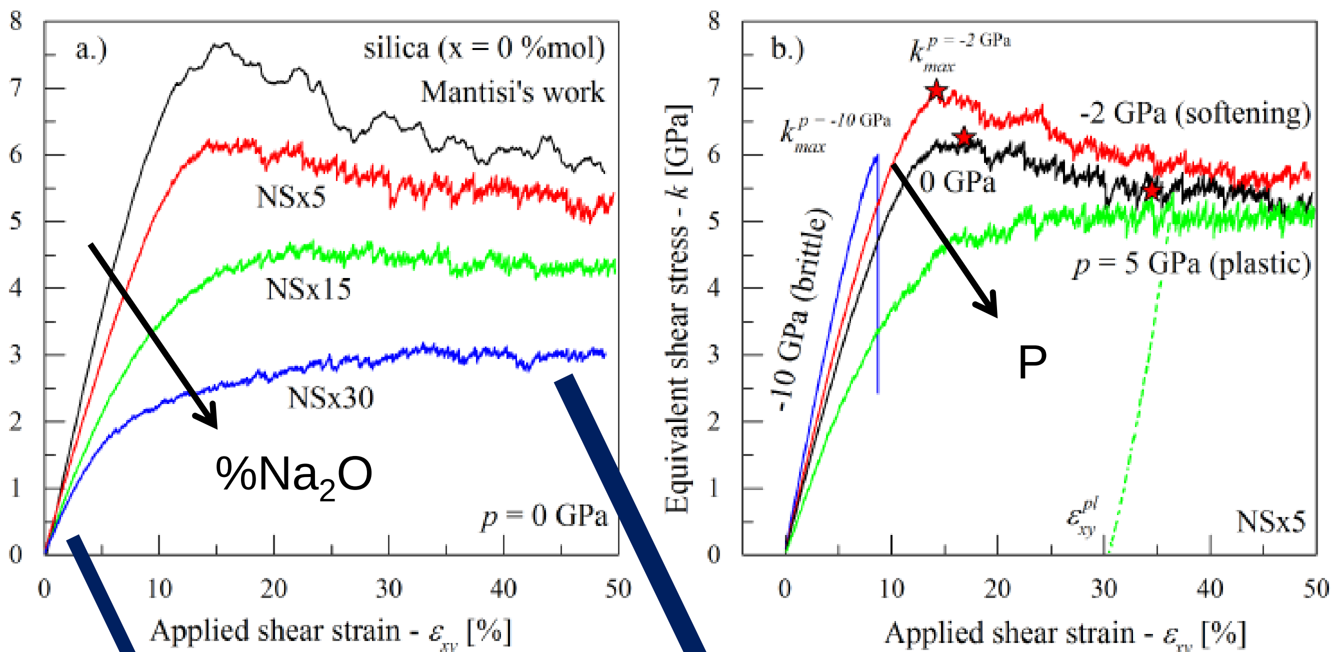
$$\delta\varepsilon_{xy} = \delta\varepsilon_{xy}^{el} + \delta\varepsilon_{xy}^{pl}$$

$$\delta\sigma_{xy}^{pl,esh+bc}(\gamma) = \frac{2G(\gamma)V_{esh}(\gamma)}{V_{cell}}\varepsilon_{xy}^{*}(\gamma)$$

$$\boxed{\delta\sigma_{xy} = 2G(\gamma)\delta\varepsilon_{xy} - 2G(\gamma)\delta\varepsilon_{xy}^{pl} = \delta\sigma_{xy}^{el} - \delta\sigma_{xy}^{pl}}$$

T. Albaret et al. (2016)

Sensitivity to **Composition** and **Pressure**
The example of sodo-silicate glass

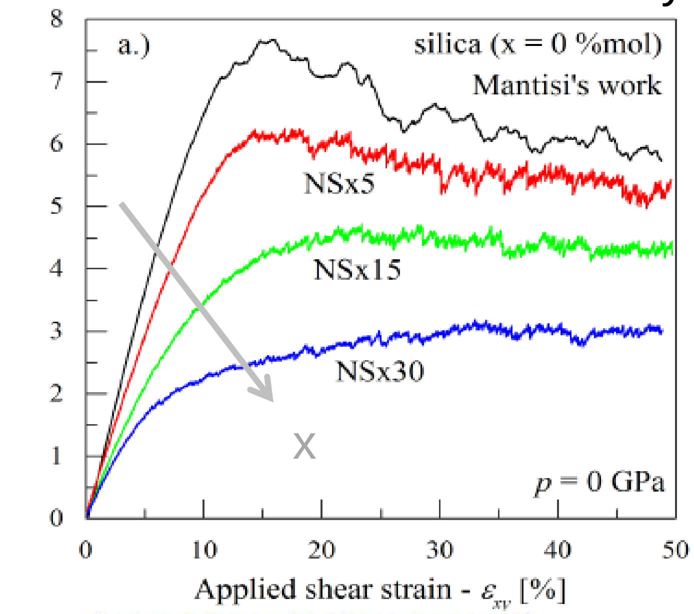


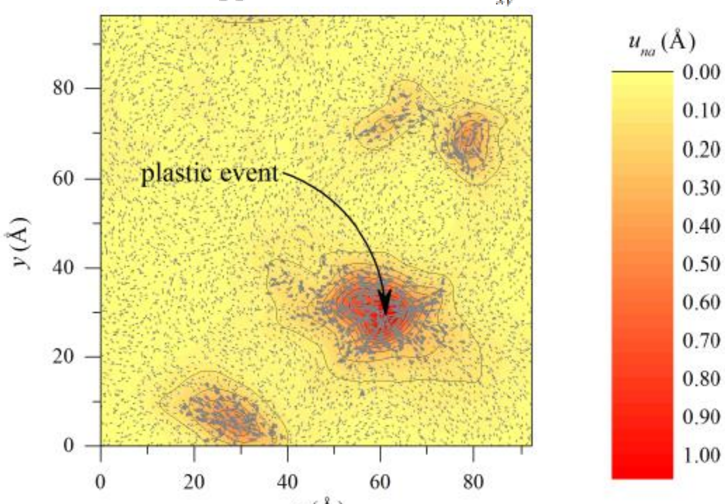
« Linear Elasticity »

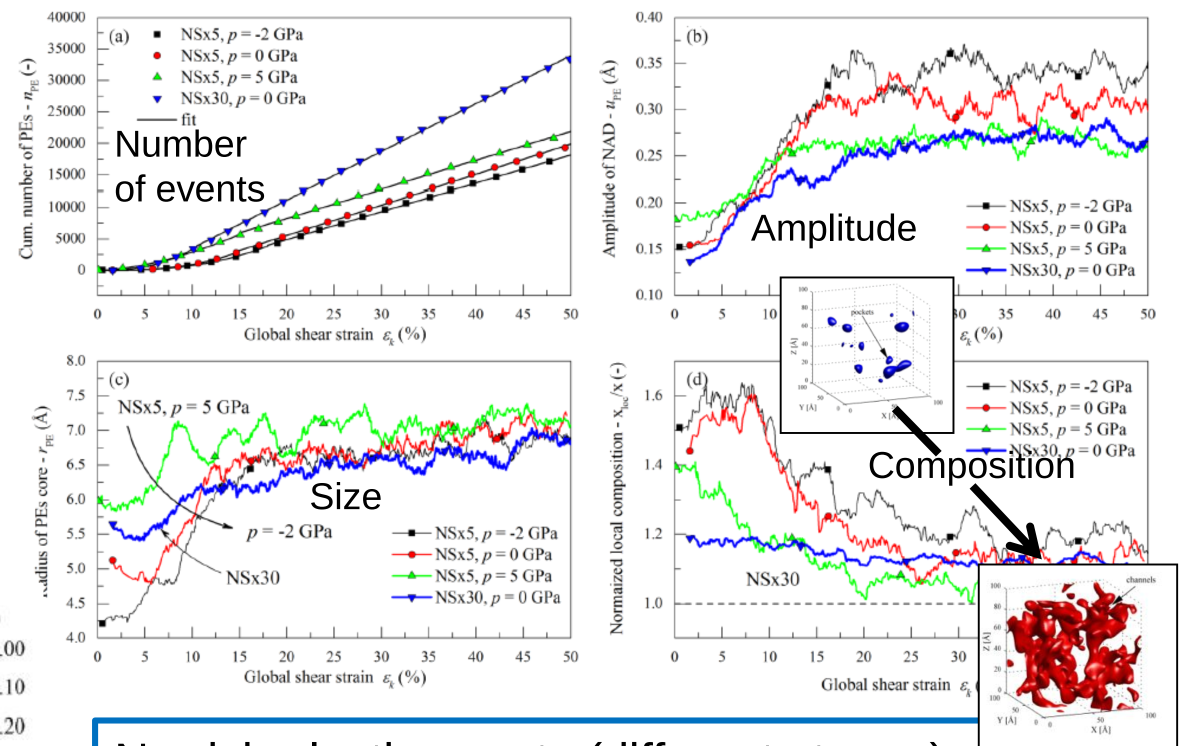
Plastic Plateau

G. Molnar et al. (2016)

Sensitivity to **Composition** and **Pressure**







Na-rich plastic events (different stages)

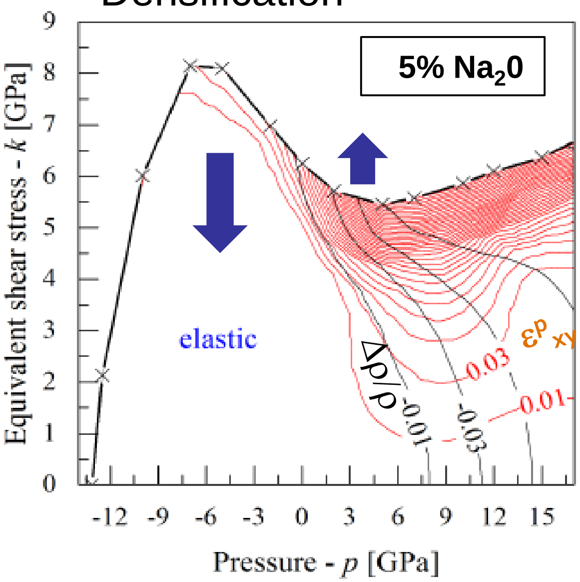
Composition controls the number of events

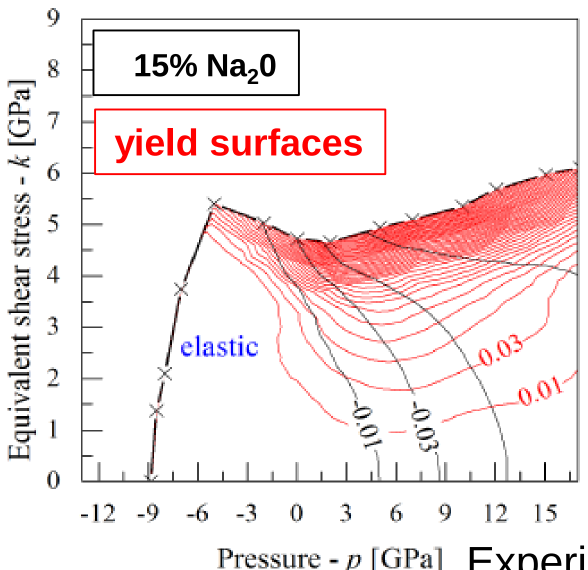
Pressure sensitivity of their size, and amplitude

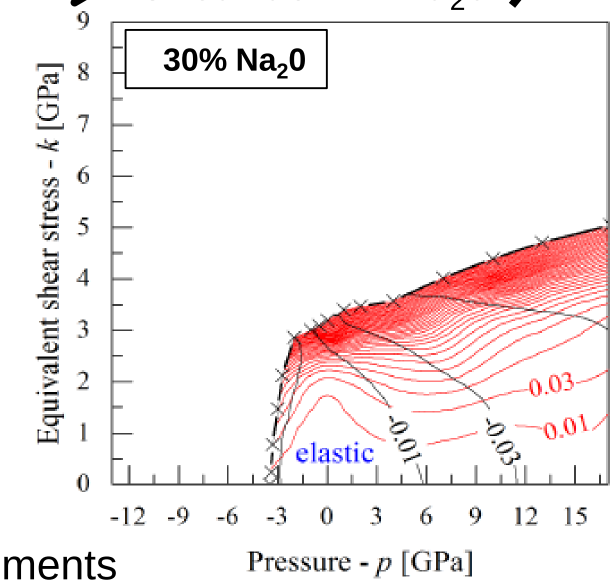
G. Molnar et al. (2017)

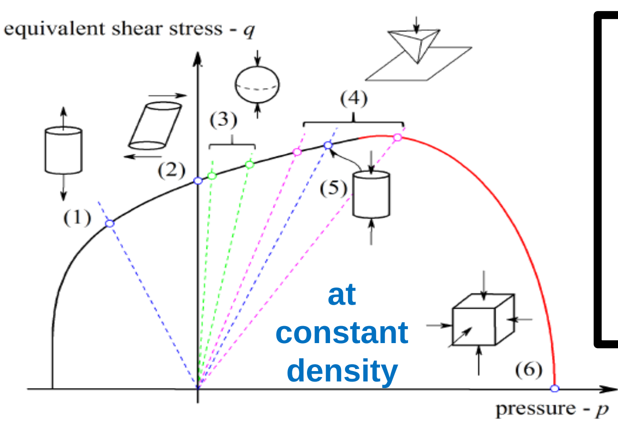
Sensitivity to **Composition** and **Pressure**

Densification → Shear as % Na_20 ↗



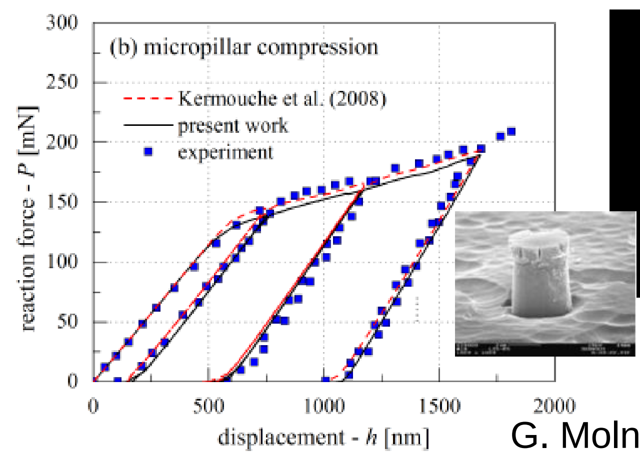


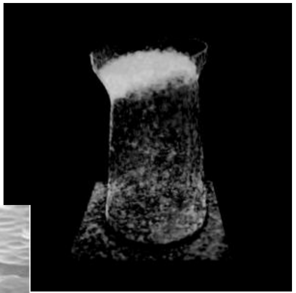




Adapt the **parameters** of the **yield surfaces** to experimental results

Experiments

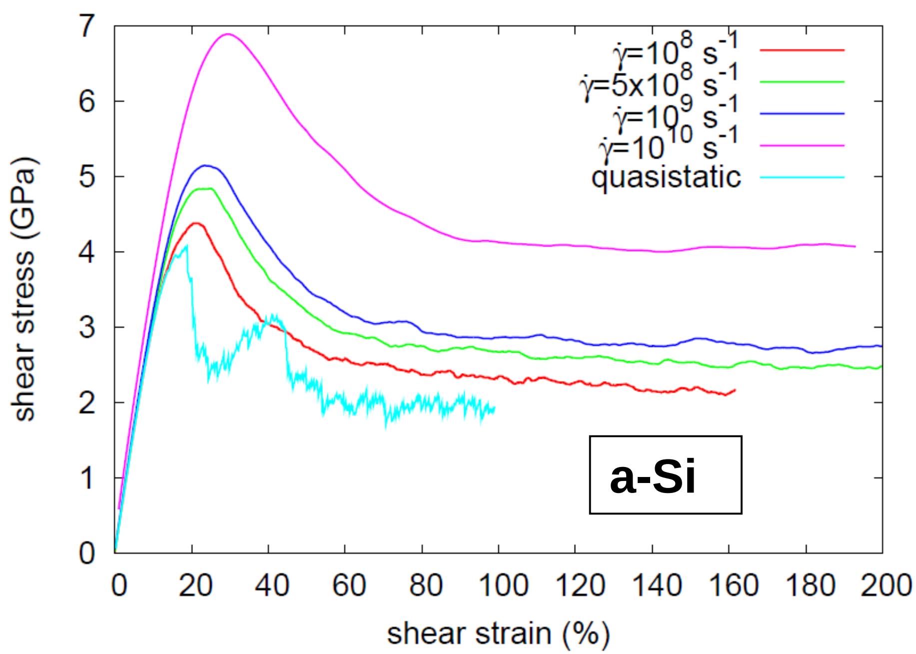


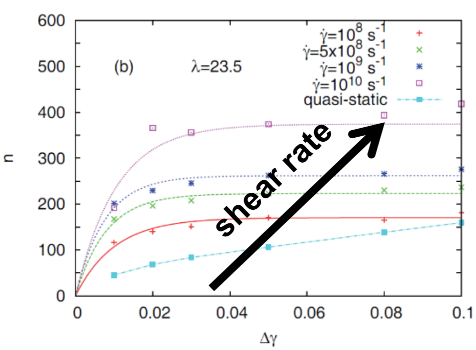


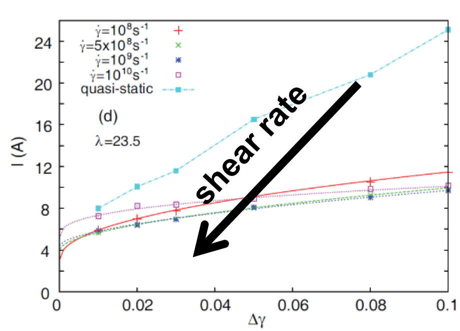
G. Kermouche. (2022)

G. Molnar et al. (2017)

Sensitivity to **Strain rate**

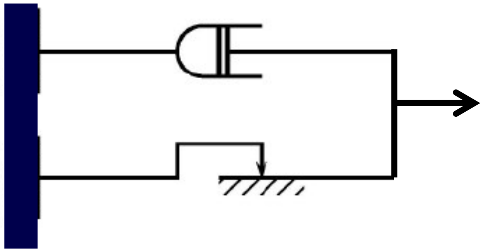


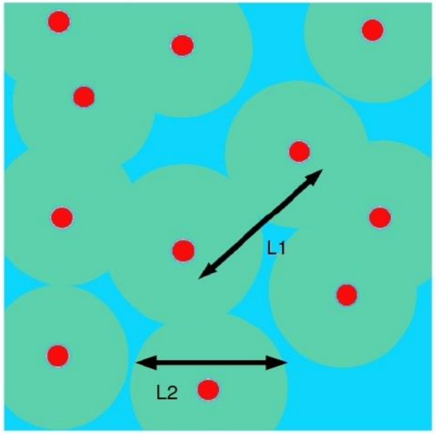




$$\sigma_F = \sigma_0 + (\dot{\gamma}/\dot{\gamma}_0)^{\beta} \quad \text{avec} \quad \beta \approx 0.4$$

Herschel-Bulkley (1926)



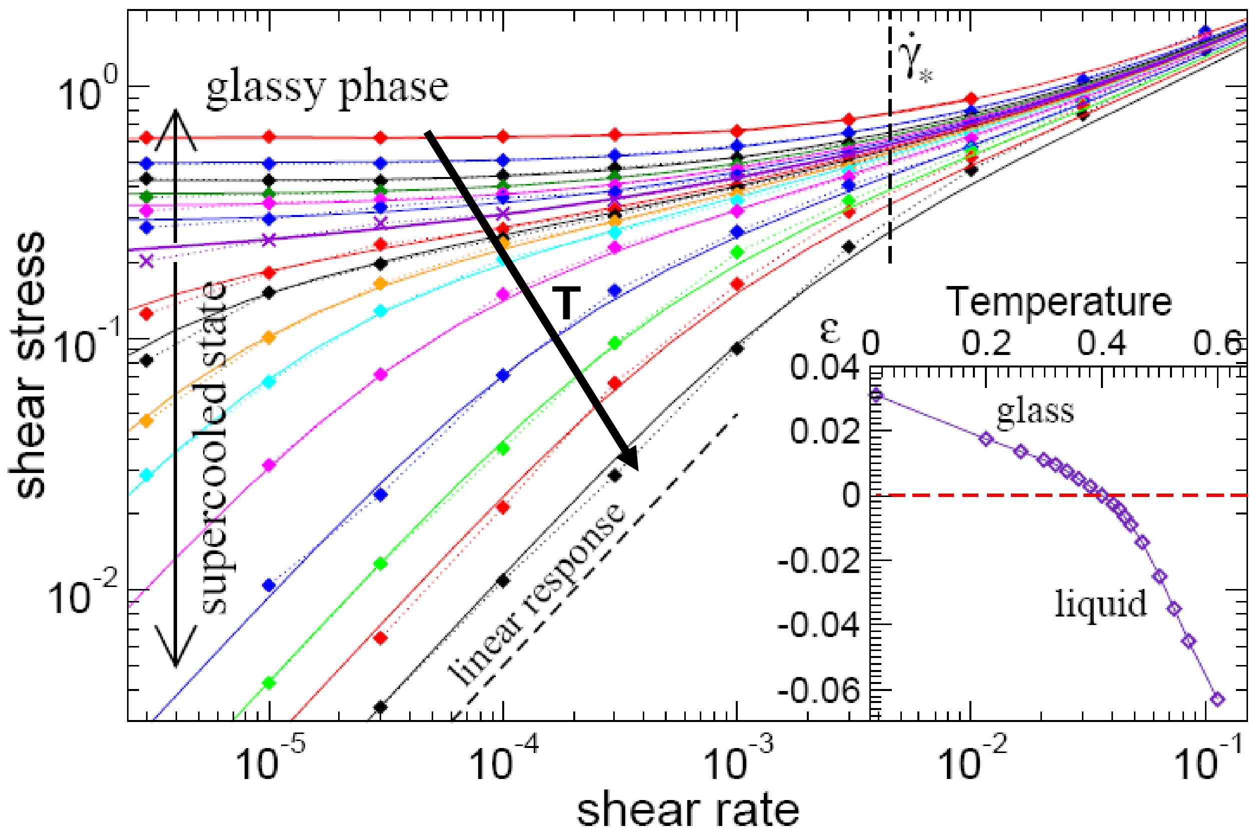


M. Tsamados (2010)
C. Fusco et al. (2013)

Rheological Properties:

Sensitivity to **Strain rate**

Flow Stress in a Lennard-Jones Glass:



~ Herschel-Bulkley

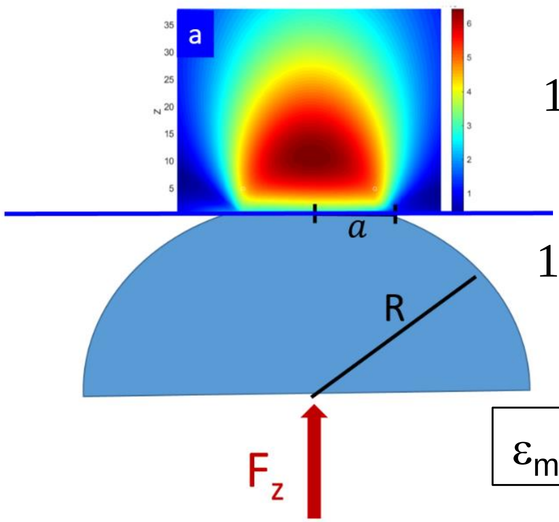
$$\sigma_F = \sigma_0 + C.\dot{\gamma}^n$$

n<1 shear thinning
n>1 shear thickenning

F. Varnik et al. (2006)

Sensitivity to **Disorder**

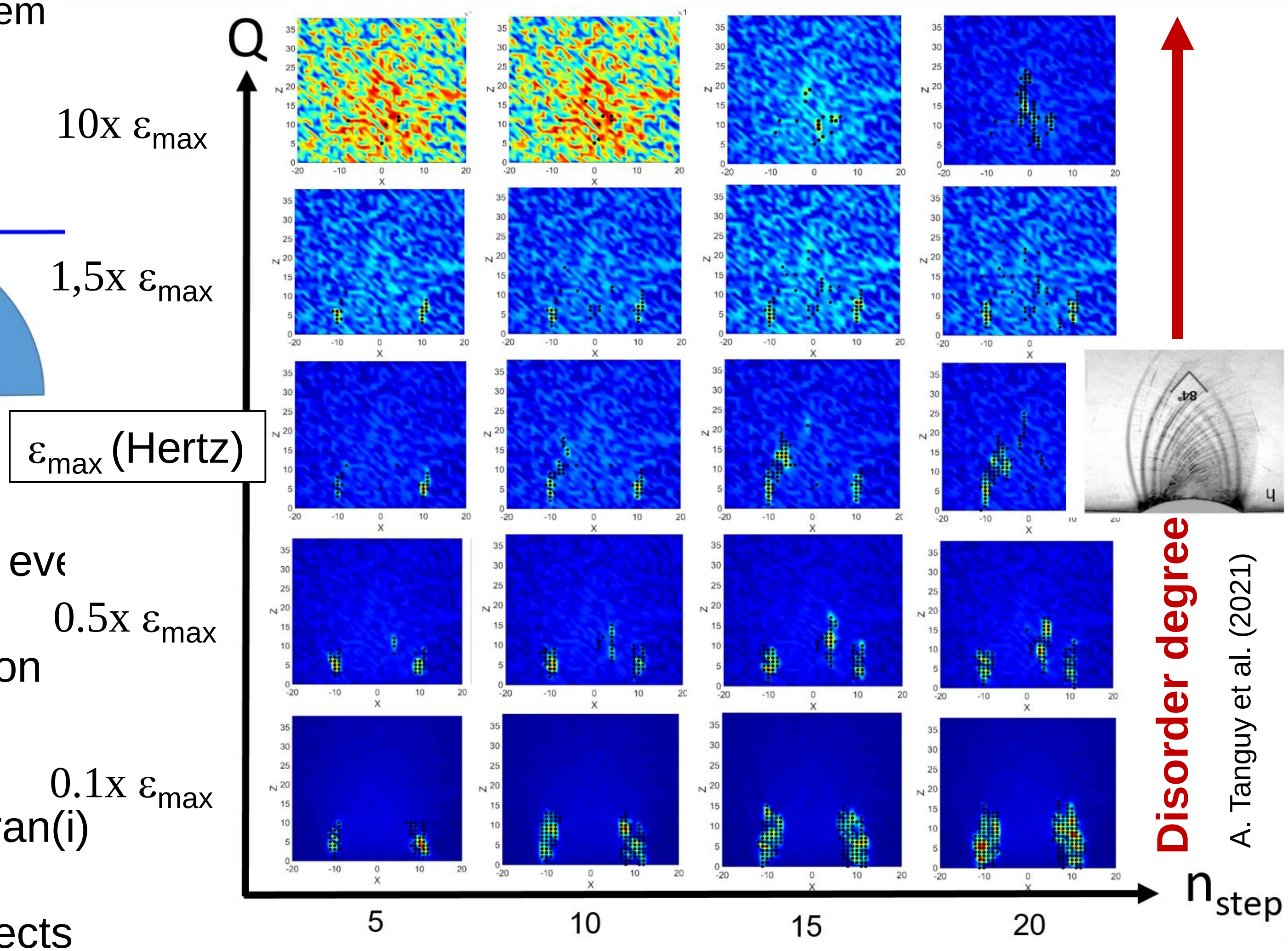
Example of **shear banding** in a **contact** problem



$\varepsilon(i) > \varepsilon^d_{thresh}(i)$: plastic eve
then : $\varepsilon(i) = \varepsilon(i) + d\varepsilon$
with stress redistribution

Random threshold:
$\varepsilon^d_{thresh}(i) = \varepsilon^0_{thresh} + Q.ran(i)$

with initial surface defects



Conclusion Mechanical Deformation

Inhomogeneous reversible elastic behaviour → Lower effective sound velocity

Localized plasticity → Low dissipation, sensitivity to local structure

In **Amorphous Materials**

- What are the **microscopic sources** of **mechanical deformation** ?
- Is it possible to define **Phonons** ?
- Is it possible to quantify **Thermal transport** ?

Cas d'un milieu continu, linéaire, homogène et isotrope:

2 modules d'élasticité, λ et μ

Phonons = (quantum) **vibrations** in crystals

stresses $\sigma_{\alpha\beta} = \sigma_{\alpha\beta}{}^{0} + \lambda . tr\underline{\underline{\varepsilon}}.\delta_{\alpha\beta} + 2\mu.\varepsilon_{\alpha\beta}$

equation of motion (momentum conservation):

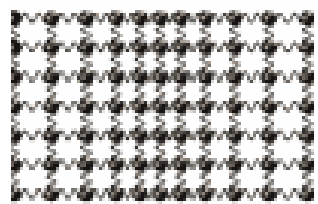
$$\rho \frac{\partial^2 \underline{u}}{\partial t^2} = (\lambda + 2\mu).\underline{grad}.div\underline{u} - \mu.\underline{rot}.\underline{rotu} + \underline{f_{ext}}$$

$$\underline{u} = \underline{grad}(\varphi) + \underline{rot}(\underline{\psi})$$

Longitudinal modes:

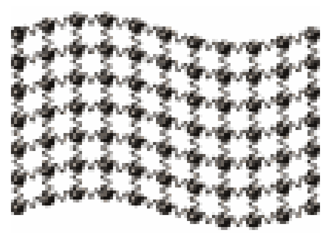
$$\ddot{\phi} = c_L{}^2.\nabla^2\phi, \quad c_L = \sqrt{\frac{\lambda + 2\mu}{\rho}}$$

$$\omega_{lmn} = c_L.k = c_L.\frac{2\pi}{L}.\sqrt{n^2 + m^2 + l^2}$$



Transverse modes:

$$\ddot{\underline{\psi}} = c_T{}^2.\nabla^2\underline{\psi}, \quad c_T = \sqrt{\frac{\mu}{\rho}} < c_L$$



Wave vector $\underline{k}$

$$k = \frac{2\pi}{L}.\sqrt{n^2 + m^2 + l^2}$$

Vibrational Density of States: $g(\omega) \sim 3\frac{\omega^2}{\omega_D{}^3}$

1. **Vibrations** in the **Harmonic** approximation of Energy

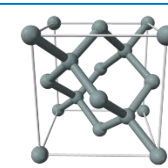
What are the Eigenmodes in Amorphous Materials**?**

Vibrational Eigenmodes in **Amorphous Materials**: the example of Amorphous Silicon

$$m_i.\frac{\partial^2 u_\alpha}{\partial t^2}\left(\underline{r}_i,t\right) = -\frac{\partial E_{total}}{\partial r_{i\alpha}} \approx -\sum_j \sqrt{m_i m_j}\, M_{ij}^{\alpha\beta}.u_\beta\left(\underline{r}_j,t\right) + f_\alpha\left(\underline{r}_i\right) \quad \text{with } M_{ij}^{\alpha\beta} \equiv \frac{1}{\sqrt{m_i m_j}}\frac{\partial^2 E_{total}}{\partial r_{i\alpha}\partial r_{j\beta}}$$

$\underline{u}\left(\underline{r}_i,t\right) \equiv \underline{r}_i(t) - \underline{r}_i^{\,0} = \underline{U}_i / \sqrt{m_i}.e^{i\omega t}$ Dynamical Matrix: **Eigenvectors** U, **eigenvalues** ω^2

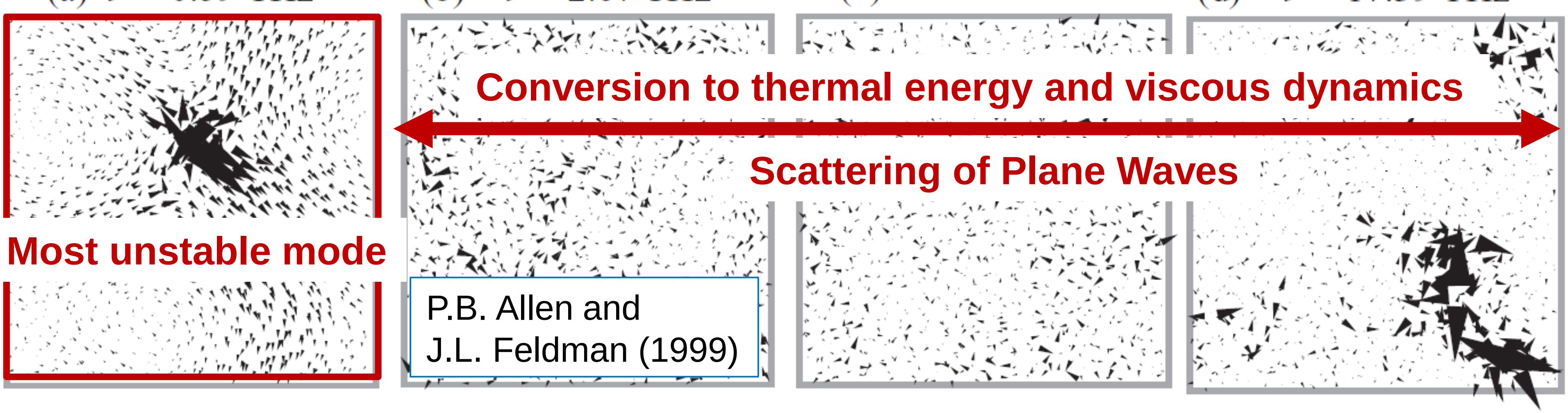
$$E_{total} = \Sigma_{(i,j)} f(r_{ij}) + \Sigma_{i,j,k}\Lambda.\left(\cos\theta_{jik} + \frac{1}{3}\right)^2 .e^{\gamma.(r_{ij}-a)^{-1}+\gamma.(r_{ik}-a)^{-1}}$$



Stillinger-Weber interatomic interactions

soft modes **diffusons** **locons**

(a) $\nu = 0.59$ THz (b) $\nu = 2.67$ THz (c) $\nu = 9.95$ THz (d) $\nu = 17.39$ THz



Conversion to thermal energy and viscous dynamics

Scattering of Plane Waves

Most unstable mode

P.B. Allen and J.L. Feldman (1999)

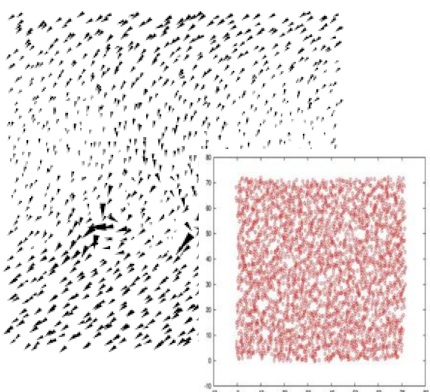
What are the Eigenmodes in Amorphous Materials**?**

Vibrational Eigenmodes in **Amorphous Materials**: the example of Silica glass SiO_2

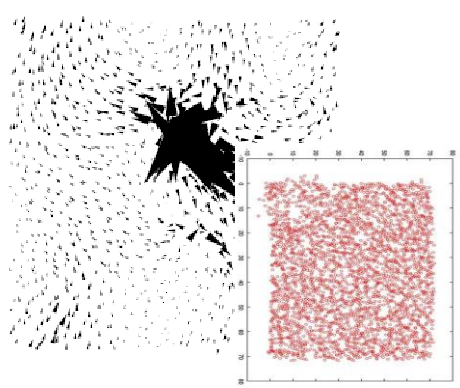
$$m_i.\frac{\partial^2 u_\alpha}{\partial t^2}\left(\underline{r_i},t\right) = -\frac{\partial E_{total}}{\partial r_{i\alpha}} \approx -\sum_j \sqrt{m_i m_j} M_{ij}^{\alpha\beta}.u_\beta\left(\underline{r_j},t\right) + f_\alpha\left(\underline{r_i}\right) \text{ with } M_{ij}^{\alpha\beta} \equiv \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 E_{total}}{\partial r_{i\alpha}\partial r_{j\beta}}$$

$$\underline{u}\left(\underline{r_i},t\right) \equiv \underline{r_i}(t) - \underline{r_i}^0 = \underline{U}_i / \sqrt{m_i}.e^{i\omega t}$$ Dynamical Matrix: **Eigenvectors** U, **eigenvalues** ω^2

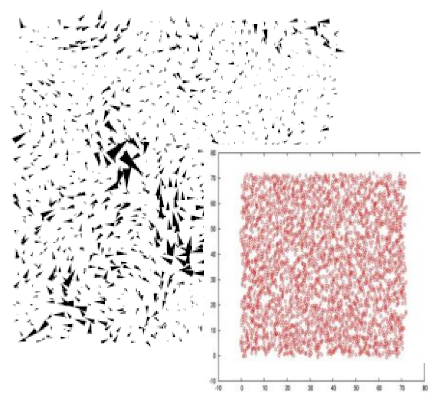
Plane Waves



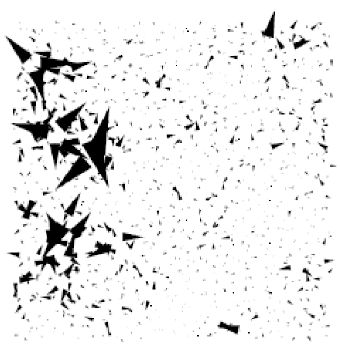
Soft Modes



Diffusons



Locons

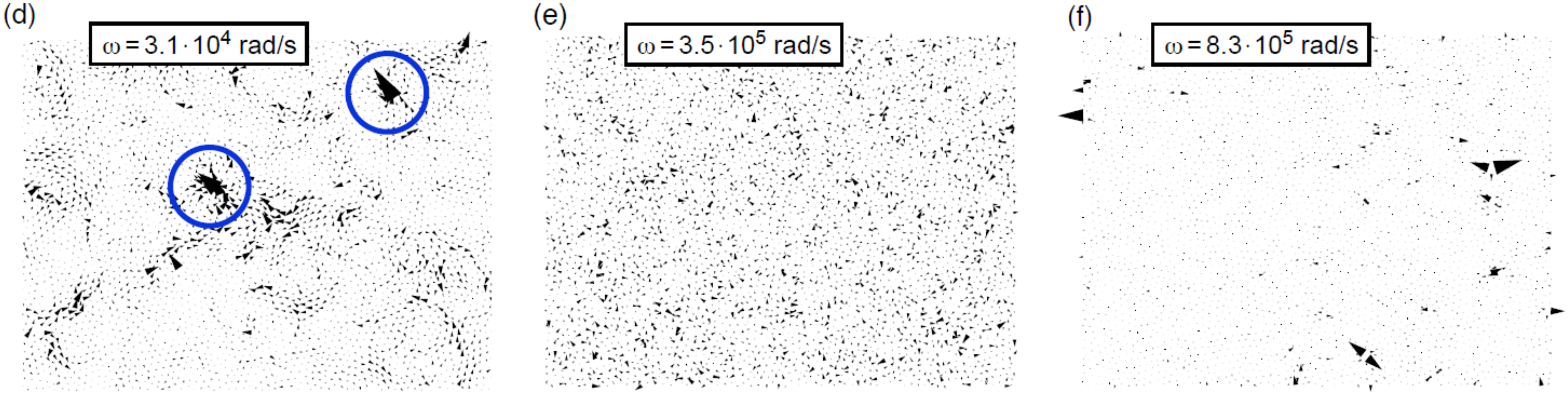


N. Shcheblanov et al. (2015)

P.B. Allen and J.L. Feldman (1999)

What are the Eigenmodes in Amorphous Materials**?**

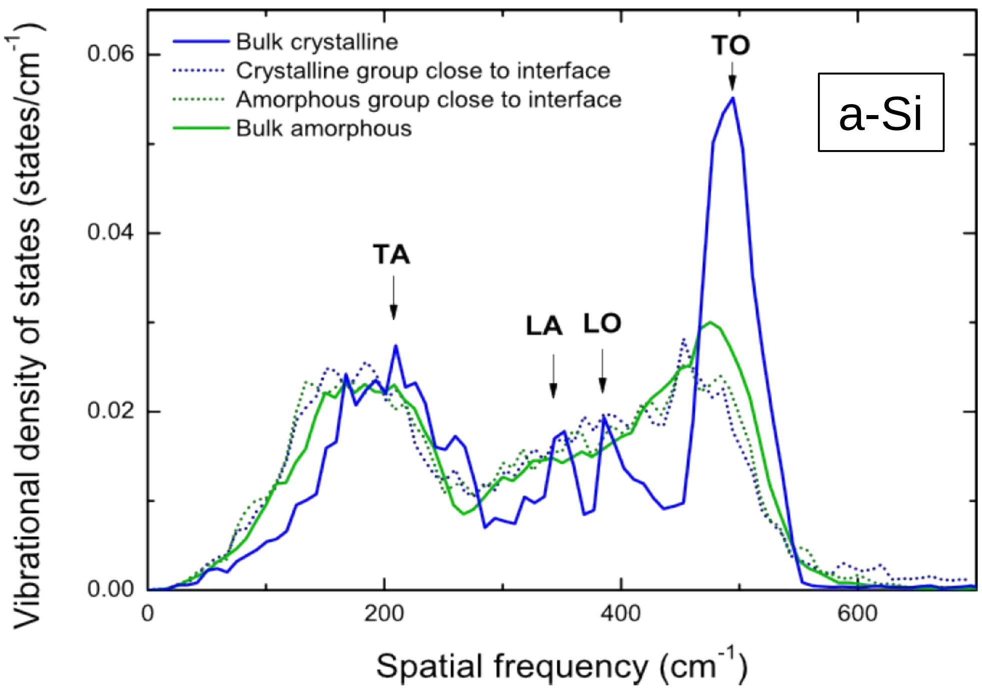
Vibrational Eigenmodes in **Amorphous Materials**: the example of Soft colloidal gel



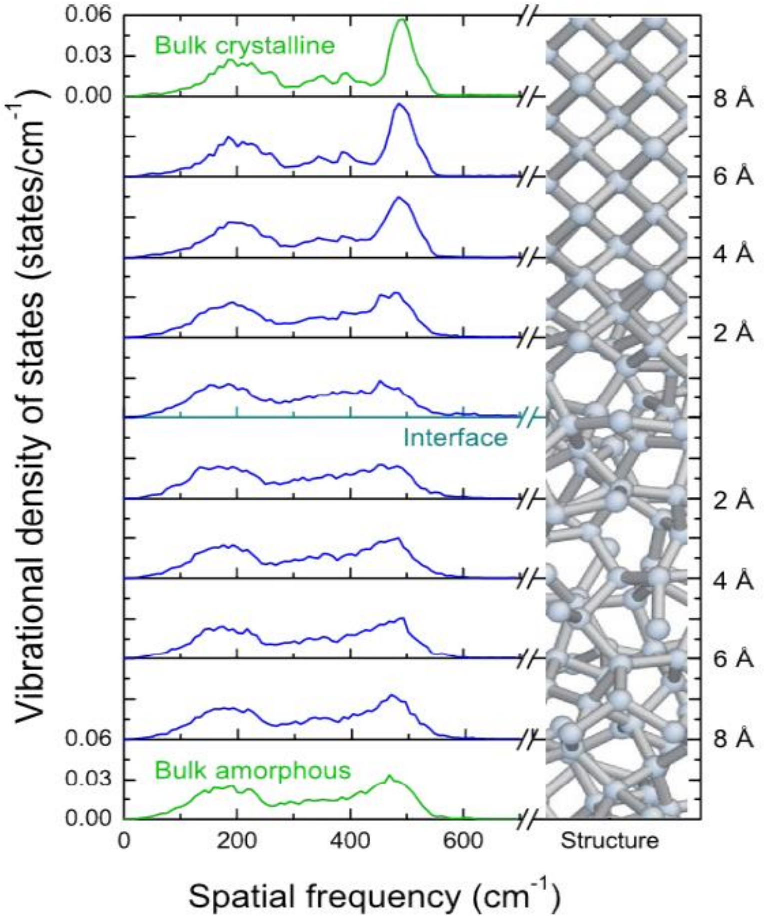
O. Dauchot et al. (2010)

Glasses vs. Crystals

Vibrational Density of States

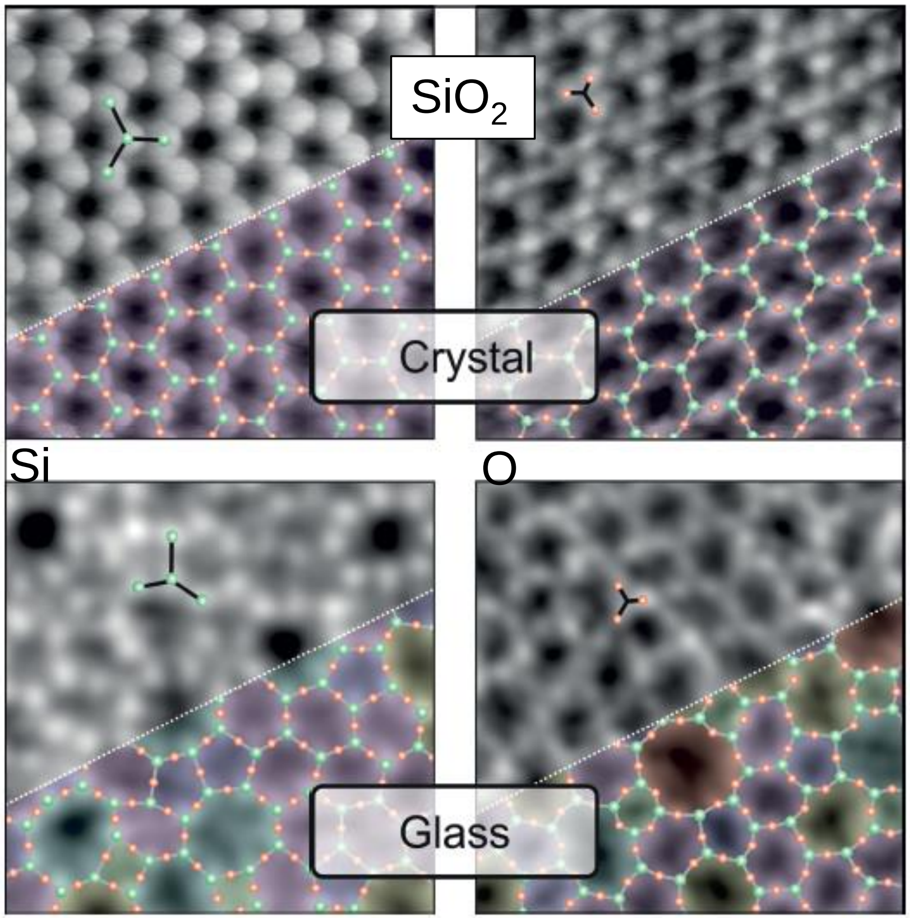


A. France-Lanord et al. (2014)

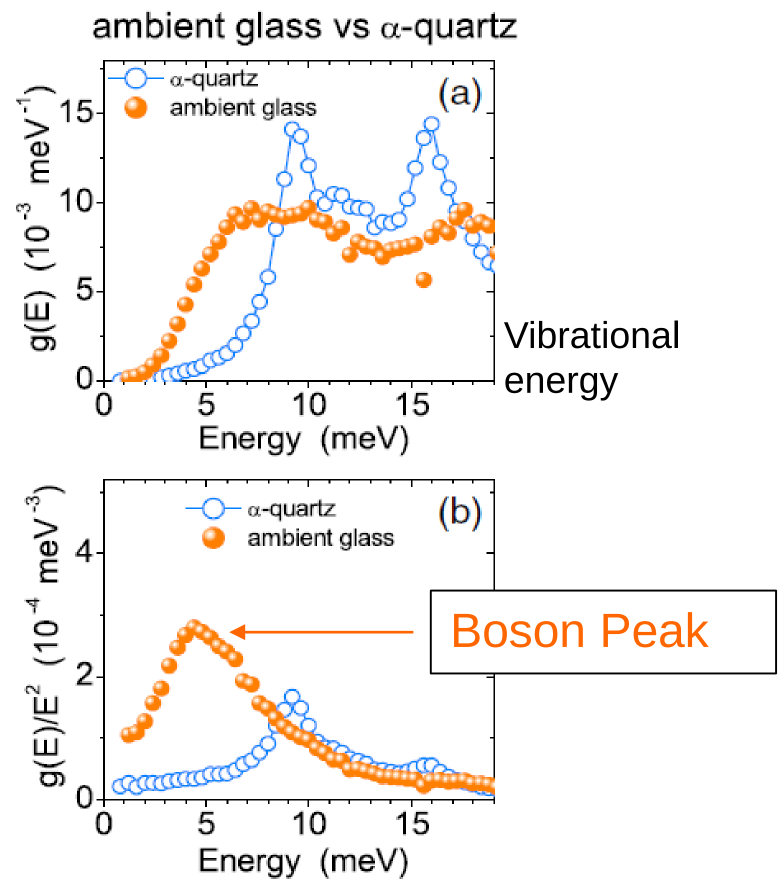


Glasses vs. Crystals

Vibrational Density of States



L. Lichtenstein et al. (2014) - STM

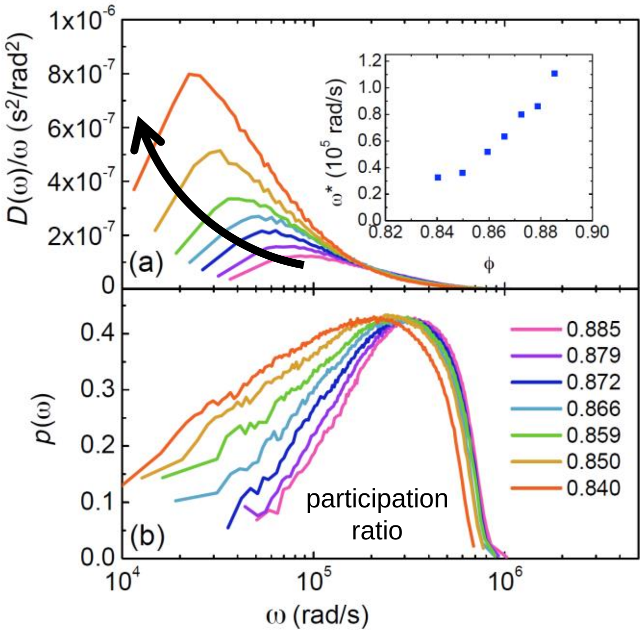


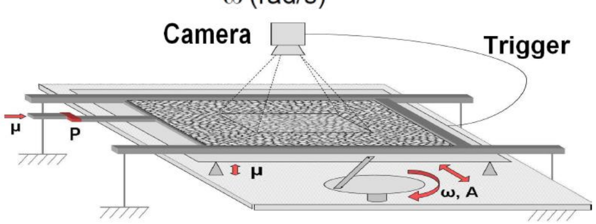
A.I. Chumakov et al. (2014)

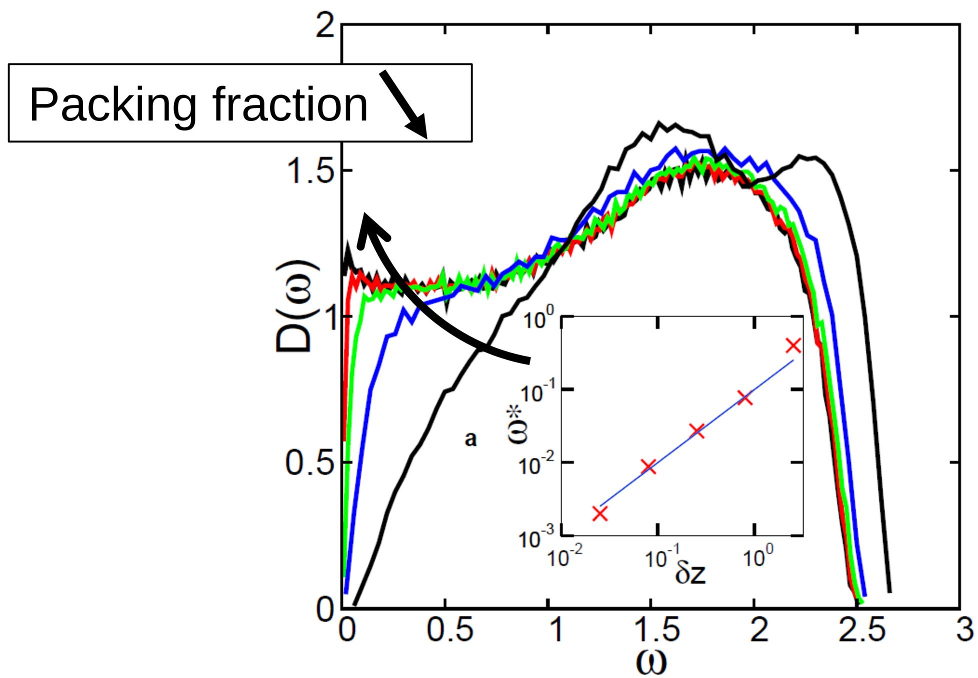
Glasses vs. Crystals

Vibrational Density of States

Soft colloidal gels / granular media, above the jamming transition







O. Dauchot et al (2010)
M. Wyart et al (2005)

Glasses vs. Crystals

Vibrational Density of States

Imaging Atomic Rearrangements in Two-Dimensional Silica Glass: Watching Silica's Dance

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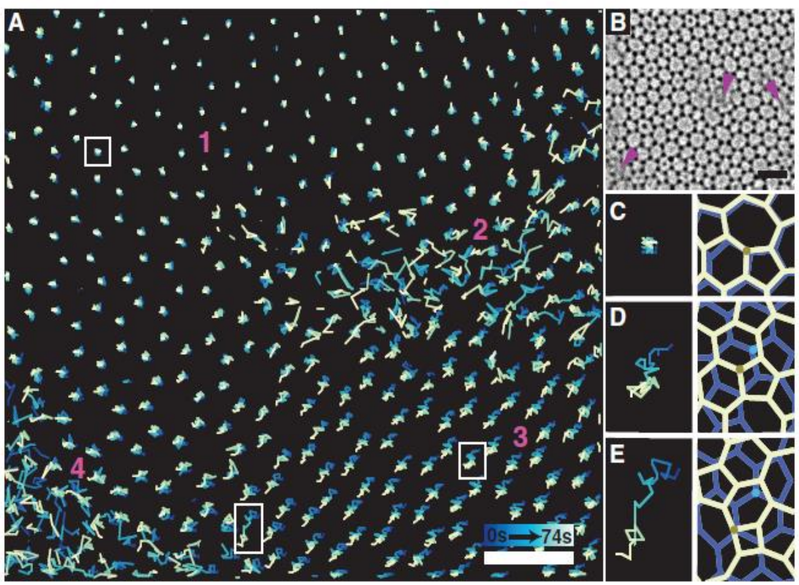


P.Y. Huang et al. Science (2013)

Inhomogeneous strain

↓

Lower **effective** sound velocity

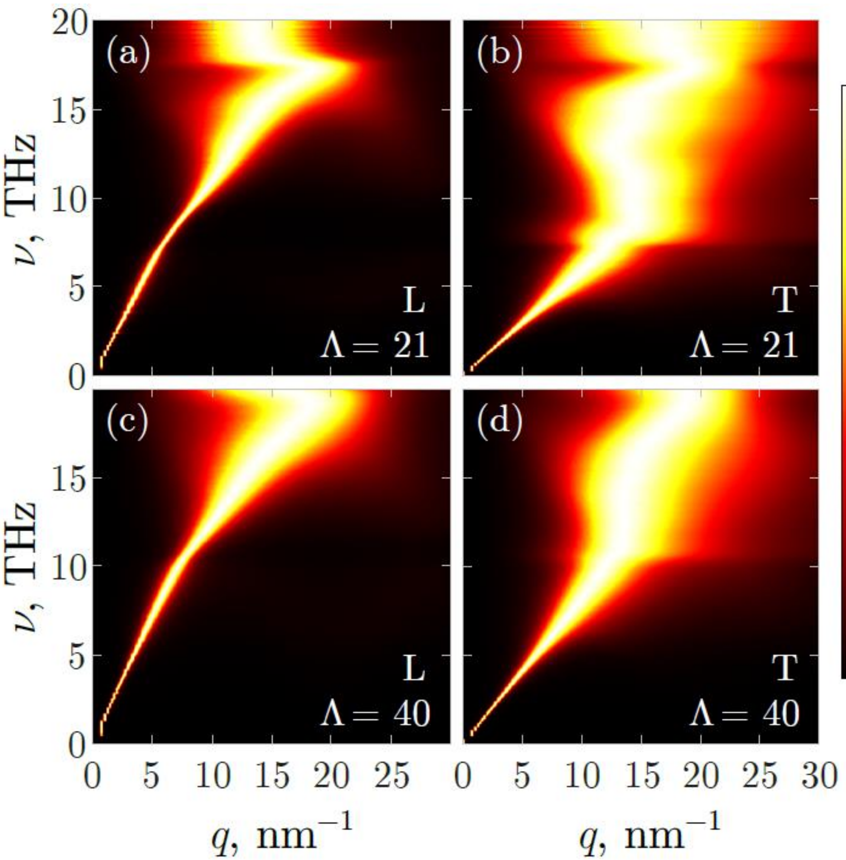
A. Tanguy et al. (2002)

Heterogeneous Elasticity

W. Schirmacher et al. (1998)
A. Reuss (1929)

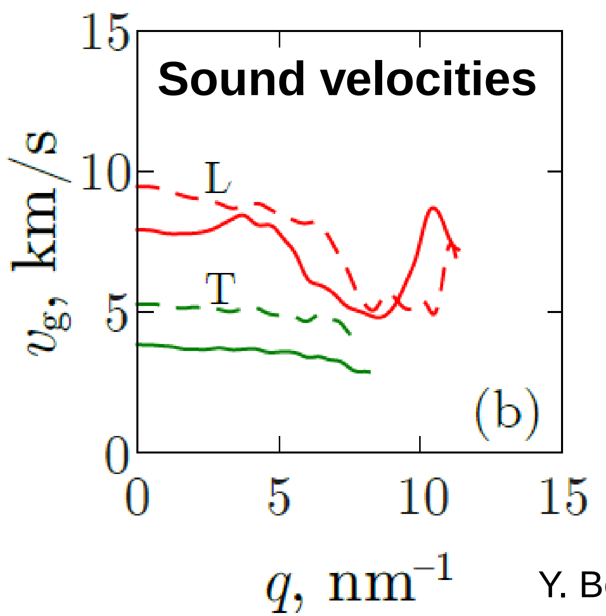
Dynamical Structure Factor in **a-Si:**

$$S_L(q,\omega) = \int e^{-i\omega t} \left\langle \rho(\bar{q},t).\rho(-\bar{q},0) \right\rangle dt$$



Damped Harmonic Osc fit:

$$S_{\mathrm{L,T}}(q,\omega) = \frac{A}{(\omega^2 - \omega^2_{\mathrm{L,T}}(q))^2 + \omega^2\Gamma^2}$$



$$v_g = \frac{d\omega_{L,T}}{dq}$$

Y. Beltukov et al. (2016)

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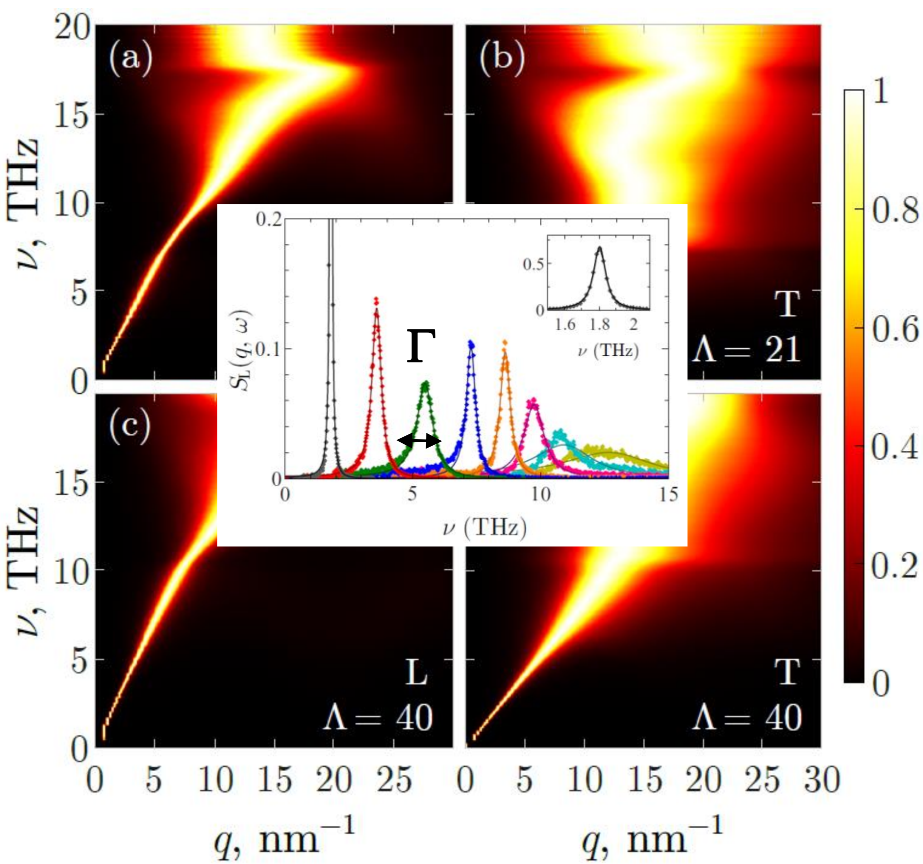
Y. Beltukov et al. (2016)



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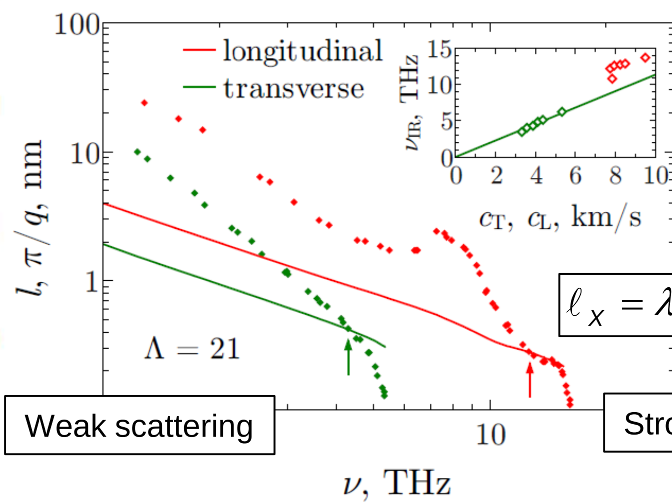


Mean-free Path

$\ell_x = v_g / \Gamma$

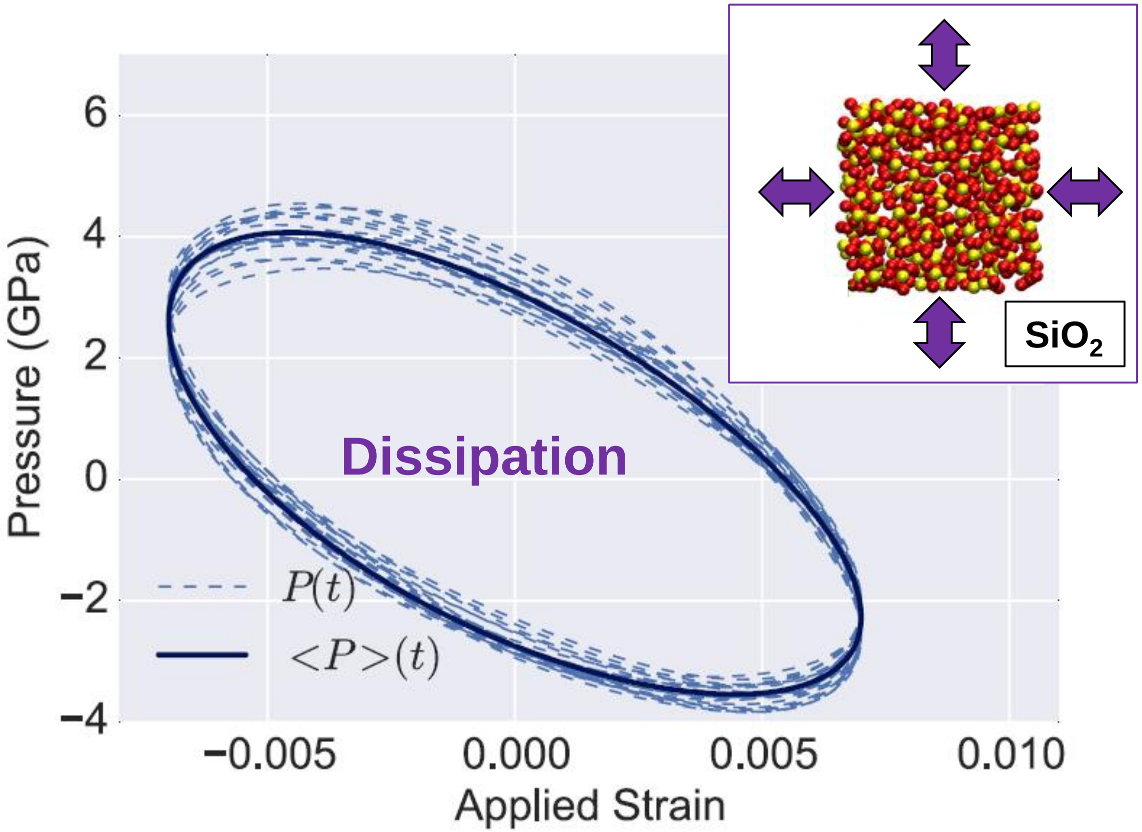
$\ell_x = \lambda / 2$ Ioffe-Regel criterion

Weak scattering

Strong scattering

Scattering of Transverse and then Longitudinal waves

Phase-shifted response of a glass to an oscillatory load



$$\varepsilon = \varepsilon_0 \sin(\omega t)$$

$$\tau = \tau_0 \sin(\omega t + \delta)$$

Elastic Modulus

$$\tau = G'(\omega).\varepsilon_0.\sin(\omega t) + G''(\omega).\varepsilon_0.\cos(\omega t)$$

Loss Modulus

Internal Friction $\tan\delta = \dfrac{G''}{G'} \propto \dfrac{\text{Dissipated Energy}}{\text{Stored Energy}} = \dfrac{1}{\omega}\dfrac{\int_0^T \langle P\rangle(t)\dot{\varepsilon}(t)dt}{\int_0^T \langle P\rangle(t)\varepsilon(t)dt}$

T. Damart et al. (2017)

$$m_i \ddot{x}_i^{\alpha} = -\left(\sum_{j\beta} D_{ij}^{\alpha\beta} R_{ij}^{\beta}\right)\epsilon - \sum_{j\beta} D_{ij}^{\alpha\beta} x_j^{\beta} - m_i \gamma \dot{x}_i^{\alpha} + F_{th}$$

Thermal Force
+ related local damping

Projection on the Eigenmodes:

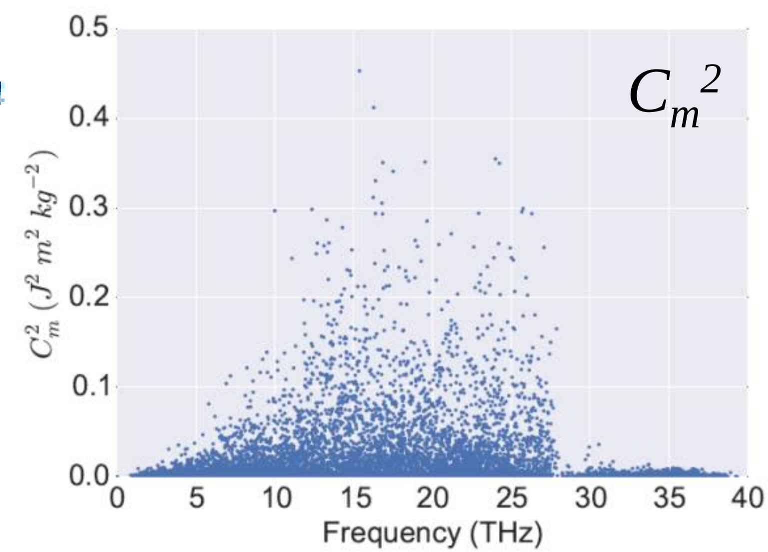
$$s_j^{\beta} = \sqrt{m_j} x_j^{\beta} = \sum_m s_m e_j^{\beta}(m).$$

$$\ddot{s}_m = C_m \epsilon - \omega_m^2 s_m - \gamma \dot{s}_m + F_m$$

$$\langle s_m \rangle(\omega) = \frac{C_m}{\omega_m^2 - \omega^2 + i\gamma\omega}\epsilon(\omega)$$

$$\boxed{C_m = \sum_{i\alpha j\beta} D_{ij}^{\alpha\beta} R_{ij}^{\alpha} \frac{e_j^{\beta}(m)}{\sqrt{m_j}}}$$

Pressure induced by the eigenmode

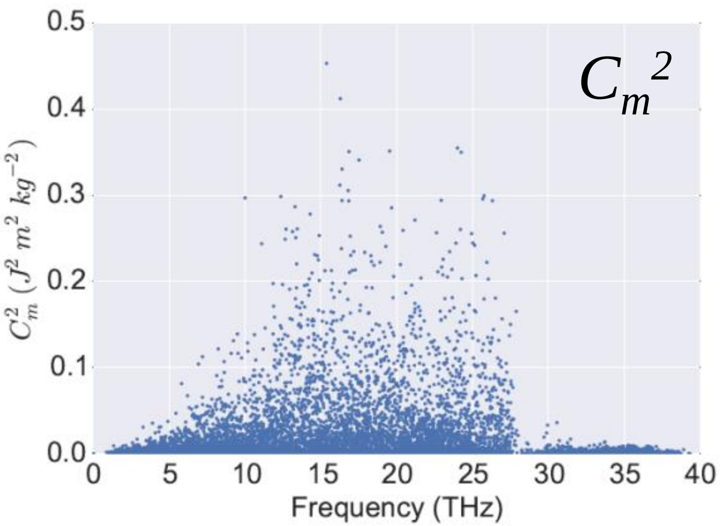


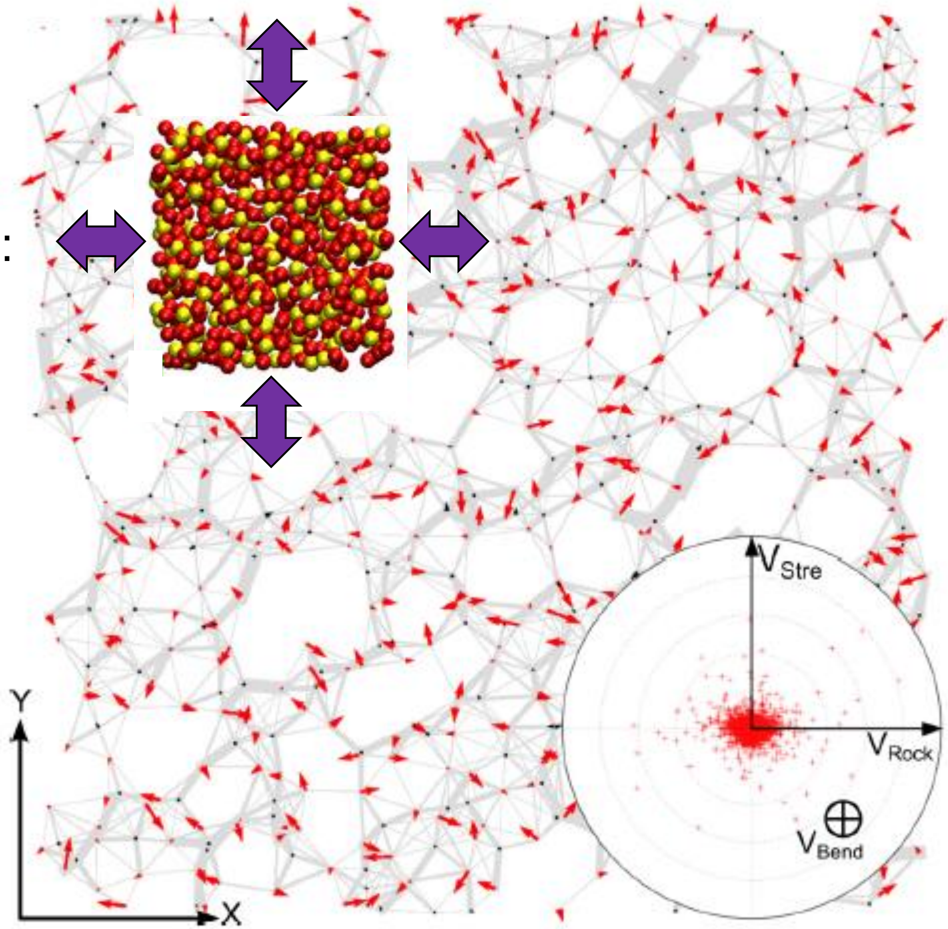
Pressure C_m induced by each eigenmode, for an applied **isotropic compression**:

$$\boxed{C_m = -\sum_{i\alpha} \Xi_i^\alpha \frac{e_i^\alpha(m)}{\sqrt{m_i}}}$$

Asymetry factor or **Non-affine force**:

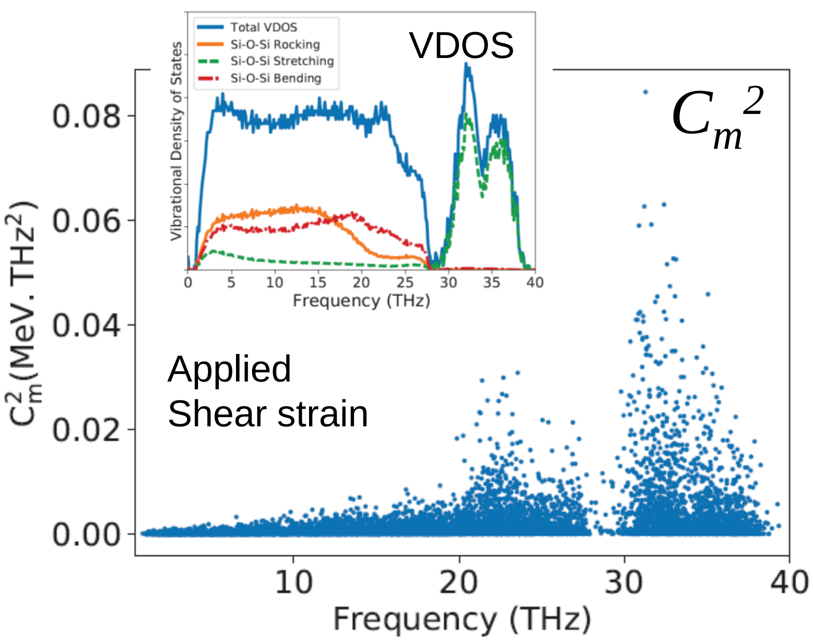
$$\Xi_i^\alpha = \frac{\partial F_i^\alpha}{\partial \epsilon} = -\sum_{j\beta} D_{ij}^{\alpha\beta} R_{ij}^\beta$$



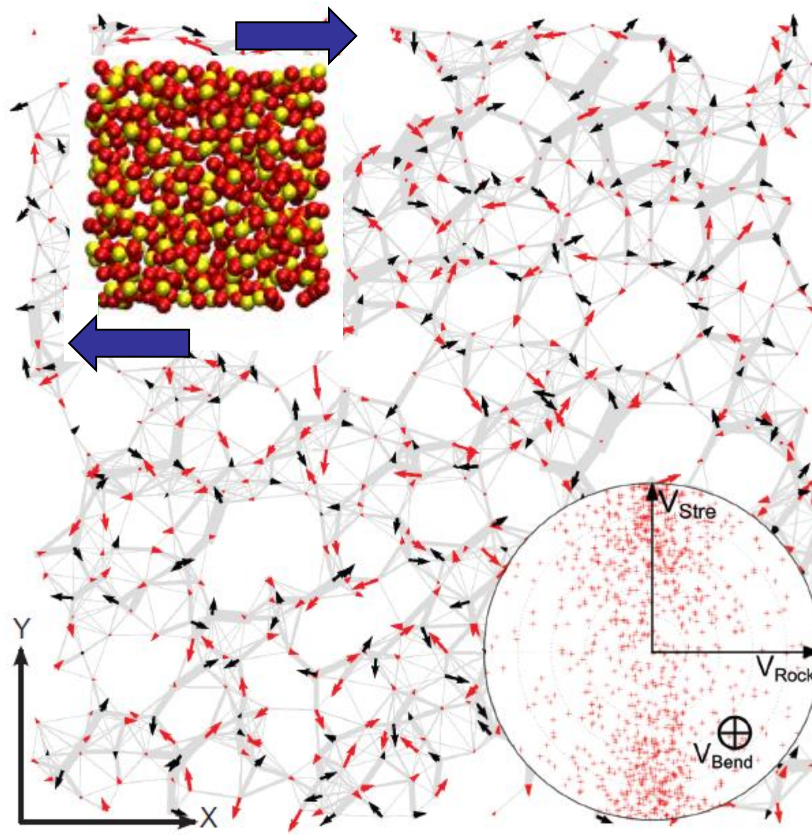


Generalized stress $C_m^{\alpha\beta}$ induced by each eigenmode:

$$C_m^{\alpha\beta} = \frac{1}{2}\sum_{ij\kappa}\left[D_{ij}^{\alpha\kappa}R_{ij}^{\beta} + D_{ij}^{\beta\kappa}R_{ij}^{\alpha}\right]\frac{e_j^{\kappa}(m)}{\sqrt{m_j}}$$



Asymetry factor or Non-affine force for an applied **shear strain**:



$$\Xi_{\alpha\beta,i}^{\kappa} = -\frac{1}{2}\sum_j\left(D_{ij}^{\kappa\alpha}R_{ij}^{\beta} + D_{ij}^{\kappa\beta}R_{ij}^{\alpha}\right)$$

Internal Friction

$$P = \frac{1}{3V} \sum_{i\alpha j\beta} D_{ij}^{\alpha\beta} (r_{ij}^{\beta} - R_{ij}^{\beta}) r_{ij}^{\alpha}$$

$$r_i^{\alpha} = (1+\epsilon) R_i^{\alpha} + x_i^{\alpha}$$

non-affine displacement

$$P = -3K^{\infty}\epsilon + \frac{2}{3V_0} \sum_{i\alpha j\beta} D_{ij}^{\alpha\beta} R_{ij}^{\alpha} x_j^{\beta}$$

Projection of the displacement on the eigenmode *m*

$$\langle P \rangle(\omega) = -3K^{\infty}\epsilon(\omega) + \frac{2}{3V_0} \sum_m C_m \langle s_m \rangle(\omega)$$

Pressure induced by the eigenmode *m*

with $\langle s_m \rangle(\omega) = \dfrac{C_m}{\omega_m^2 - \omega^2 + i\gamma\omega}\epsilon(\omega)$

$$\tan\delta = \frac{G''(\omega)}{G'(\omega)} = \frac{\sum_m C_m^2 \frac{\omega\gamma}{(\omega_m^2-\omega^2)^2+(\gamma\omega)^2}}{\frac{9V_0}{2}K^{\infty} - \sum_m C_m^2 \frac{\omega_m^2-\omega^2}{(\omega_m^2-\omega^2)^2+(\gamma\omega)^2}}$$

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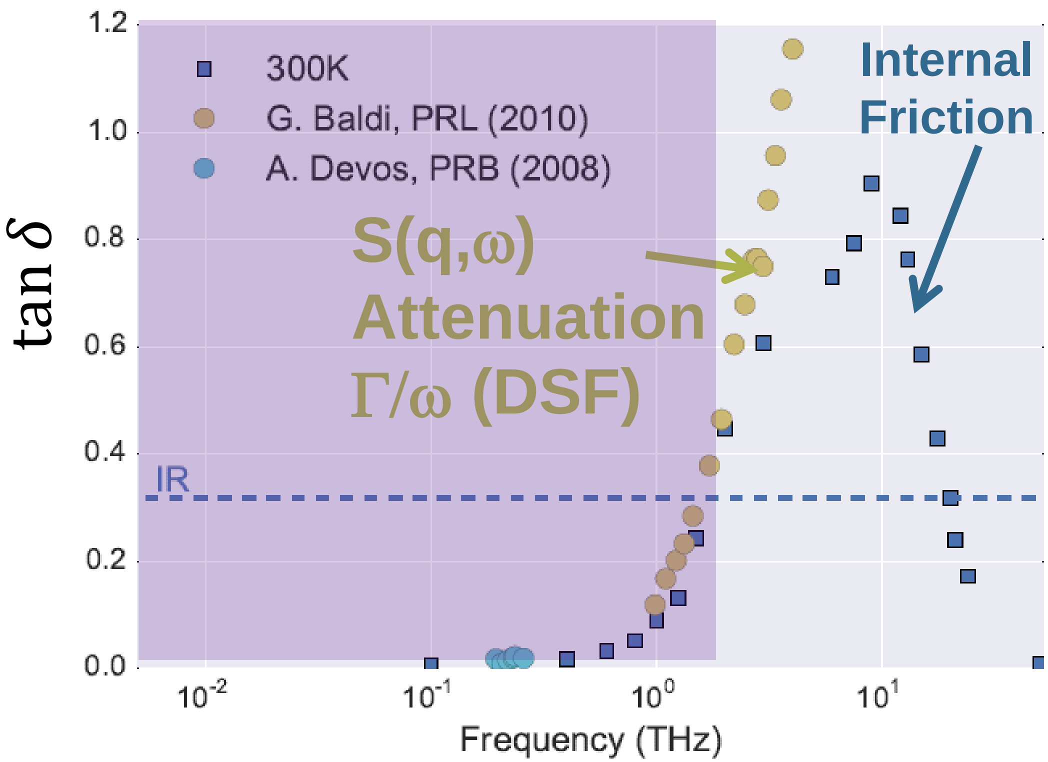


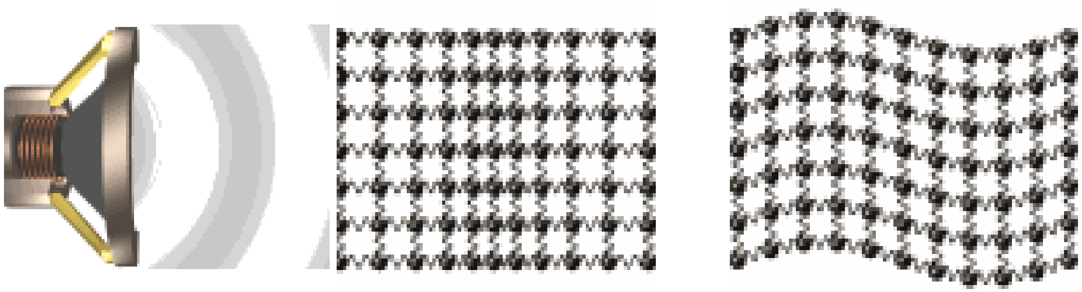
In the harmonic approximation,
the **internal friction** is due to the
sensitivity of the **stress** on
the local shape of the **eigenmodes**

In **glasses**, the non trivial shape of the
eigenmodes explains its
non-monotonous **frequency**
dependence

Comparable to the apparent Mean-free
path below the **Ioffe-Regel** frequency

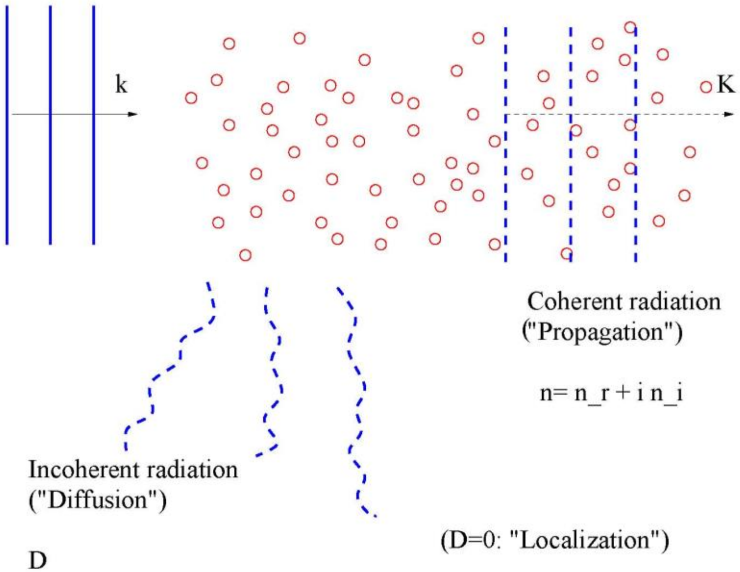
T. Damart et al. (2017)

Apparent Acoustic Attenuation in Glasses



crystal

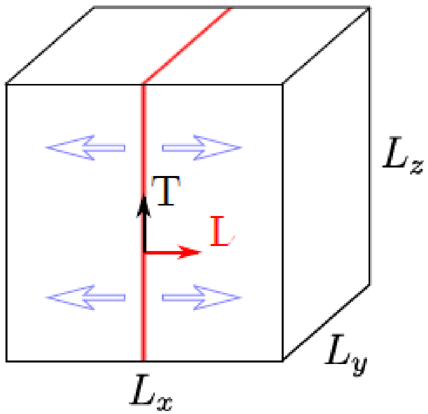
MULTIPLE SCATTERING

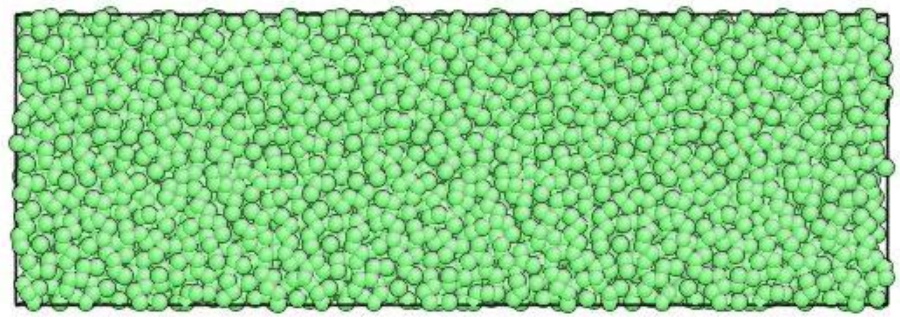


glass

F. Lund et al. (2012)
T. Damart et al. (2015)

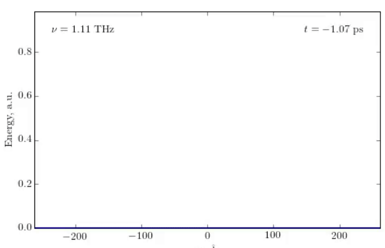
Wave-Packets Dynamics in **a-Si:**

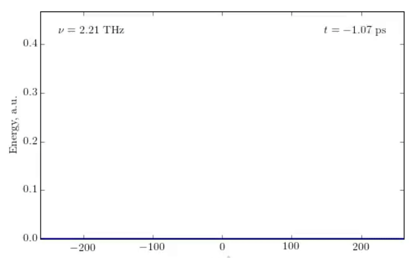


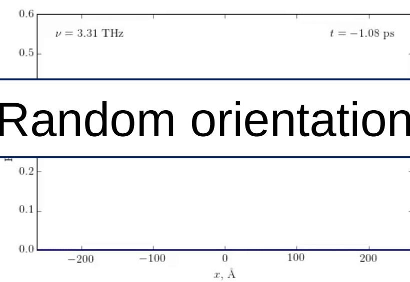


$$\mathrm{f}_i^{\mathrm{exc}}(\omega, t) = \mathrm{f}_\eta \exp\left(i\omega t - \frac{t^2}{2\tau_{\mathrm{exc}}^2} - \frac{x_i^2}{2w^2}\right)$$

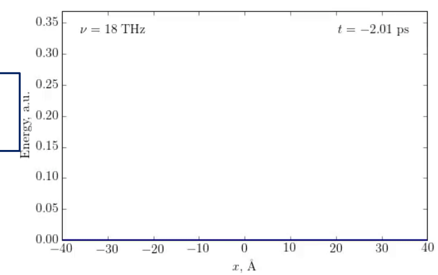
$\omega \nearrow$







Random orientations



Ballistic Regime
Propagons
$\omega \ll \omega_{IR}$

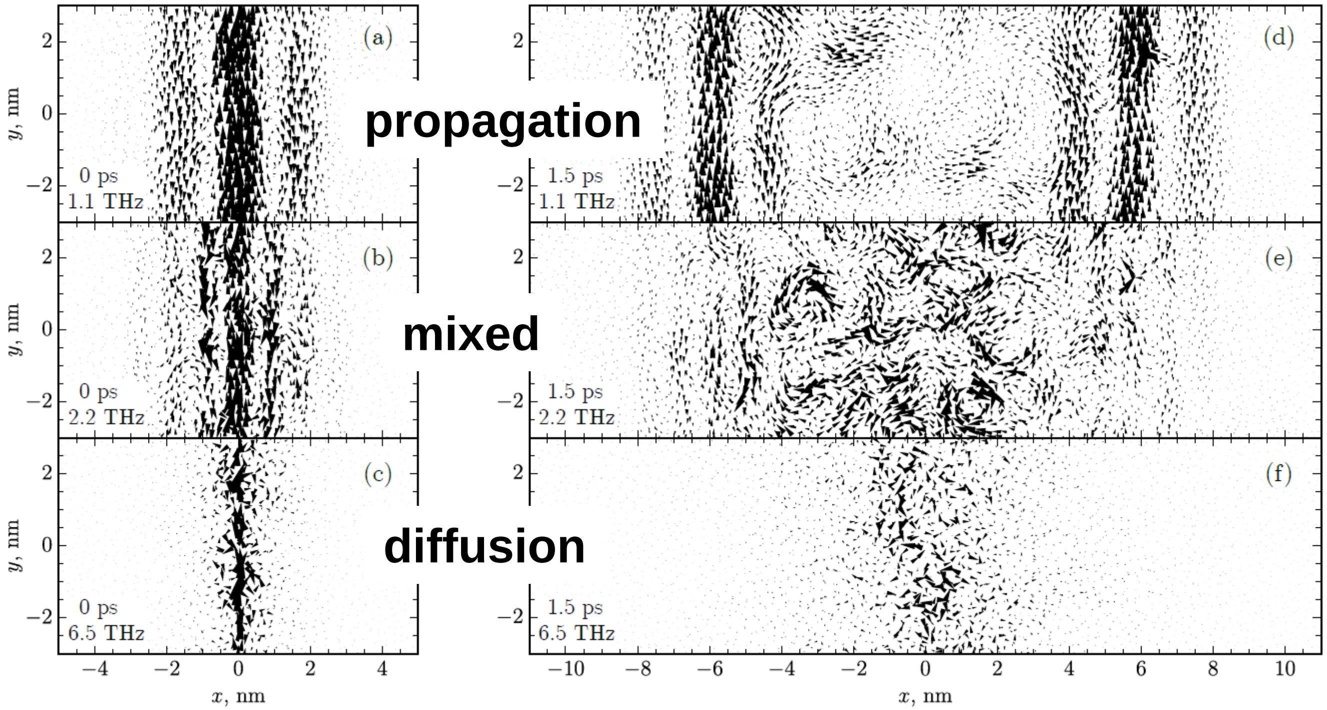
Mixed Regime
(Boson Peak)

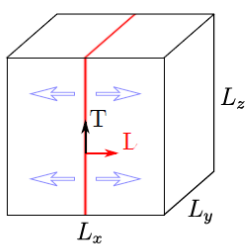
Diffusive Regime
Diffusons
$\omega > \omega_{IR}$

Localisation
Locons

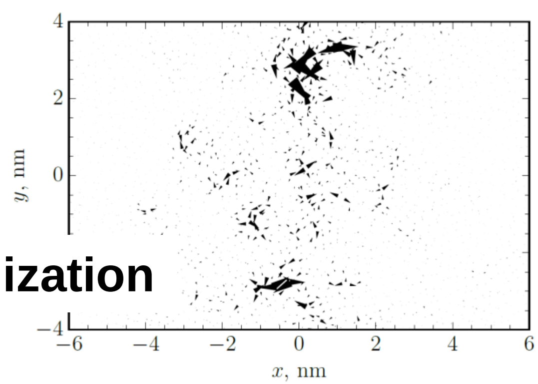
Y. Beltukov et al. (2018)

Wave Packet excitation





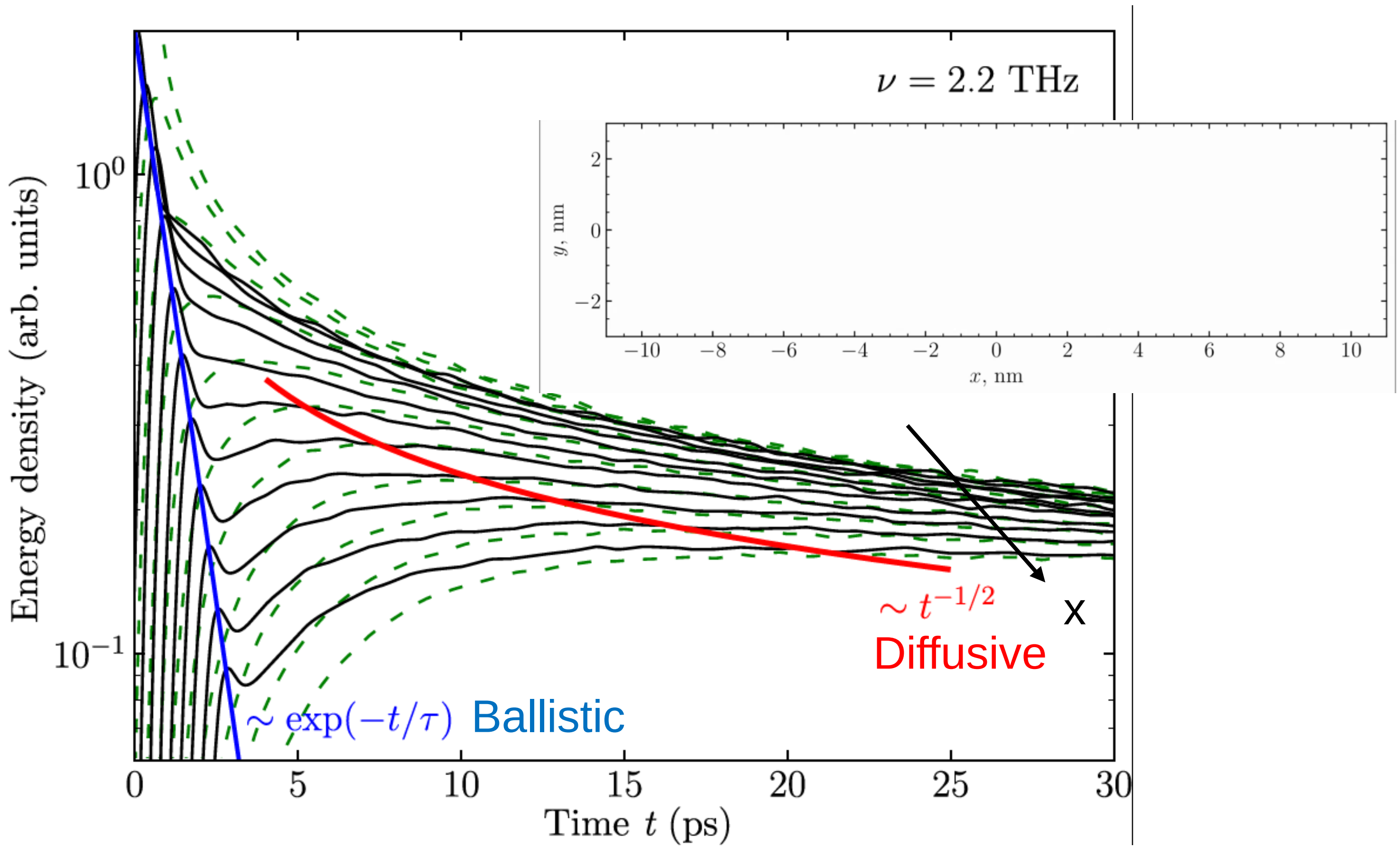
localization



Wave packets are supported by a combination of Normal Modes

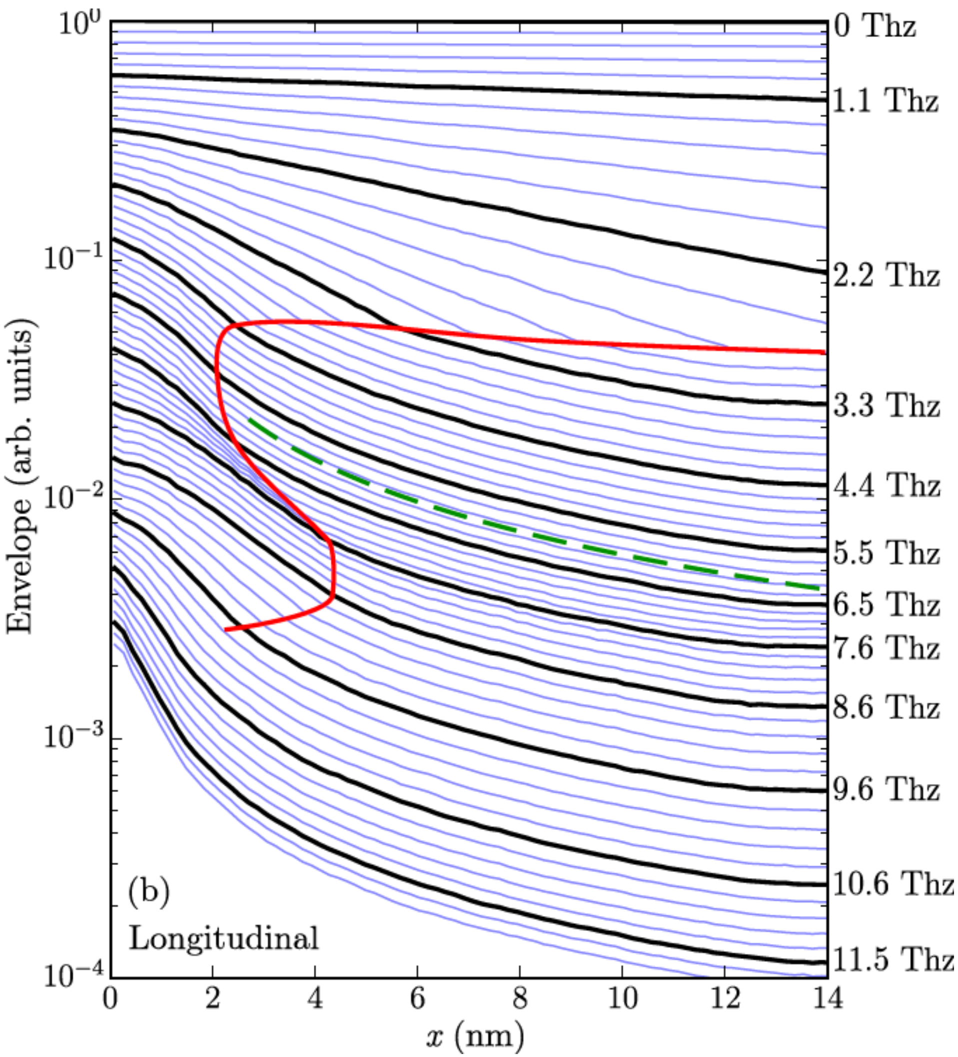
Y. Beltukov et al. (2018)

After-shocks in the Mixed Regime



Y. Beltukov et al. (2018)

Enveloppe of Energy



Ballistic Regime:

Beer-Lambert Attenuation

$$E_{\text{prop}}(x,t) = \frac{\mathcal{E}_0}{\sqrt{\pi v^2 \tau_{\text{exc}}^2}} \exp\left(-\frac{x}{l} - \frac{(x-vt)^2}{v^2\tau_{\text{exc}}^2}\right)$$

$$\boxed{P_{\text{prop}}(x) = E_{\text{prop}}(x, x/v) = \frac{\mathcal{E}_0}{\sqrt{\pi v^2 \tau_{\text{exc}}^2}} e^{-x/l}}$$

Diffusive Regime:

Power-law Attenuation

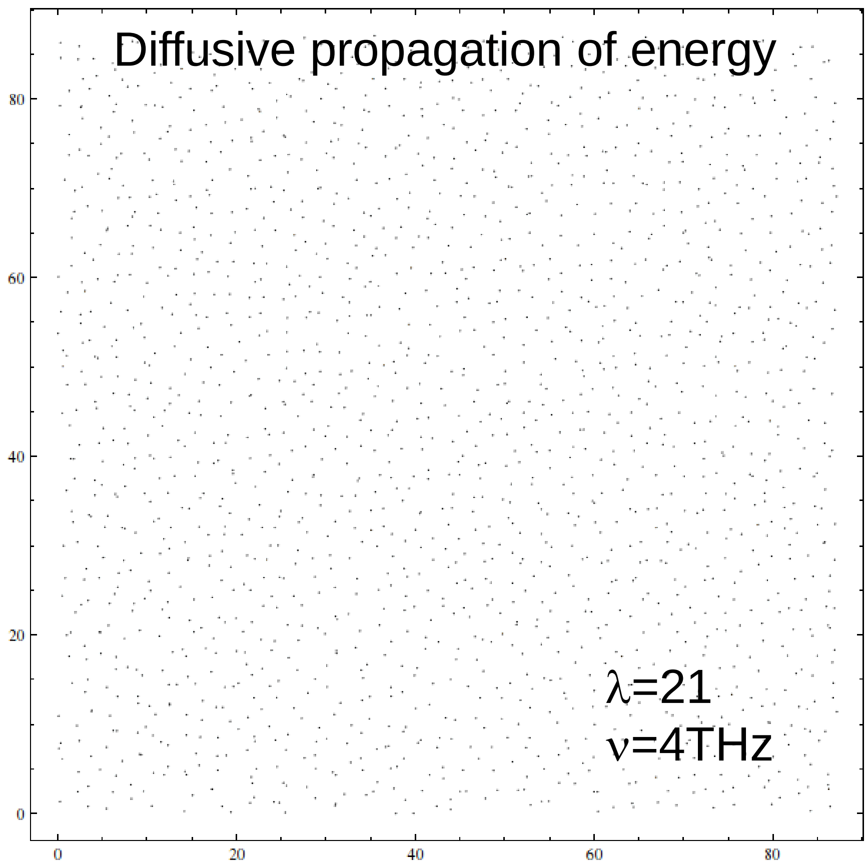
$$E_{\text{diff}}(x,t) = \frac{\mathcal{E}_0}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

max at $t^* = x^2/2D$

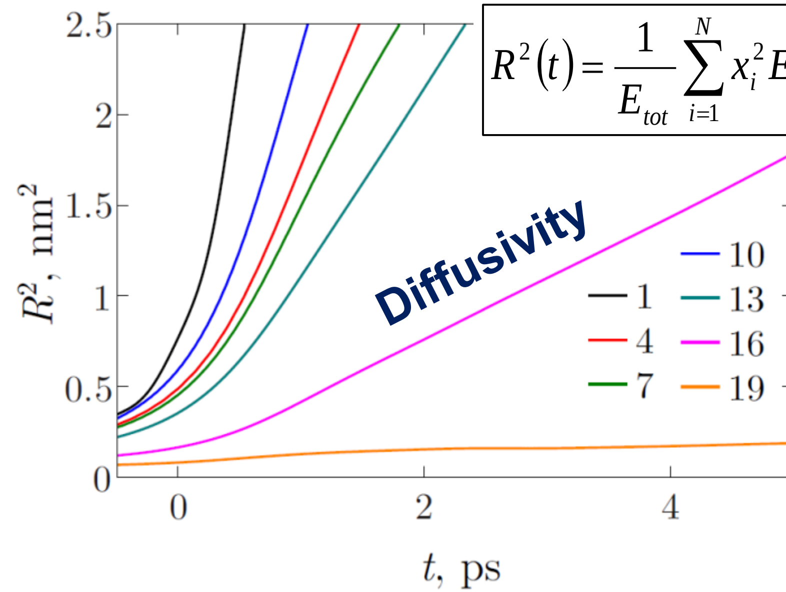
$$\boxed{P_{\text{diff}}(x) = E_{\text{diff}}(x, t^*) = \frac{\mathcal{E}_0}{\sqrt{2\pi e}} \frac{1}{x}}$$

Y. Beltukov et al. (2018)

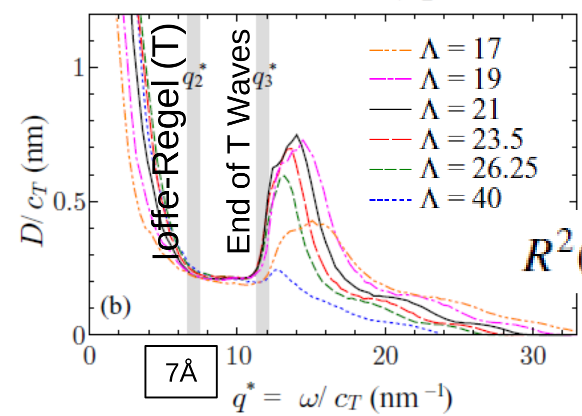
Random Excitations and Diffusivity of Kinetic energy



Diffusive transport due to the **departure from plane waves**



$$R^2(t) = \frac{1}{E_{tot}} \sum_{i=1}^{N} x_i^2 E_i(t) \approx D.t$$



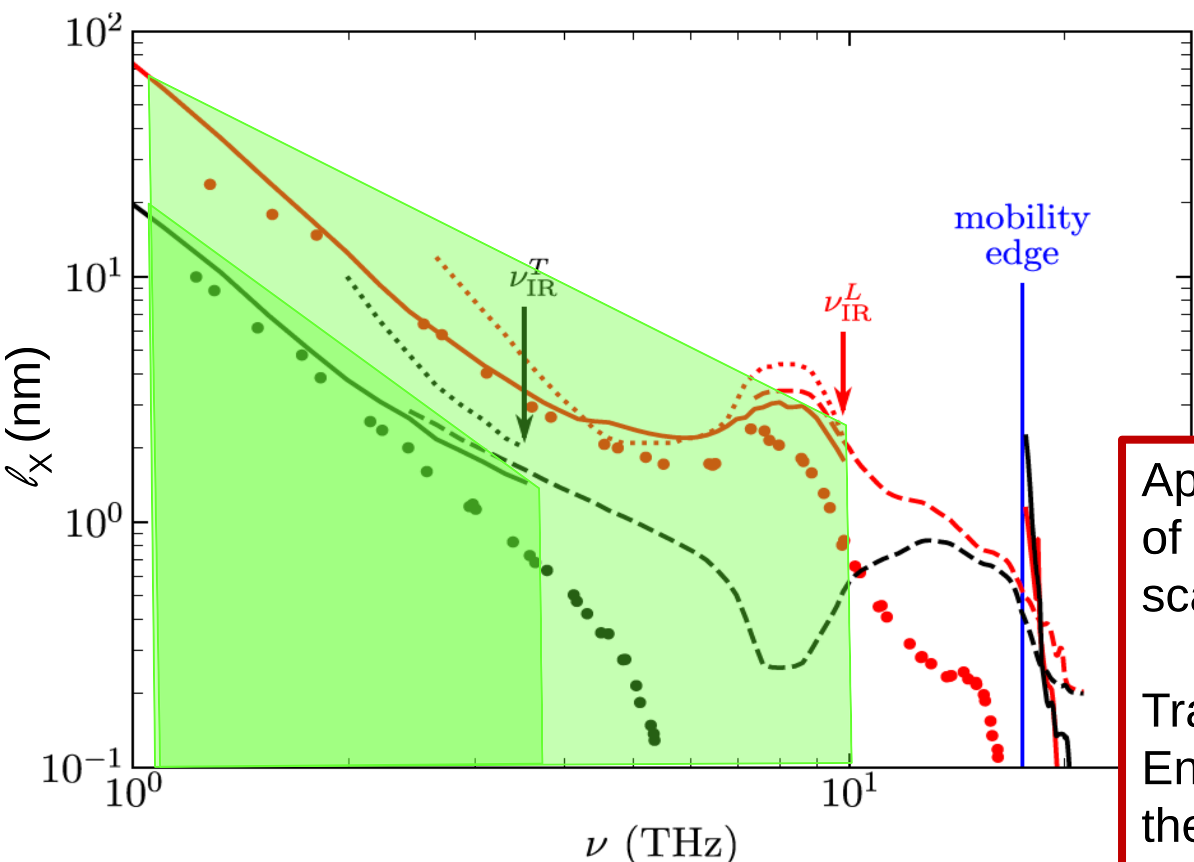
a-Si

$$R^2(t) = 2D(\omega)t$$

Allen and Feldman (1999)

Attenuation Length

Comparison of Wave Packet propagation, to the Dynamical Structure Factor



Attenuation length (WP)
$P_{diff\text{-}prop}(l)=P_{diff\text{-}prop}(0)/e$

Mean-free path (WP)
(Beer-Lambert)

Mean-free path (DSF)
$\ell_X = c_{L,T}/\Gamma$

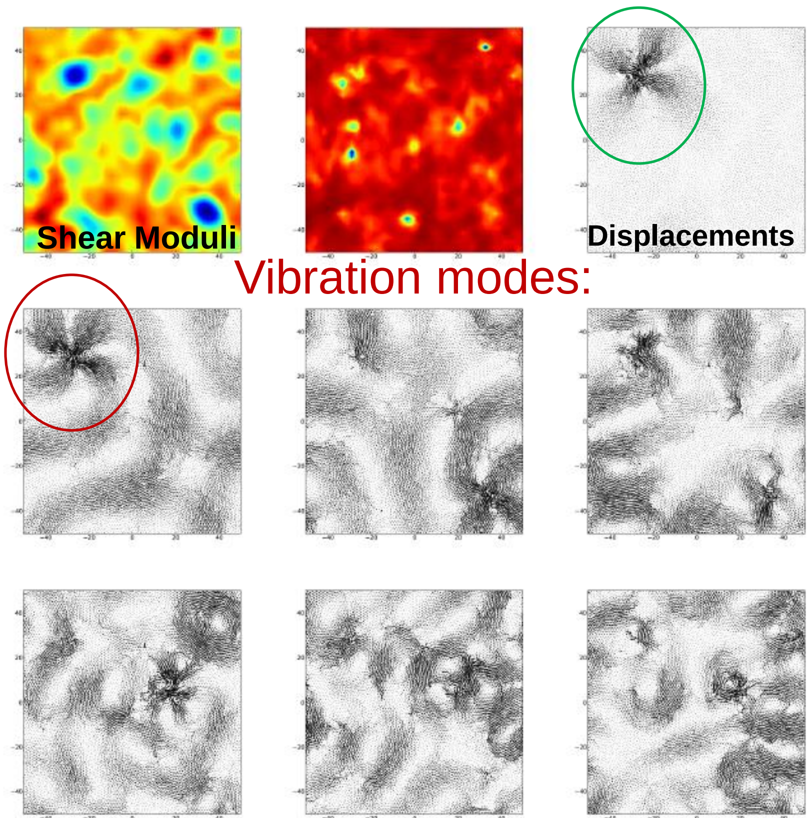
Apparent **attenuation** (MFP) of the Wave Packets due to scattering in the Ballistic regime

Transportation of Energy even **beyond** the Ioffe-Regel frequency (Diffusive regime)

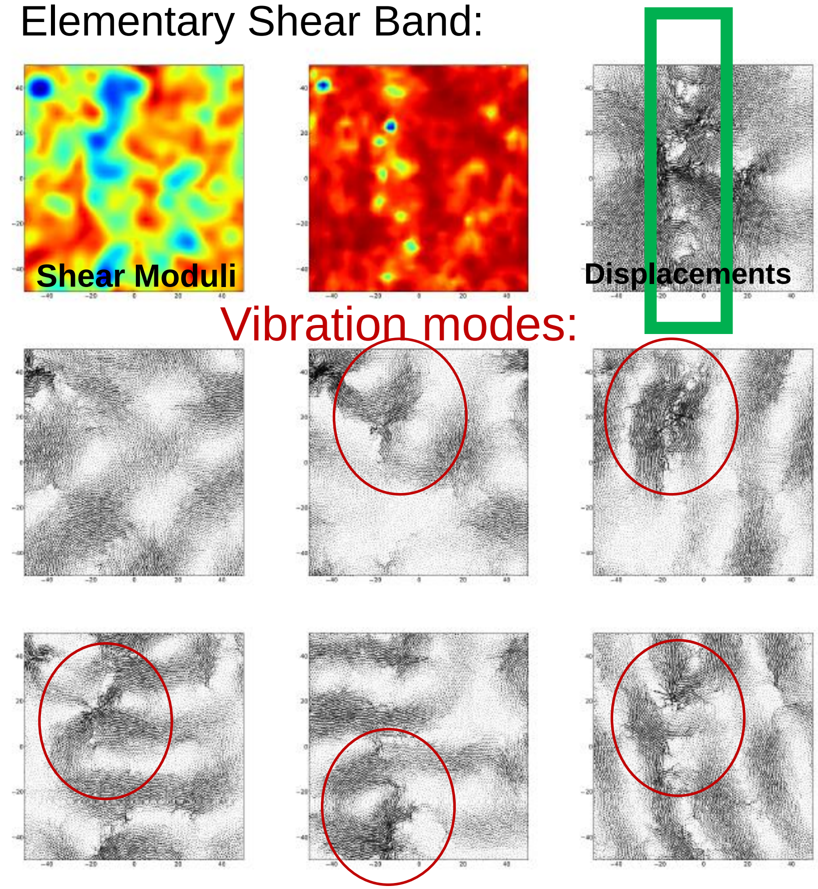
Y. Beltukov et al. (2018)

2. **Vibrations** and **anhamonicity**

Eshelby Inclusion:



Elementary Shear Band:

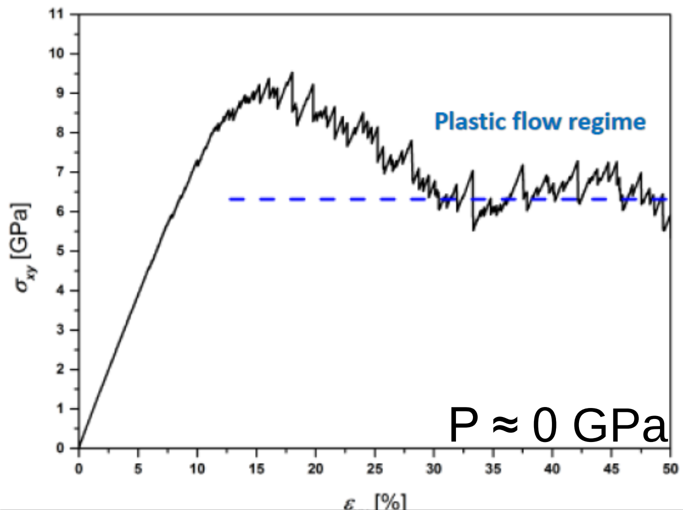


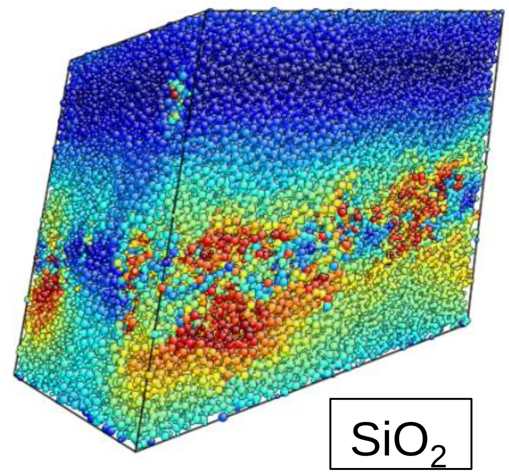
A *single* localized mode

A. Lemaitre (2004)
A. Tanguy et al. (2010)

Superposition of localized modes, on percolating soft zones

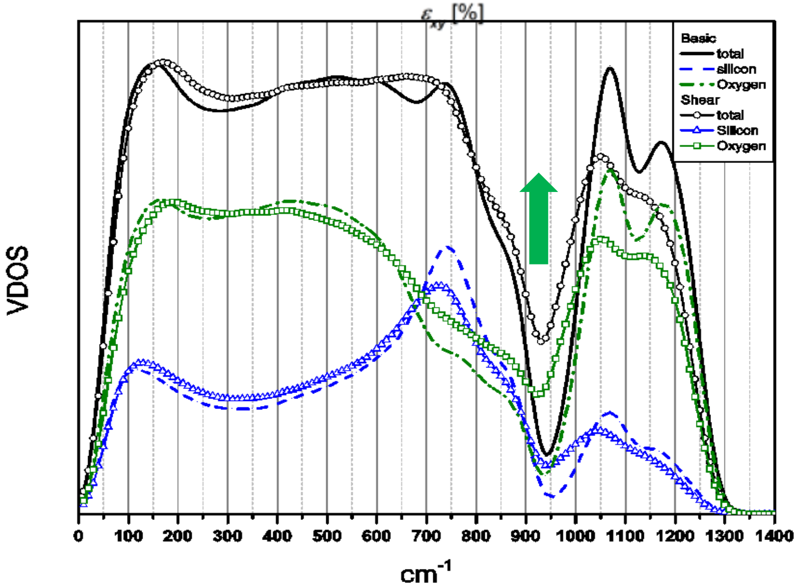
Effect of **Plasticity** on vibrations through Raman Scattering in sheared SiO_2 glass:

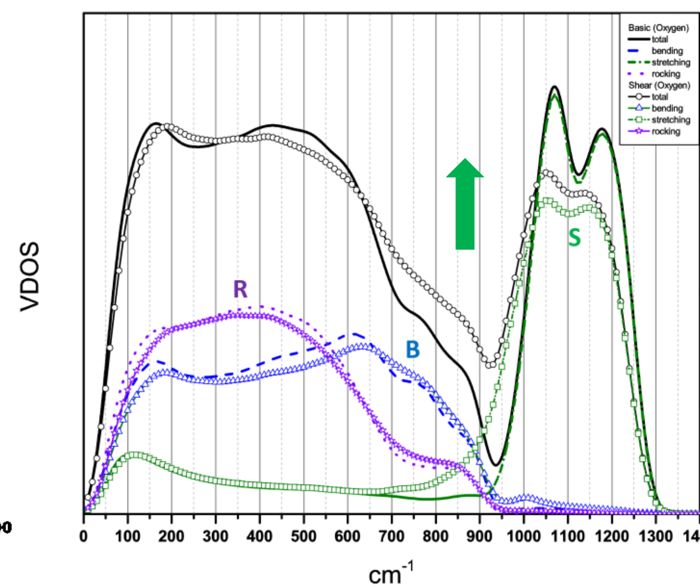


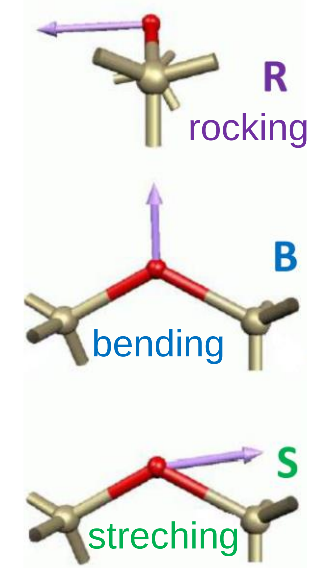


In the plastic plateau

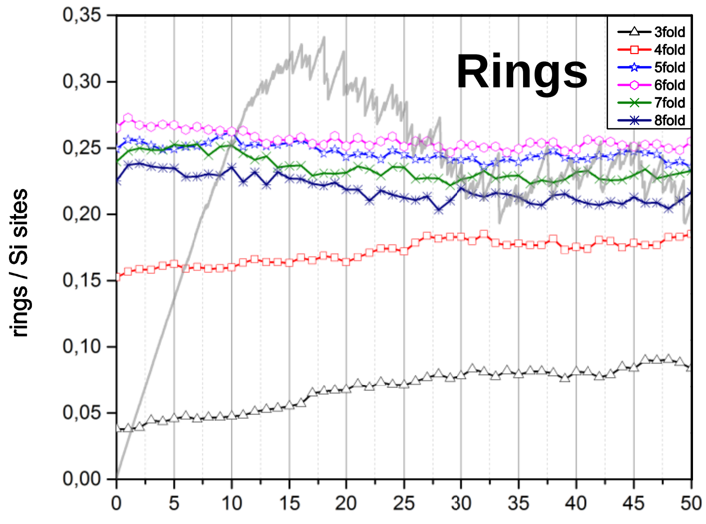
B. Mantisi et al. (2012)
N. Shcheblanov et al. (2015)

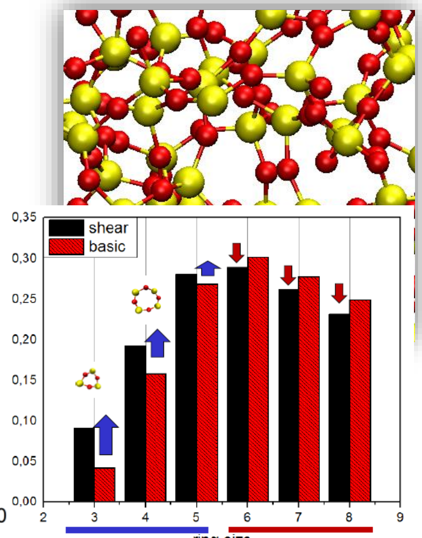


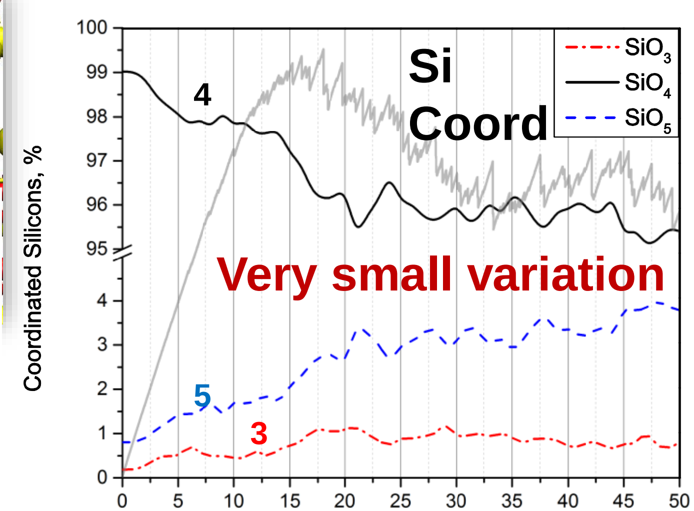


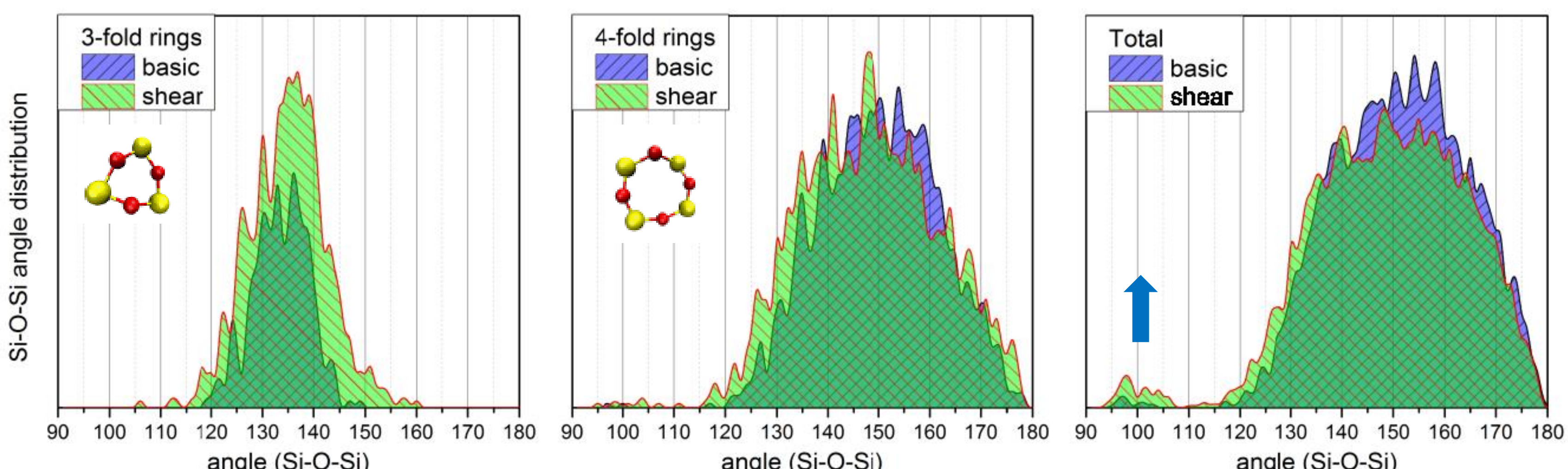


Structural changes in plastified a-SiO2

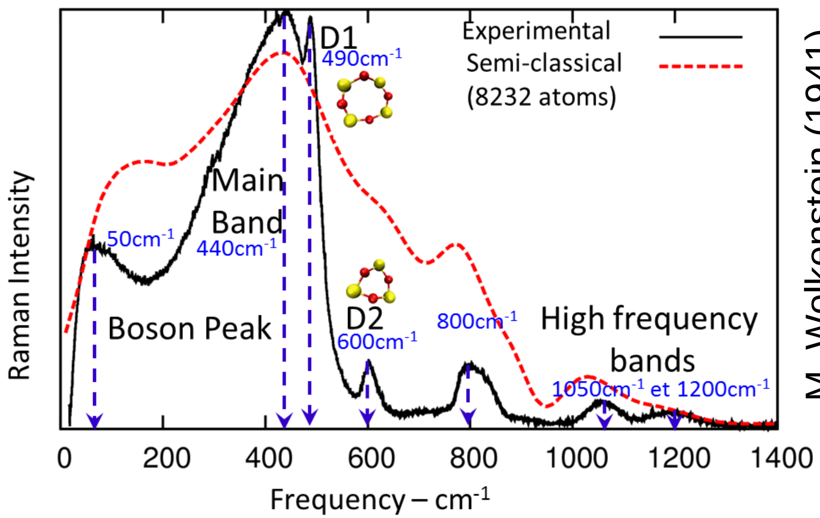








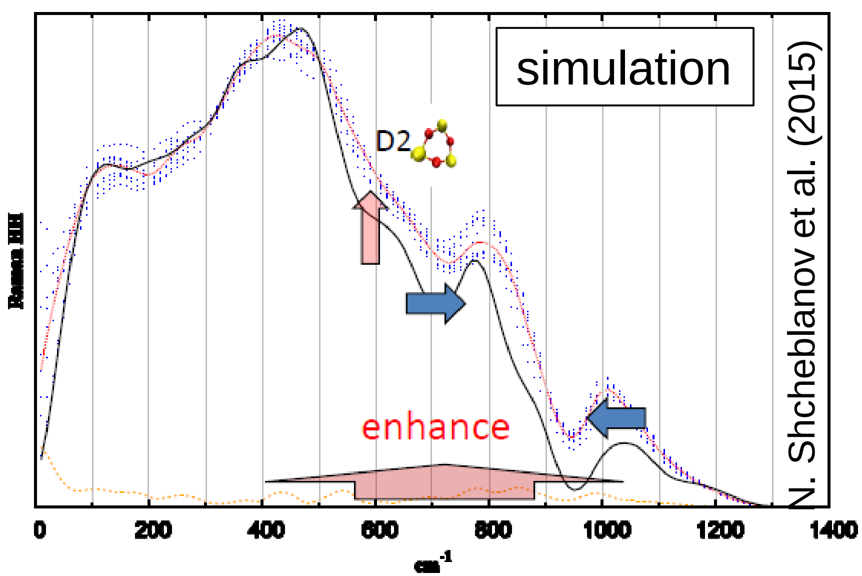
Semi-classical calculation:



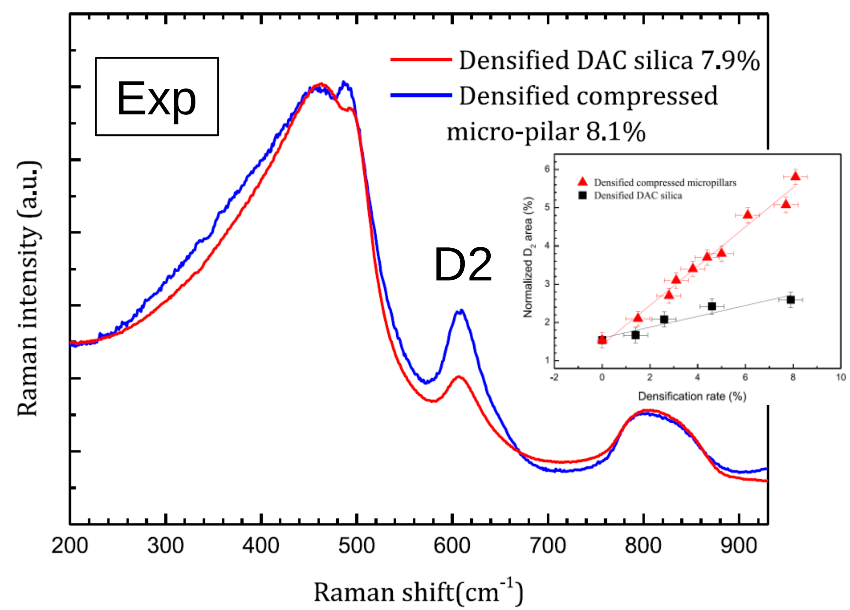
M. Wolkenstein (1941)

Effect of **Shear** induced **Irreversible Structural changes**:

Enhanced contribution of Stretching modes supported by Oxygen atoms, increasing D2 band



N. Shcheblanov et al. (2015)

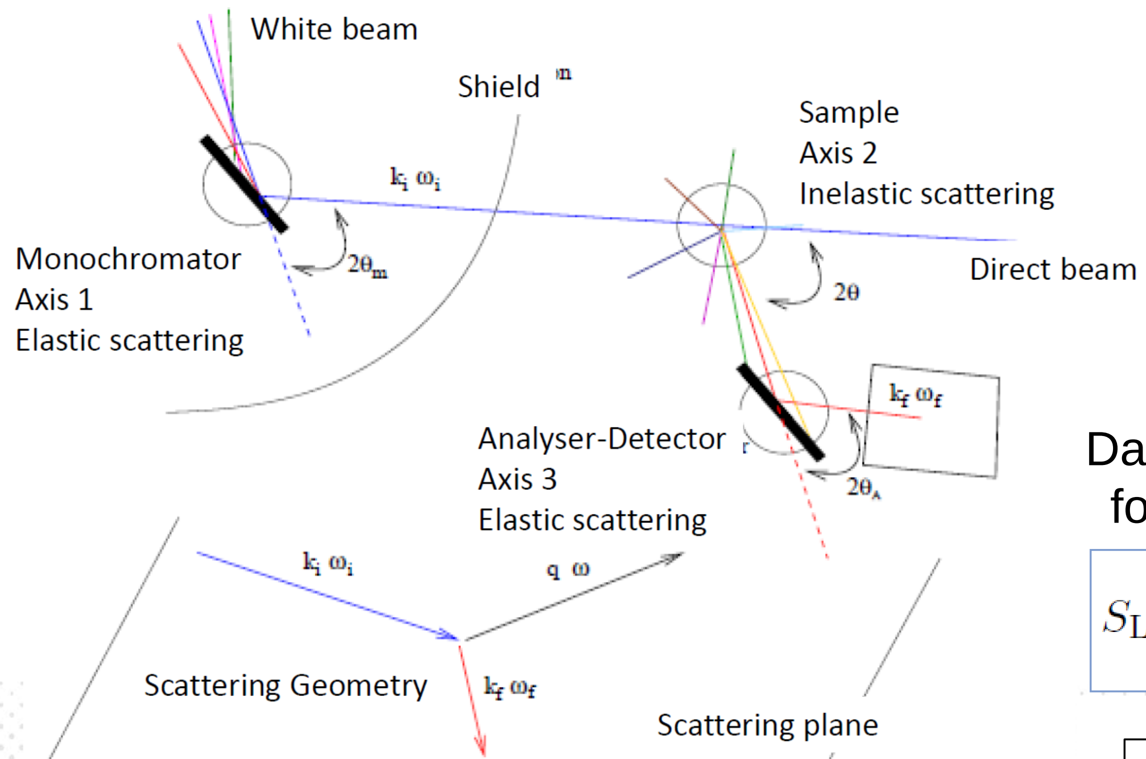


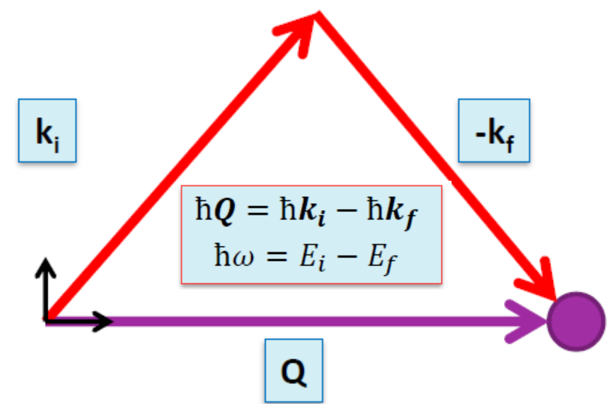
C. Martinet et al. (2020)

Measurement of Acoustic Attenuation in Glasses

Inelastic Neutron or X-ray scattering

is based on wave-vector assumption





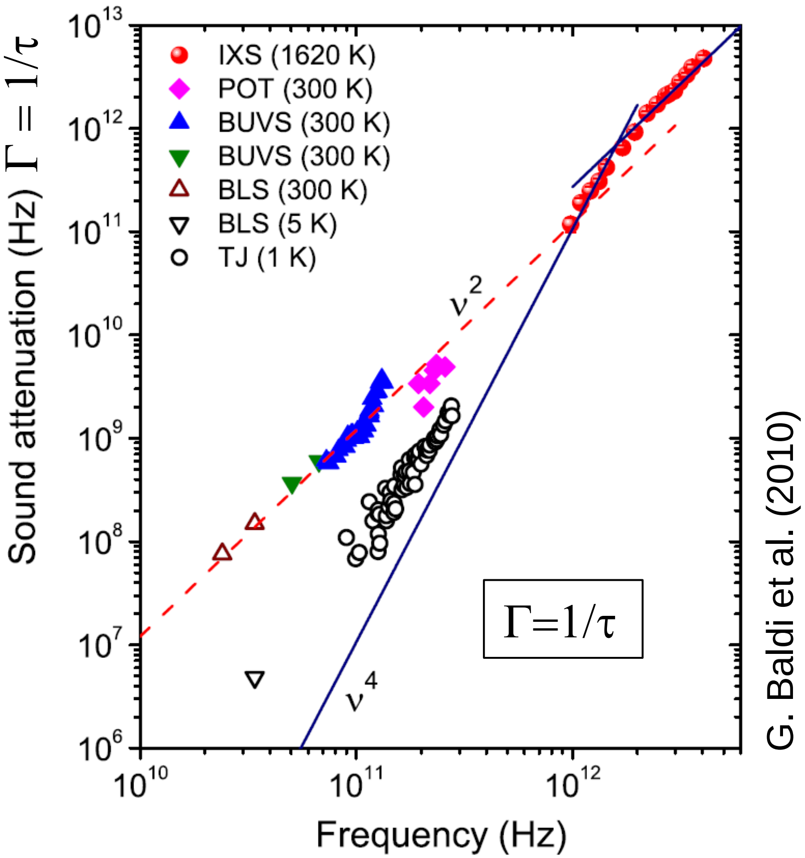
Damped Harmonic Oscillator Model for the Dynamic Structure Factor

$$S_{\mathrm{L,T}}(q,\omega) = \frac{A}{(\omega^2 - \omega_{\mathrm{L,T}}^2(q))^2 + \omega^2\Gamma^2}$$

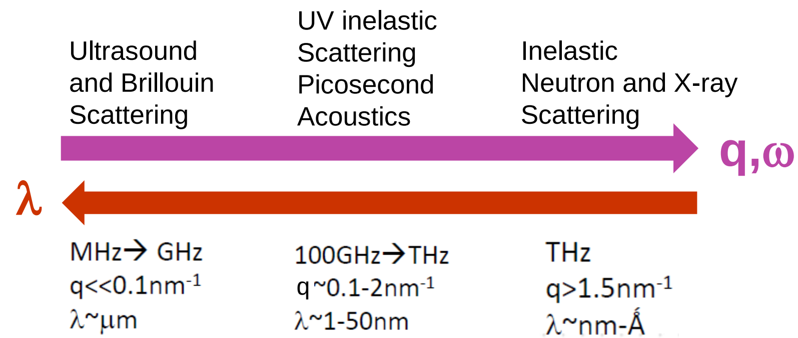
eigenfrequency

attenuation

Measurement of Acoustic Attenuation in Glasses



IXS: Inelastic X-ray Scattering
POT: picosecond optical technique
BUVS /BLS: Brillouin Ultraviolet/Light Scattering
TJ: Tunneling Junction



Inverse Attenuation Time:

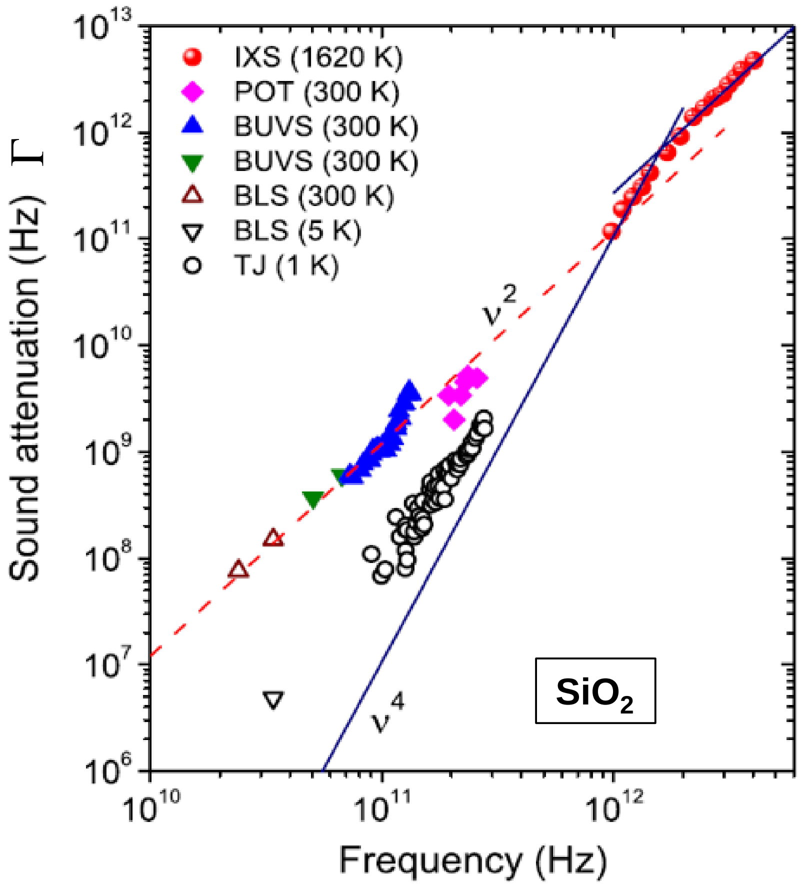
$$\Gamma = \frac{1}{\tau} \propto \omega^2 ; \omega^4 ; \omega^2$$

Origin of the frequency dependence of the Acoustic attenuation Time:

Anharmonicity ? Low Scattering ?
Strong Scattering ?

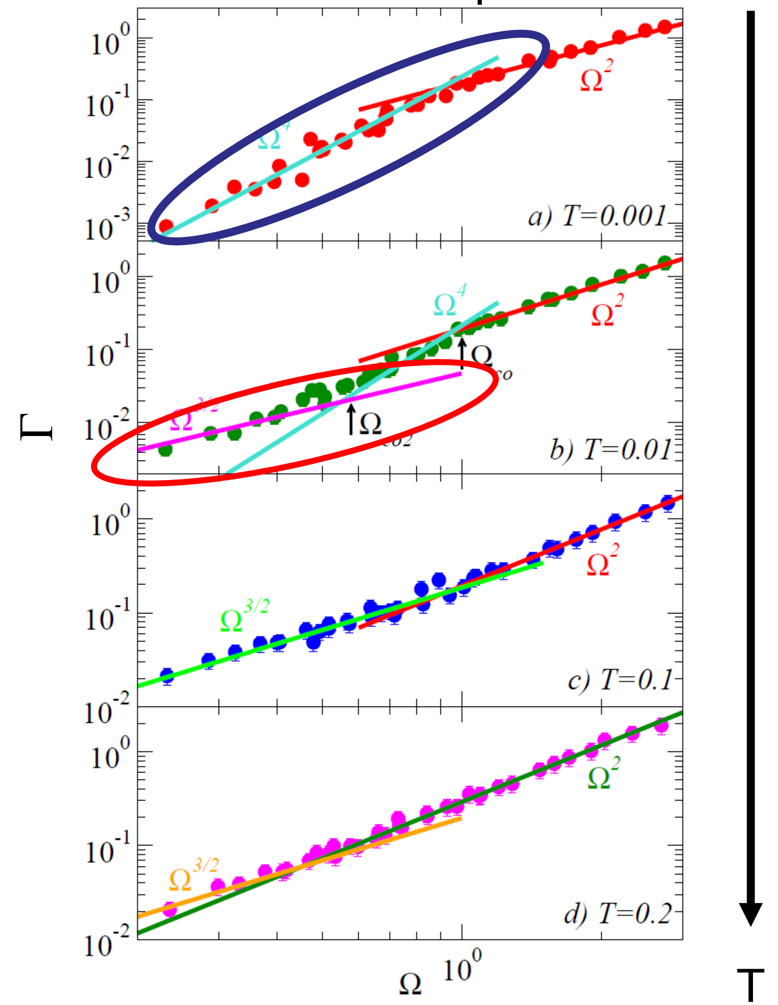
Experimental Results

$$S_{\mathrm{L,T}}(q,\omega) = \frac{A}{(\omega^2 - \omega^2_{\mathrm{L,T}}(q))^2 + \omega^2\Gamma^2}$$



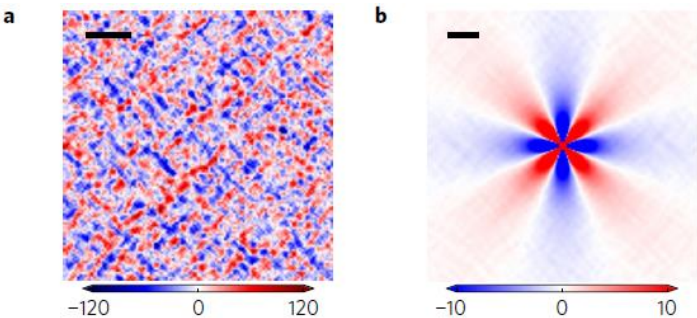
G. Baldi et al. (2010)

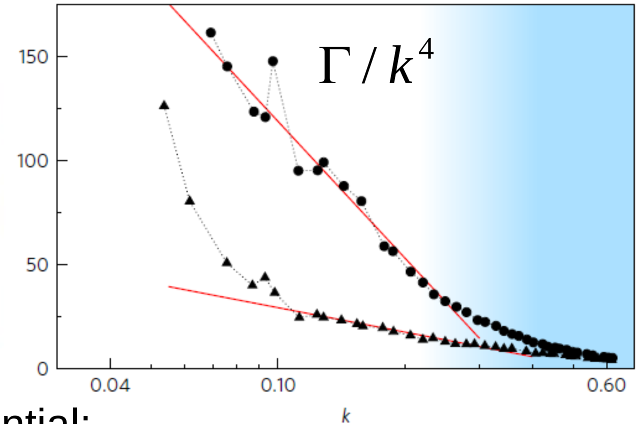
Molecular Dynamics Simulations at different Temperatures



H. Mizuno, et al.(2020)

- (Anomalous) Rayleigh Scattering





$\Gamma \propto -k^4 \ln(k)$ for 3D

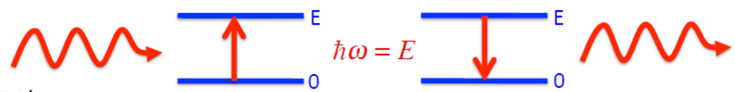
Structural stress anisotropy
Long-rang correlations

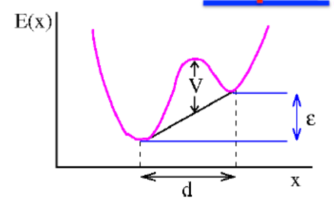
A. Lemaitre et al (2016)

- Anharmonicity on double well potential:

Fermi Golden rule scattering rate of phonons with tunneling

$$\left.\begin{aligned} \ell_X &= v_g / \Gamma \propto 1/\omega \\ \hbar\omega &\propto k_B T \\ C(T) &\propto T^3 \end{aligned}\right\} \Rightarrow \kappa \propto T^2$$

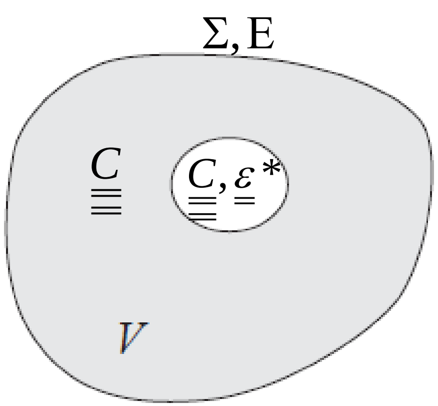


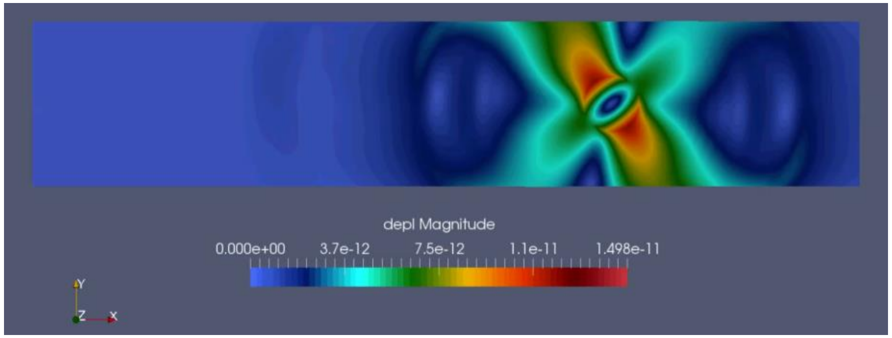


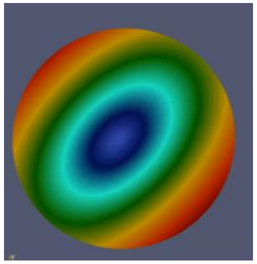
P. Anderson et al,
W.A. Philipps (1972)

- Scattering on Esheby Inclusions (plastic defect):

$$\rho \frac{\partial^2 u}{\partial t^2} = div\left(\underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}\right) + f\left(\underline{\underline{\varepsilon}}^*\right) \quad \text{with} \quad f\left(\underline{\underline{\varepsilon}}^*\right) = \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}^* . \underline{n}\ \delta\left(S'\right)$$

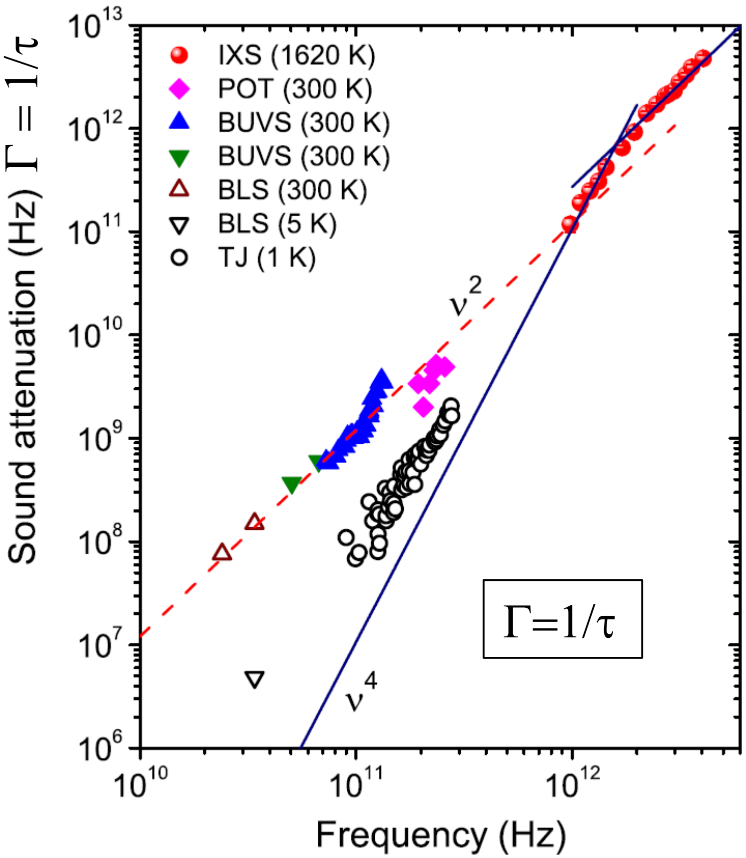






F. Lund et al (2021)

Effective modeling of Acoustic Attenuation in Glasses



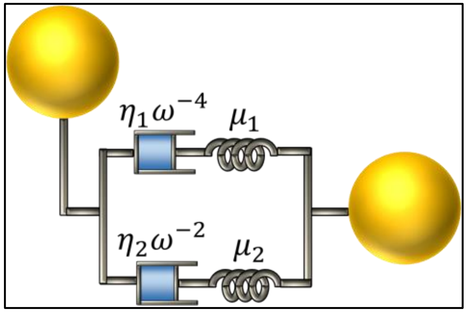
G. Baldi et al. (2010)

IXS: Inelastic X-ray Scattering
POT: picosecond optical technique
BUVS /BLS: Brillouin Ultraviolet/Light Scattering
TJ: Tunneling Junction

Sound attenuation = Inverse Attenuation Time:

$$\Gamma = \frac{1}{\tau} \propto \omega^2 ; \omega^4 ; \omega^2$$

Effective modelling: two parallel processes



Quality factor (Q^{-1})

$$\frac{G''}{G'}(\omega) = \Phi(\omega, \alpha, \tau_1, \tau_2)$$

$$\frac{\Gamma}{\omega}(\omega) = Q^{-1}(\omega)$$

3 parameters:

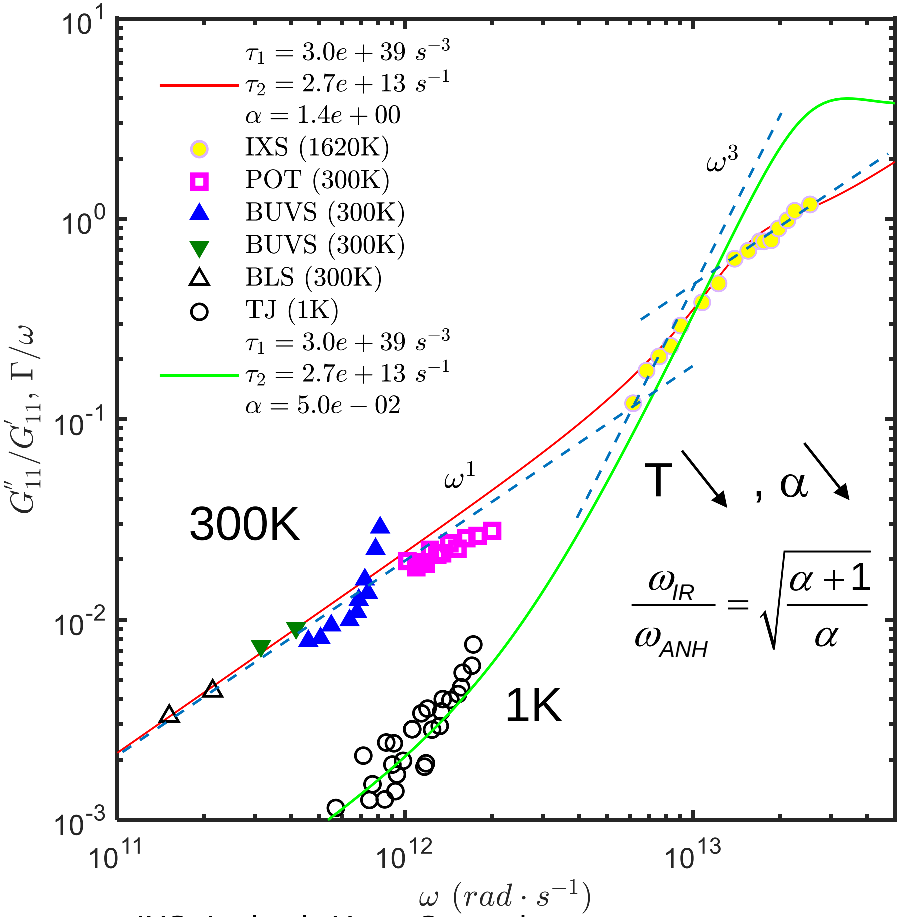
$$\alpha = \frac{\mu_2}{\mu_1}, \tau_1 = \frac{\eta_1}{\mu_1}, \tau_2 = \frac{\eta_2}{\mu_2} \quad \text{with} \quad \alpha(\mathrm{T}) \nearrow$$

H. Luo, et al (2021)

LaMCoS Unité Mixte de Recherche 5259 — cnrs — INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON — UNIVERSITÉ DE LYON

Laboratoire de Mécanique des Contacts et des Structures

Effective modeling of Acoustic Attenuation in Glasses



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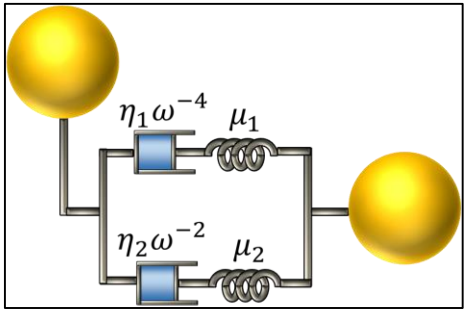

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H. Luo, et al (2021)

Conclusion Phonons in Amorphous Materials

No wave-vector in disordered materials → Apparent Attenuation and Internal friction

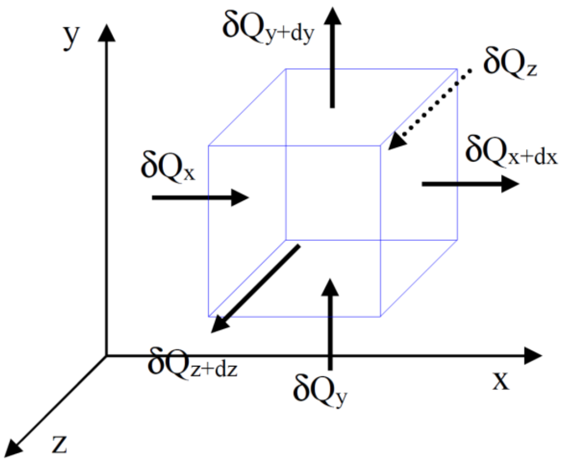
Anharmonic Processes → Different Frequency dependences of attenuation

In **Amorphous Materials**

- What are the **microscopic sources** of **mechanical deformation** ?
- Is it possible to define **Phonons** ?
- Is it possible to quantify **Thermal transport** ?

Out-of-Equilibrium Fluxes:

J.-B. J. Fourier (1768-1830)

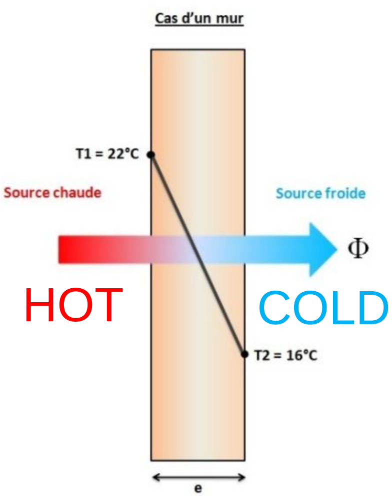


Flux of heat

Fourier's Law

$$\delta Q_x = -k_x \frac{\partial T}{\partial x} dydzdt$$

Thermal Conductivity



Energy Conservation:

$$\delta Q_x + \delta Q_y + \delta Q_z + qdVdt = \delta Q_{x+dx} + \delta Q_{y+dy} + \delta Q_{z+dz} + \rho C.dV.\frac{\partial T}{\partial t}dt$$

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) + q = \rho C \frac{\partial T}{\partial t}$$

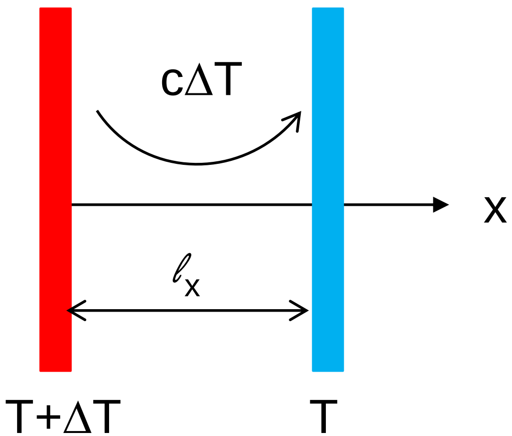
$$\Delta T + \frac{q}{k} = \frac{1}{D}\frac{\partial T}{\partial t} \qquad D = \frac{k}{\rho C}$$

Diffusivity

Thermal Conductivity in crystals (Kittel)

In crystals, phonons = quantum of vibrational energy $\left(n+\frac{1}{2}\right)\hbar\omega$ with wave vector **K**
Thermal energy transfer = random diffusive process

Kinetic Theory of Thermal Conductivity:



$$\Delta T = \frac{dT}{dx}\ell_x = \frac{dT}{dx}v_x\tau$$

ℓ_x, phonons mean free path

Net flux of Energy: $j_q = -\frac{N}{V}\langle v_x c\Delta T\rangle = -\frac{N}{V}\left\langle v_x c\frac{dT}{dx}\ell_x\right\rangle \approx -\frac{1}{3}\frac{N}{V}c\|v\|\ell_x\frac{dT}{dx}$

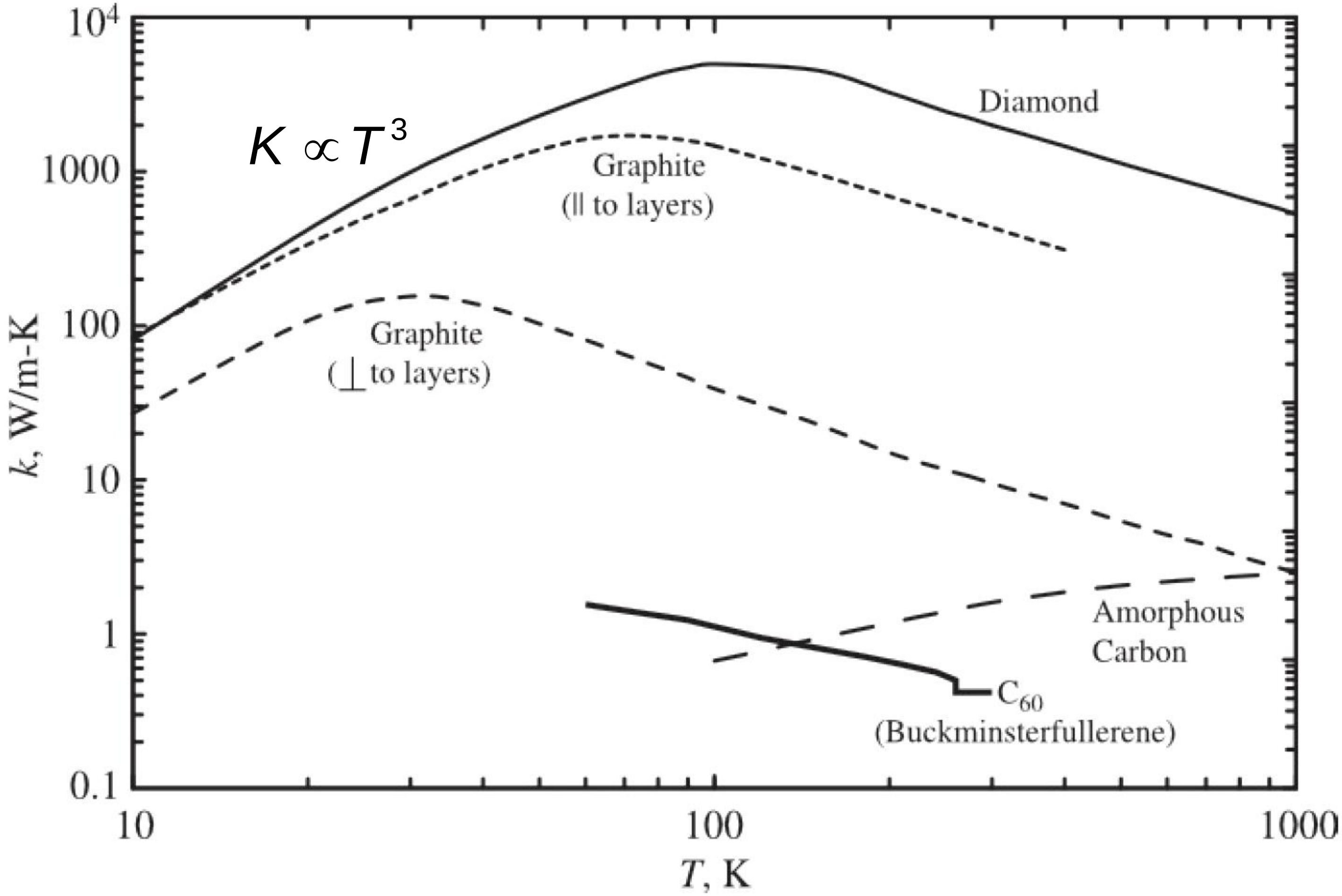
$$\Rightarrow \boxed{K \approx \frac{1}{3}C\|v\|\ell_x}$$ Heat Conductivity

In **Crystals** ℓ_x

Geometrical scattering: $\ell_x \approx L \quad K \propto C \propto T^3$
crystal boundary, lattice imperfections…

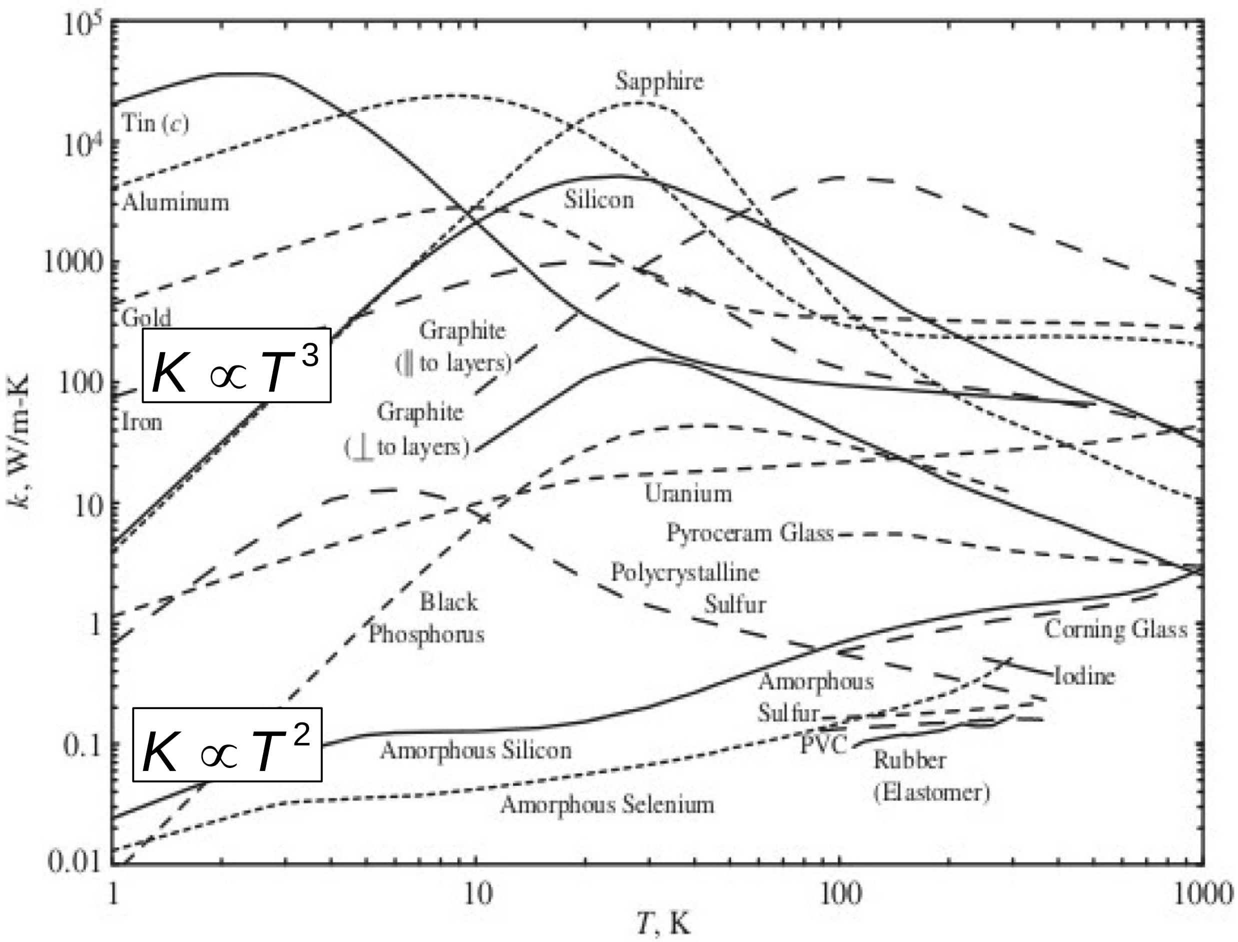
Scattering by other phonons: $\ell_x \propto \frac{1}{n_{phonons}} \propto \frac{1}{T}$
anharmonicity, umklapp processes…

Some Measurements of Thermal Conductivity



Y. Touloukian, Thermophysical Properties of Matter

Some Measurements of Thermal Conductivity



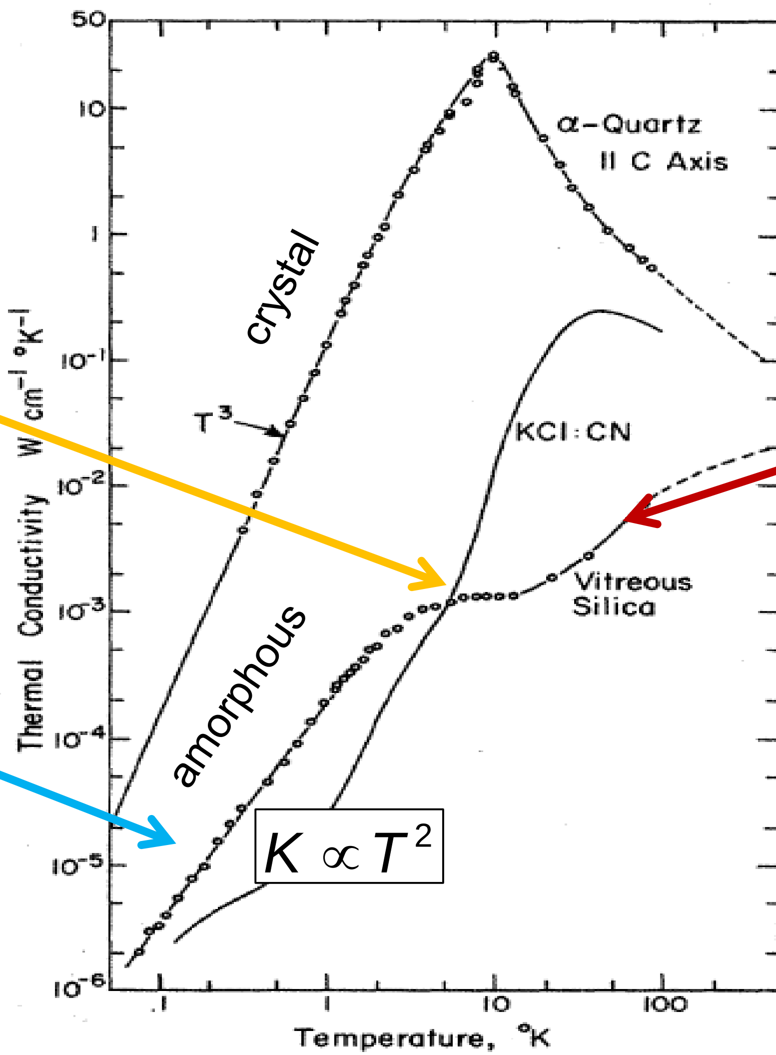
Y. Touloukian, Thermophysical Properties of Matter

Thermal Conductivity

plateau:
Resonant scattering of phonons by « quasi-local vibrations»?
(Buchenau et al. 1992)

Strongly scattered modes?
(Wyart et al. 2010)

Resonant scattering of phonons on « 2-level systems »?
(Hunklinger et al 1986)



Diffusion mechanism for heat transfer due to clusters vibrating with random phases?
(Cahill et al 1988)

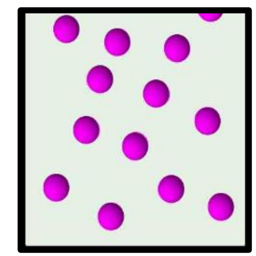
D. Parshin (2013)

Transportation of Energy: Boltzmann Equation in Glasses

$\boxed{f_1(\vec{r},\vec{p},t)d\vec{r}d\vec{p}}$ = Mean number of particles which, at time t, are in the phase space at (**r**,**p**) within d**r**d**p**

$$\rho(\vec{r},t) = m\frac{N}{V}\int f_1(\vec{r},\vec{p},t)d\vec{p}$$

$$f_1(\vec{r}_1,\vec{p}_1,t) = \frac{1}{(N-1)!}\int f_N(\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_N,\vec{p}_N,t)d\vec{r}_2d\vec{p}_2\ldots d\vec{r}_Nd\vec{p}_N$$



Equations of motion: $\vec{r},\vec{p} \rightarrow \vec{r}+\vec{p}\frac{dt}{m}, \vec{p}+\vec{F}dt$ for each particle

$f(\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_N,\vec{p}_N,t)$ is such that $\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f,H\} = 0$ with $H = \sum_{i=1}^{N}\frac{p_i^2}{2m} + U_{pot}(\vec{r}_i) + \sum_{i<j}u(\vec{r}_i-\vec{r}_j)$

that is

$$\boxed{\left[\frac{\partial}{\partial t} + \frac{\vec{p}_1}{m}\frac{\partial}{\partial \vec{r}_1} + \vec{F}(\vec{r}_1)\frac{\partial}{\partial \vec{p}_1}\right]f_1(\vec{r}_1,\vec{p}_1,t) = \int d\vec{r}_2 d\vec{p}_2 \frac{\partial u(\vec{r}_1-\vec{r}_2)}{\partial \vec{r}_1}\frac{\partial}{\partial \vec{p}_1} f_2(\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2,t)}$$

one-particle   interactions   BBGKY

Boltzmann Equation: $\frac{\partial f_1}{\partial t} + v_g.\nabla_x f_1 = -\frac{f_1 - f_{eq}}{\tau_{coll}}$ (collision) is no longer valid

Transportation of Energy: Boltzmann Equation and BBGKY Hierarchy

Conservation of the total average energy:

$$\frac{\partial\left(\rho u^{tot}\right)}{\partial t}+\vec{\nabla}.\left(\rho u^{tot}\vec{v}+\vec{j}_q\right)=-\left(\underline{\underline{P}}^{cin}+\underline{\underline{P}}^{dyn}\right):\left(\underline{\underline{\nabla\vec{v}}}\right)\quad\text{with}\quad \vec{j}_q=\vec{j}_q^{\,cin}+\vec{j}_q^{\,pot,1}+\vec{j}_q^{\,pot,2}$$

$$\vec{v}(\vec{r},t)=\frac{N}{\rho(\vec{r},t)V}\int\vec{p}f_1(\vec{r},\vec{p},t)d\vec{p};\quad \vec{j}_q^{\,cin}=\frac{N}{V}\int\frac{\vec{p}-m\vec{v}}{m}\frac{\left|\vec{p}-m\vec{v}\right|^2}{2m}f_1(\vec{r},\vec{p},t)d\vec{p},$$

$$\vec{j}_q^{\,pot,1}=\frac{1}{2}\left(\frac{N}{V}\right)^2\int\frac{\vec{p}-m\vec{v}}{m}u(\vec{r}-\vec{r}_1)f_2(\vec{r},\vec{p},\vec{r}_1,\vec{p}_1,t)d\vec{r}_1d\vec{p}_1d\vec{p};$$

$$\vec{j}_q^{\,pot,2}=-\frac{1}{4}\left(\frac{N}{V}\right)^2\int_0^1d\lambda\int d\vec{r'}_{12}\frac{\vec{r'}_{12}\vec{r'}_{12}}{r'_{12}}.\frac{\vec{p}+\vec{p}_1-2m\vec{v}}{m}f_2\left(\vec{r}+(1-\lambda)\vec{r'}_{12},\vec{p},\vec{r}-\lambda\vec{r'}_{12},\vec{p}_1,t\right)d\vec{p}_1d\vec{p}$$

Out-of-equilibrium Linear expansion of the distribution functions f_1 and f_2:

$$f_1(\vec{r},\vec{p},t)=f_1^{(eq)}(\vec{r},\vec{p},t)+A(|\vec{p}-m\vec{v}|)\left[\frac{(\vec{p}-m\vec{v})\underline{\underline{e}}(\vec{p}-m\vec{v})}{\left|\vec{p}-m\vec{v}\right|^2}-\frac{1}{3}\vec{\nabla}_r.\vec{v}\right]+B\frac{\vec{p}-m\vec{v}}{\left|\vec{p}-m\vec{v}\right|}.\vec{\nabla}T\ldots$$

$$\vec{j}_q^{\,cin}\approx\frac{1}{6}\frac{N}{V}\int\frac{|q|^3}{m^2}B(|q|,r)d\vec{q}\vec{\nabla}T(\vec{r},t);\vec{j}_q^{\,pot,1}\approx 0;\vec{j}_q^{\,pot,2}\approx\frac{-1}{18}\int C(r_{12})r_{12}\frac{du}{dr_{12}}(r_{12})d\vec{r}_{12}\vec{\nabla}T\Rightarrow\boxed{\vec{j}_q\approx-k\vec{\nabla}T}$$

The thermal conductivity results from lattice dynamics, and particles motion …

The theory of **Allen and Feldman** for Thermal Conductivity in Glasses

Heat current density operator S

$$\frac{\partial h(x)}{\partial t} + \nabla \cdot \mathbf{S}(x) = 0$$

$$\mathbf{S} = \frac{1}{2V} \sum_{l,m} \sum_{\alpha,\beta} (\mathbf{R}_l - \mathbf{R}_m) \frac{p_{l\alpha}}{m_l} \frac{\partial^2 E}{\partial u(l\alpha) \partial u(m\beta)} u(m\beta)$$

Thermal Conductivity κ

$$\kappa_{\mu\nu} = \frac{V}{T} \int_0^\beta d\lambda \int_{-\infty}^0 dt \langle e^{\lambda H} S_\mu(t) e^{-\lambda H} S_\nu(0) \rangle$$

$$\kappa_{\mu\nu}(\omega) = \frac{\pi V}{T} \sum_{i,j} \frac{n_i - n_j}{\hbar(\omega_i - \omega_j)} (S_\mu)_{ij} (S_\nu)_{ji} \delta(\omega_i - \omega_j - \omega)$$

Diffusivity

$$D_i = \frac{4\pi^2 V^2}{3h^2 \omega_i^2} \sum_{j \neq i} |S_{ij}|^2 \delta(\omega_i - \omega_j)$$

$$\kappa = \kappa^{\mathrm{I}} + \kappa^{\mathrm{II}} ,$$

$$\kappa^{\mathrm{I}}(\omega) = \frac{iV}{T} \sum_{i \neq j} \frac{n_i - n_j}{\hbar(\omega_i - \omega_j)} \frac{|S_{ij}|^2}{\omega_i - \omega_j - \omega - i\eta} \approx \frac{1}{V} \sum_i C_i(T) D_i$$

« Interband » conductivity due to coupling between extended phonons (propagons?)

$$\kappa^{\mathrm{II}}(\omega) = \frac{iV}{\hbar T} \frac{1}{\omega + i\eta} \sum_i \left[-\frac{\partial n_i}{\partial \omega_i} \right] S_{ii}^2 \approx \frac{1}{3} C v \ell$$

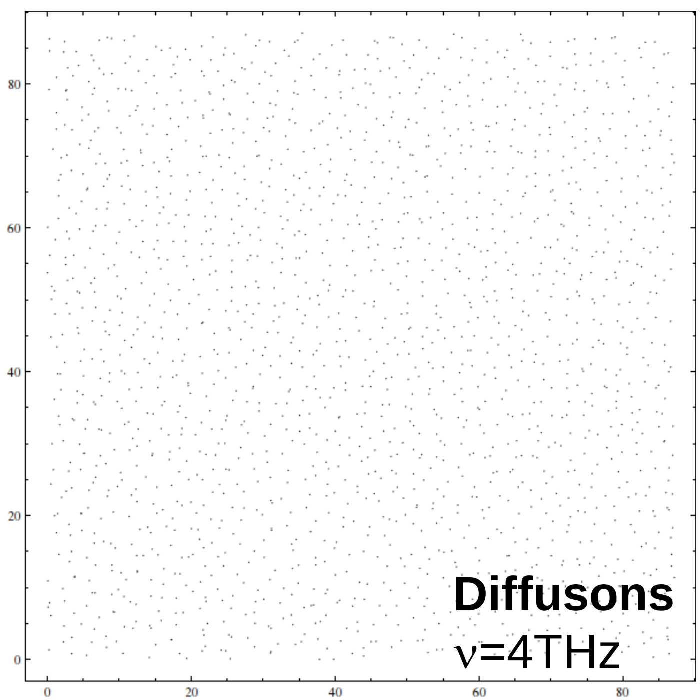
usual « intraband » conductivity

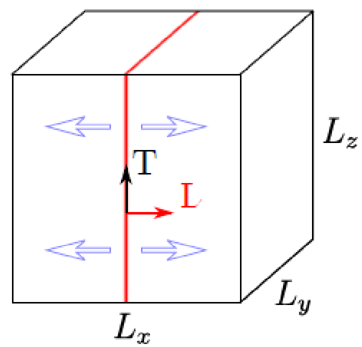
P.B. Allen and J.L. Feldman (1993)

Mechanical to **Thermal** Energy Conversion in Glasses

In crystals, phonons describe the atoms vibrations as plane waves.

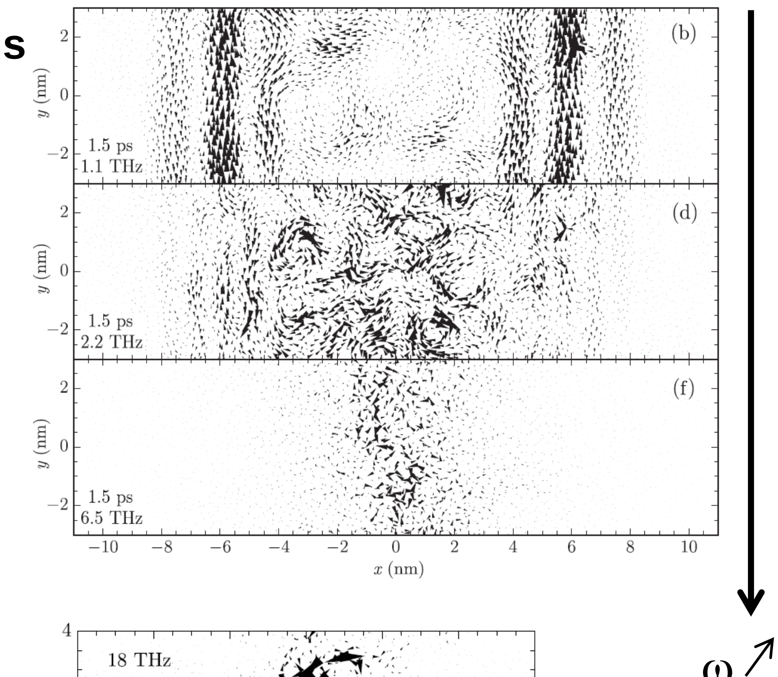
In disordered materials, plane waves are scattered on the vibrational modes known as propagons, diffusons, and locons.



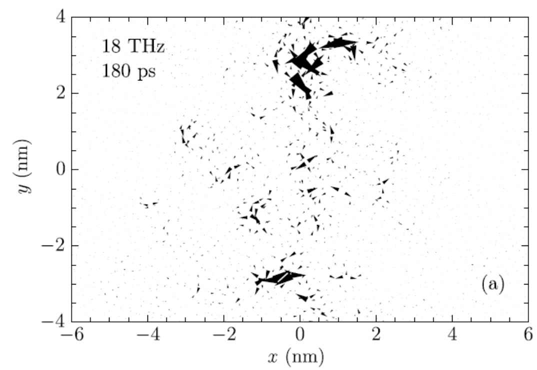


Propagons

Diffusons



Locons



Y. Beltukov et al (2018)

Mechanical to **Thermal** Energy Conversion in Glasses

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Thermal conductivity:

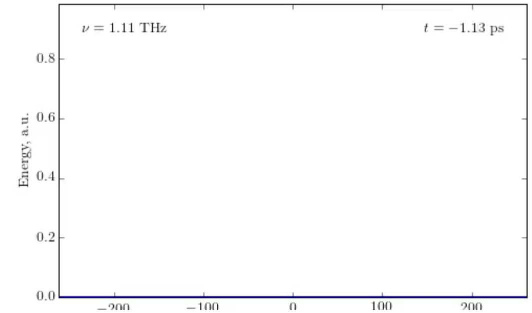
$$k_T = k_T^{prop} + k_T^{diff}$$

$$k_T^{prop} = \frac{1}{3}\int_0^{\omega_{IR}} C(T,\omega) v(\omega) l(\omega) g(\omega)\, d\omega$$

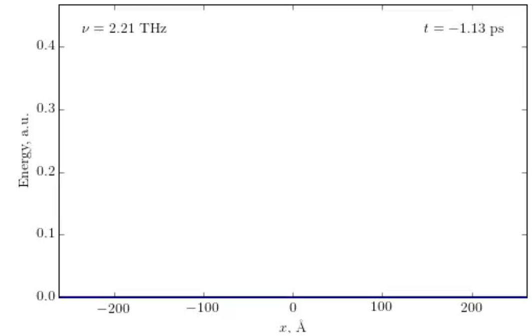
$$k_T^{diff} = \int_{\omega_{IR}}^{\omega_{max}} C(T,\omega) D(\omega) g(\omega)\, d\omega$$

$C(T,\omega)$: phonon specific heat.
$g(\omega)$: density states.
$v(\omega)$: sound speed.
$l(\omega)$: mean free path.
$D(\omega)$: diffusivity.

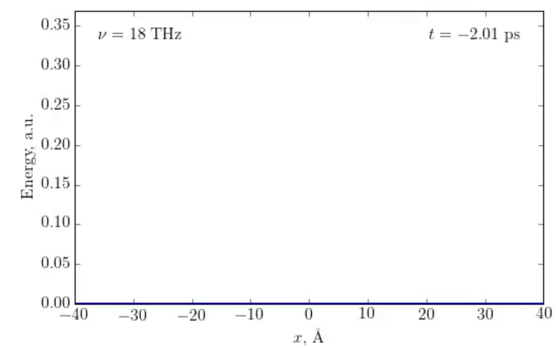
Propagons



Diffusons



Locons

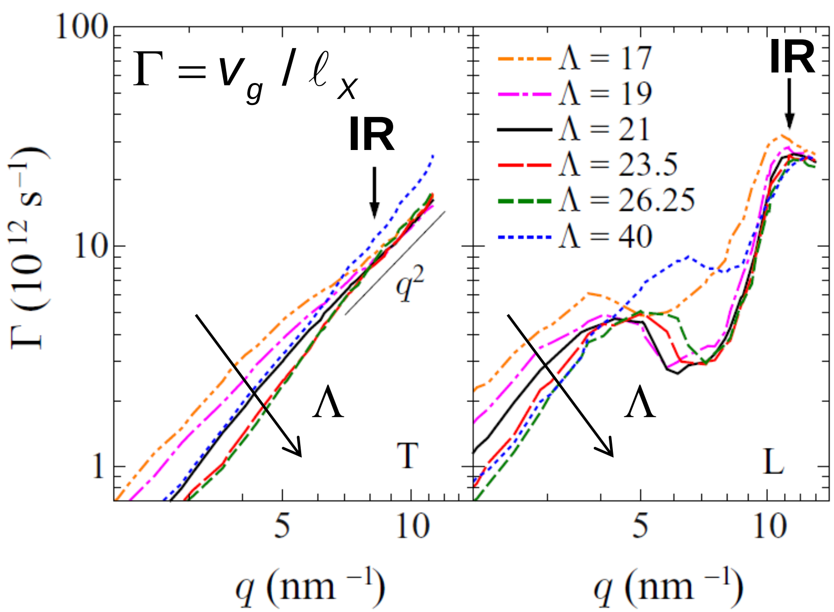


Y. Beltukov et al (2018)

Application to **Thermal Conductivity** in Glasses

Ballistic Regime

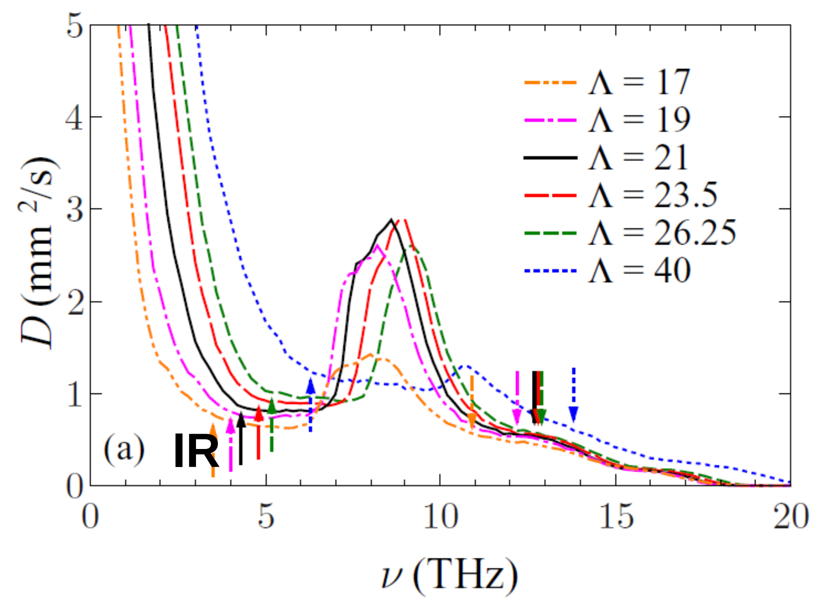
Attenuation for $\omega<\omega_{IR}$



$$\kappa^{prop}(T) = \frac{1}{3}\int_0^{\omega_{IR}} C(\omega,T)\, v_g^2(\omega)\, \Gamma^{-1}(\omega)\, g(\omega)\, d\omega$$

Diffusive Regime

Diffusivity for $\omega>=\omega_{IR}$

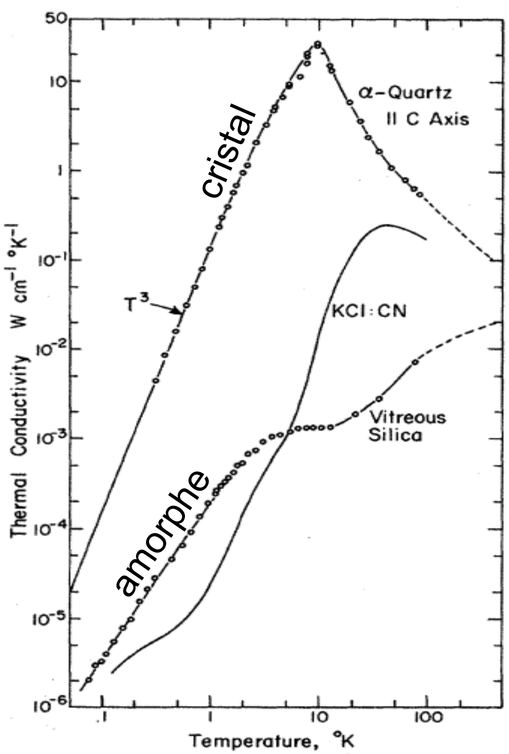


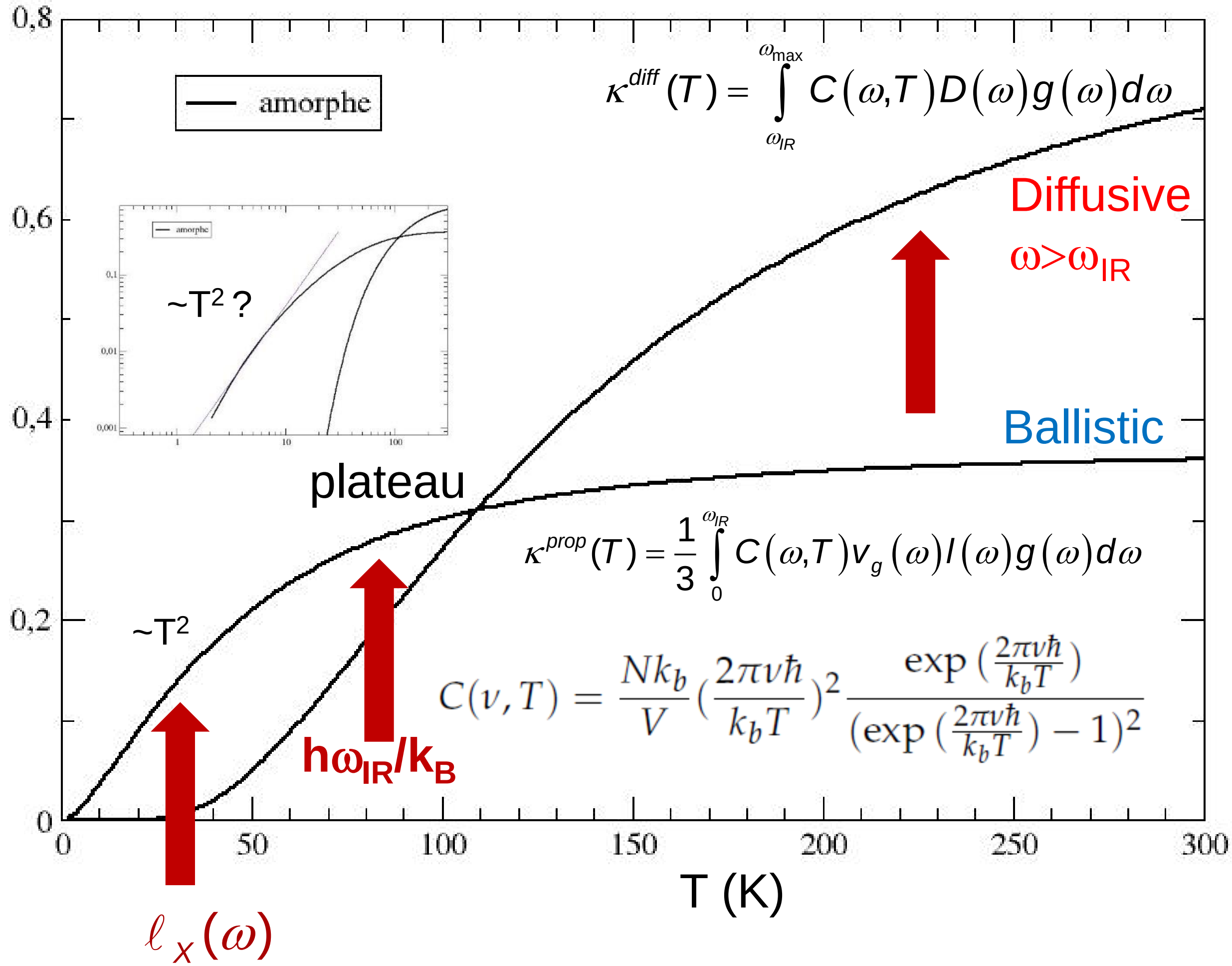
$$\kappa^{diff}(T) = \int_{\omega_{IR}}^{\omega_{max}} C(\omega,T)\, D(\omega)\, g(\omega)\, d\omega$$

Y. Beltukov et al. (2018)

Thermal Conductivity in Glasses

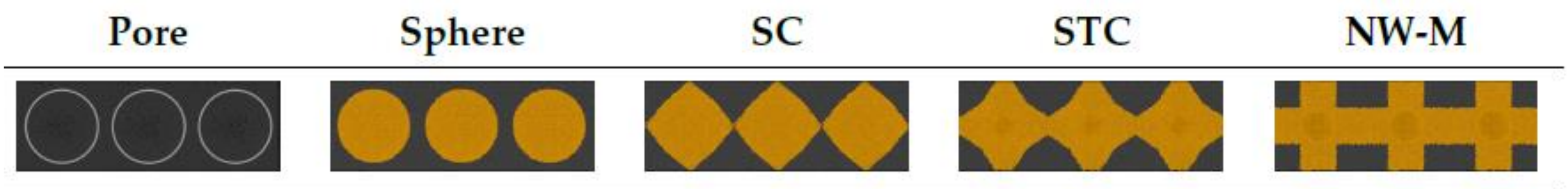
R.C. Zeller (1971)

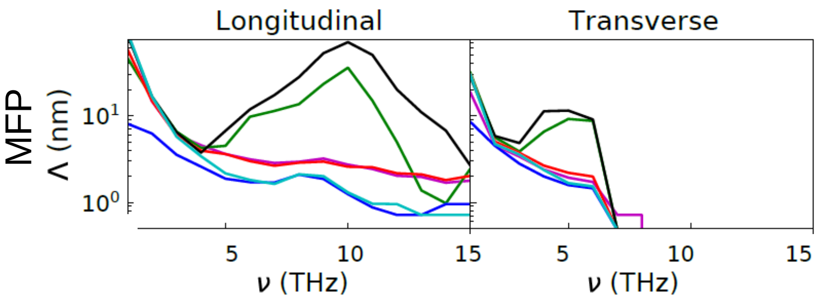




A. Tlili et al. (2019)

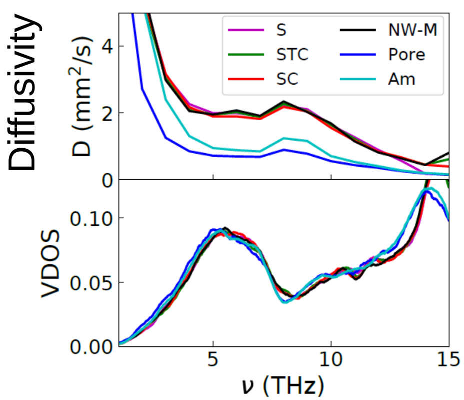
Wave-Packets Attenuation in nano-composites a-Si/c-Si
The role of the nanostructuration

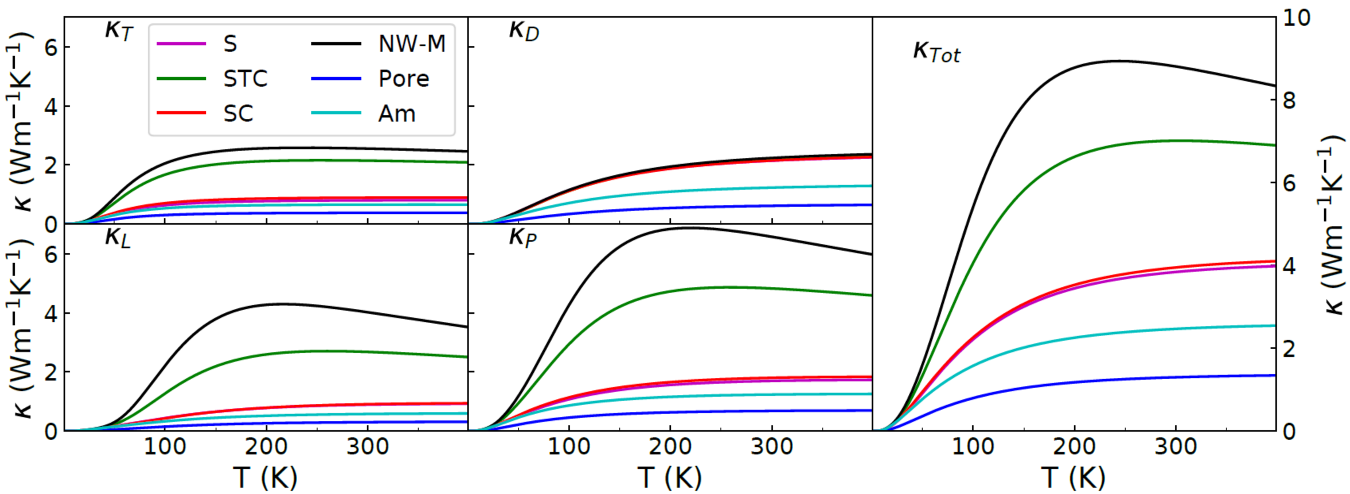




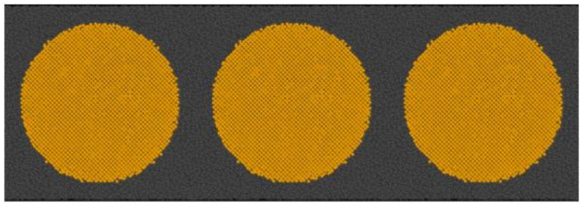
$$\boxed{\tau^{-1} = \tau_{geom}^{-1} + \tau_{ph-ph}^{-1}} \qquad \tau_{ph-ph}^{-1} = P(2\pi\nu)^2 T \exp(-C_U/T)$$

P. Desmarchelier et al. (2021)





Thermal Conductivity in a-Si / c-Si nanocomposite

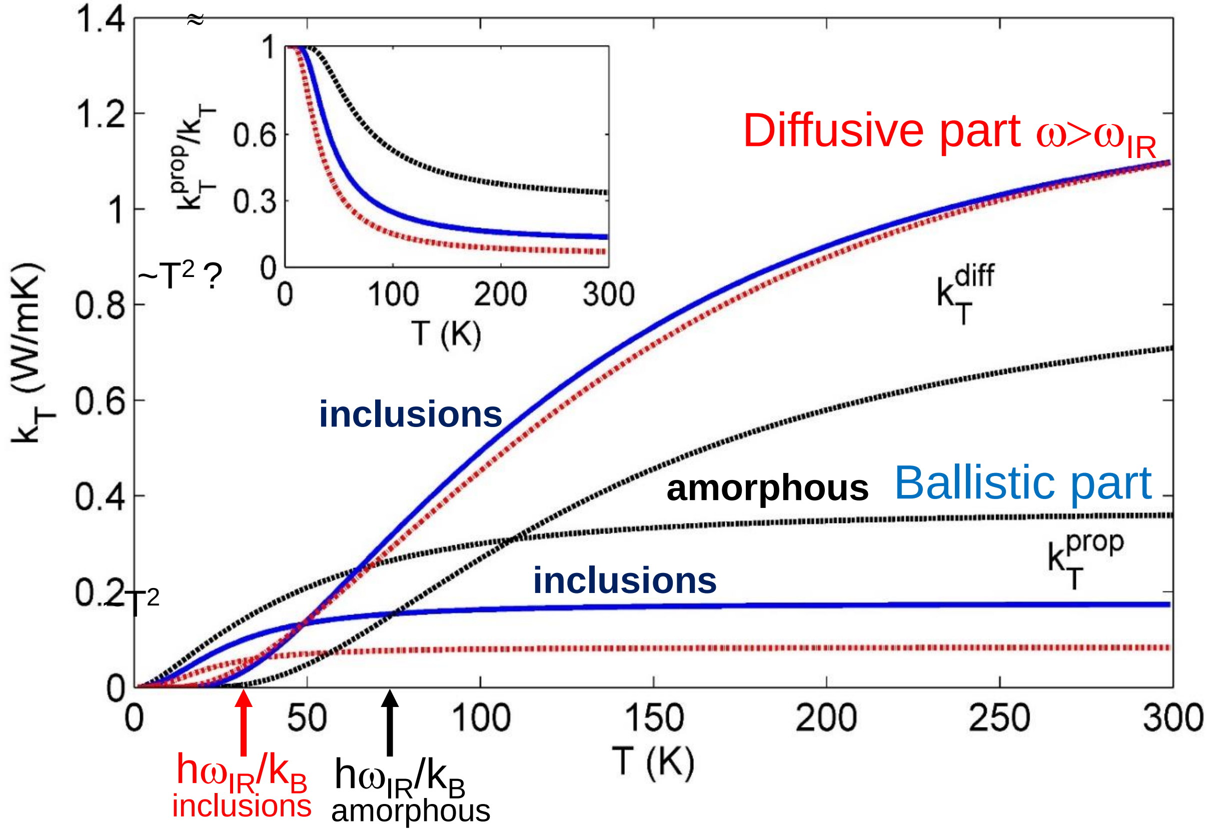


Rigidity contrast:

$E_i / E_m \approx 1$ (blue line)

$E_i / E_m \approx 4.6$ (red line)

The transition frequency to multiple scattering ω_{IR} is smaller ↘

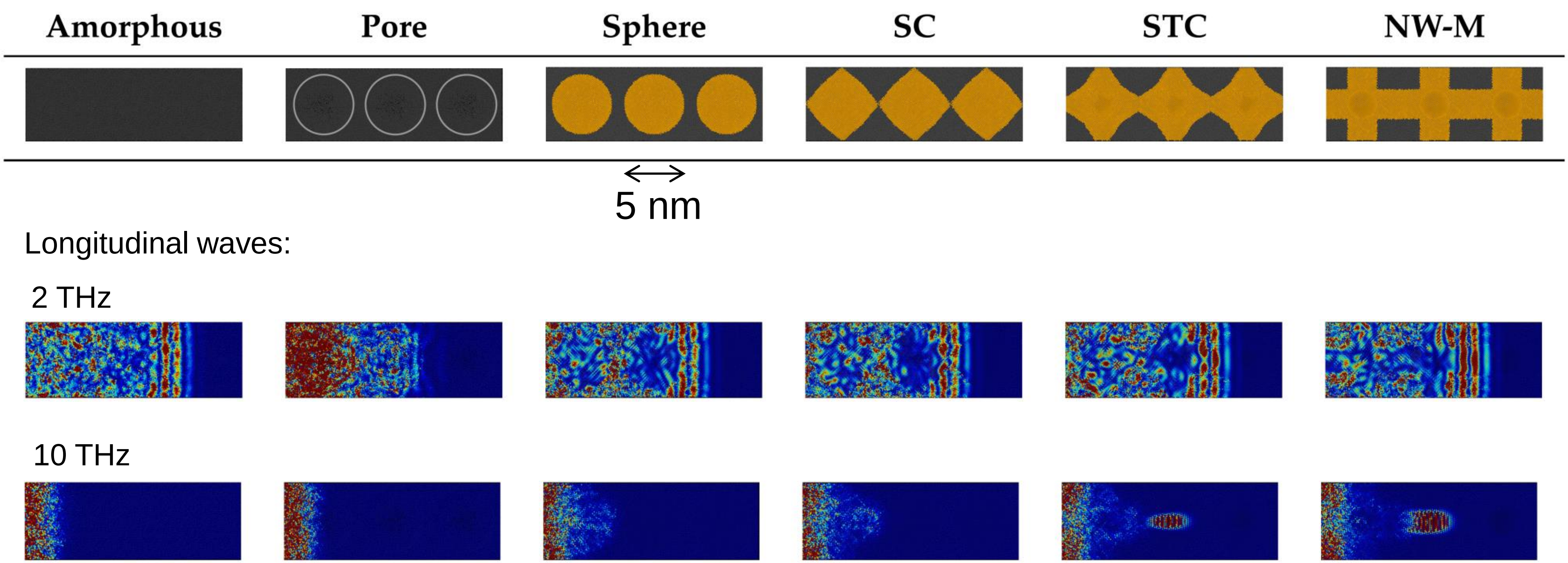


Enhancement of the diffusive contribution to Thermal conductivity in the nanocomposite

A. Tlili et al. (2019)

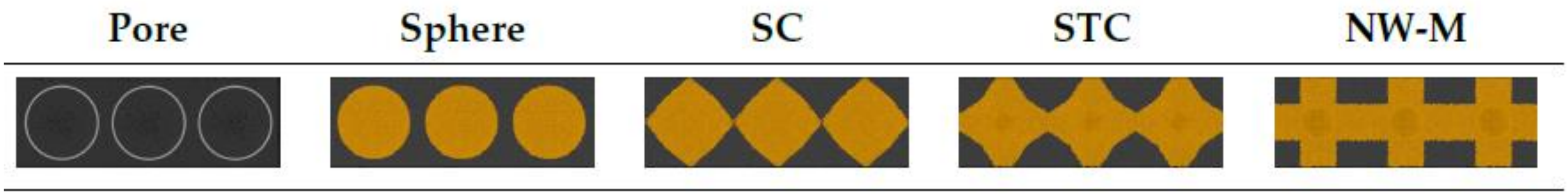
Thermal Conductivity in a-Si / c-Si nanocomposite

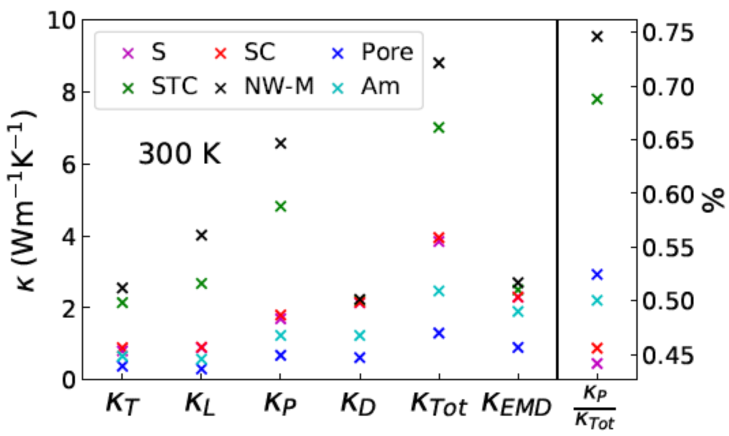
Role of the interconnections between the inclusions

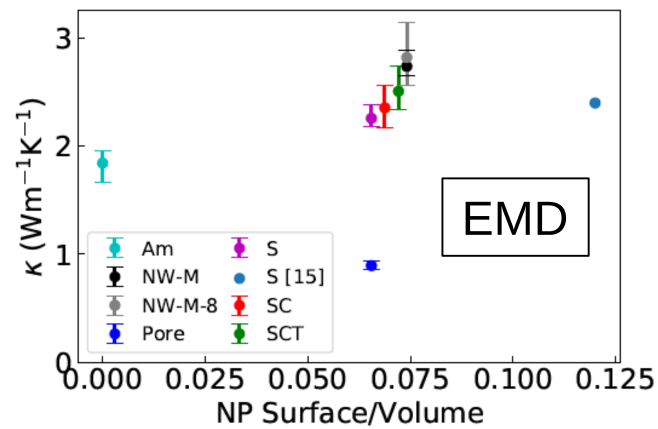


P. Desmarchelier et al. (2021)

Thermal Conductivity in a-Si / c-Si nanocomposite







P. Desmarchelier et al. (2021)

Conclusion Thermal Conductivity in Amorphous Materials

Departure of Vibrations from Plane Waves → Contribution of Propagons and Diffusons

Nanostructuration of matter (for ex. plasticity) → Affects the Thermal conductivity

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