

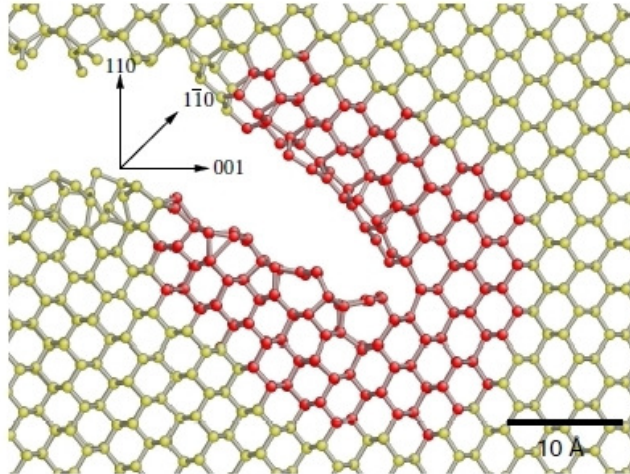
Modélisation Moléculaire de la Réponse Mécanique de Matériaux Amorphes

A.Tanguy

<http://www-lpmcn.univ-lyon1.fr/~atanguy>

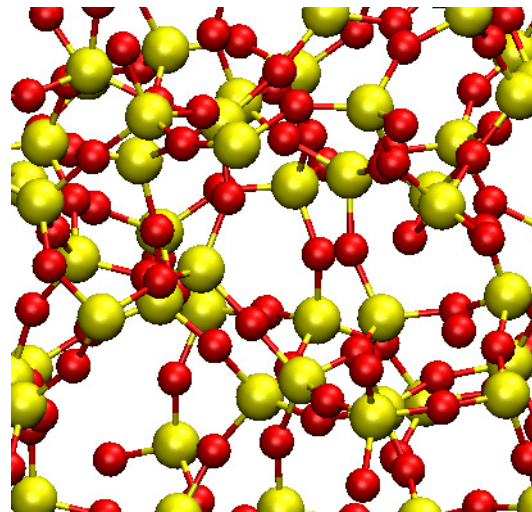
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*Institut Lumière Matière
Equipe Théorie et Modélisation
Etude Multi-échelle de la réponse mécanique des matériaux solides
Université Claude Bernard – Lyon 1
(France)*



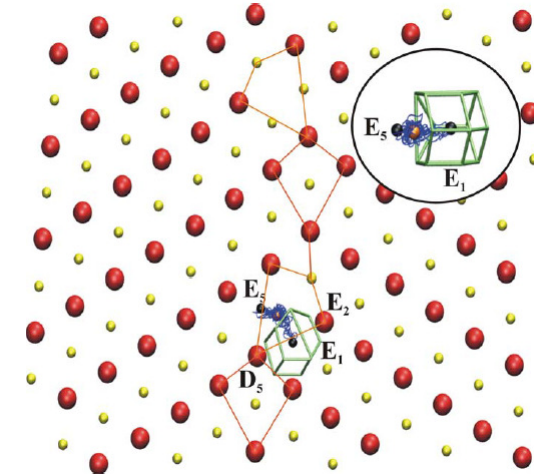
T. Albaret

Simulations Multi-échelles
Méthode LOTF.



A. Tanguy

Physique statistique et Réponse Mécanique
Matériaux Désordonnés



D. Tanguy

Simulations Monte-Carlo
Défauts - Joints de grain.

Modélisation Moléculaire de la Réponse Mécanique de Matériaux Amorphes

Exemples de Matériaux Amorphes.

Réponse sous cisaillement d'un verre de Lennard-Jones

Hétérogénéités de déformation

Dynamique Locale et bandes de cisaillement

Modules d'élasticité locaux et modes de vibration

Effet de la pression sur la réponse de la silice

Courbe de charge

Comportement en compression

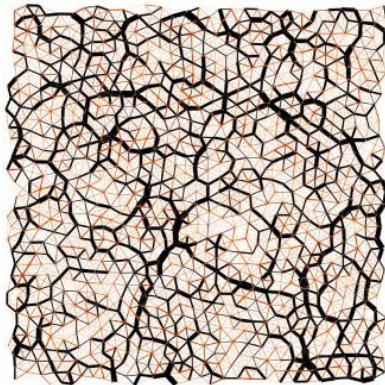
Rôle de la directionalité des liaisons

Réponse rhéologique

Réponse acoustique

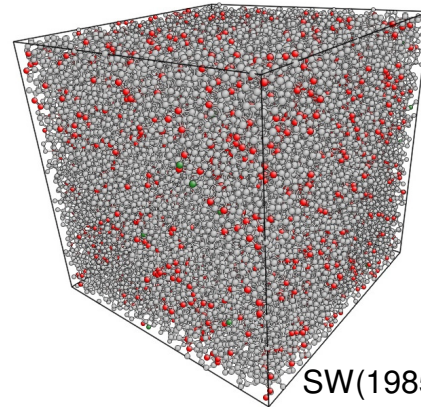
Exemples de Matériaux Amorphes.

Lennard-Jones Glasses



N = 100 to 400 000 particles
L: 10 α to 630 α (2D)
5 α to 74 α (3D)
 ρ : 0.87 to 1.4

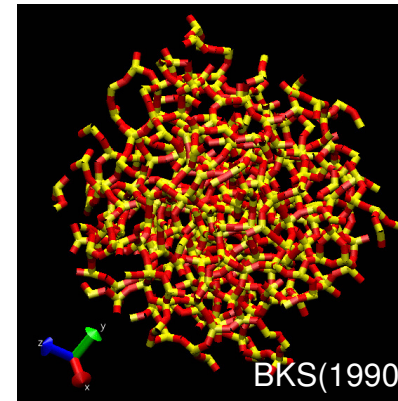
Amorphous « silicon »



SW(1985)

N = 32 768 atoms
L = 84.8 Å
 ρ = 2.4 g/cm³

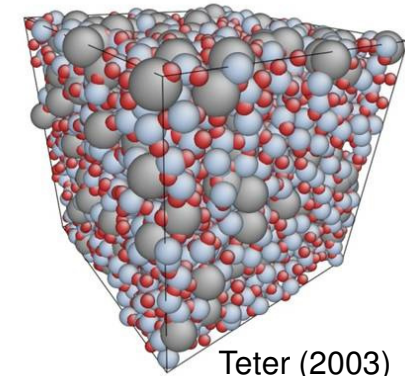
Silica glass



BKS(1990)

N = 3 000 to 375 000 atoms
L = 36 to 180 Å
 ρ = 2.2 to 3 g/cm³

Sodo-silicate glass (1-x)SiO₂ + x Na₂O



Teter (2003)

N = 2 400 to 8 100 atoms
L = 33 to 49 Å
 ρ = 2.29 g/cm³
x=5% to 30%

$$V_{ij}(r) = 4\epsilon_{ij} \left\{ \left(\frac{\sigma_{ij}}{r} \right)^{12} - \left(\frac{\sigma_{ij}}{r} \right)^6 \right\} E_{SW} = \sum_{i,j} (A_{ij} r_{ij}^{-4} - B) \cdot e^{-(r_{ij}-a)^{-1}} + \sum_{i,j,k} \lambda (\cos \theta_{jik} + 1/3)^2 \cdot e^{\gamma \cdot (r_{ij}-a)^{-1} + \gamma \cdot (r_{ik}-a)^{-1}}$$

$$E_{BKS}(r) = \frac{q_i q_j}{4\pi\epsilon_0 r} + A_{ij} e^{-B_{ij}r} - \frac{C_{ij}}{r^6}$$

with (i, j) ∈ {Si, O}

$$V(r) = A \exp(-r/\rho) - C/r^6$$

i-j	Short-range parameters			Atomic charges
	A _{ij} (eV)	b _{ij} (Å ⁻¹)	c _{ij} (eV Å ⁶)	
O-O	1388.7730	2.76000	175.0000	q _O = -1.2
Si-O	18003.7572	4.87318	133.5381	q _{Si} = 2.4

Interaction	A/eV	$\rho/\text{Å}$
O ^{-1.2} -O ^{-1.2}	1844.7458	0.343645
Si ^{2.4} -O ^{-1.2}	13702.905	0.193817
Na ^{0.6} -O ^{-1.2}	4383.7555	0.243838

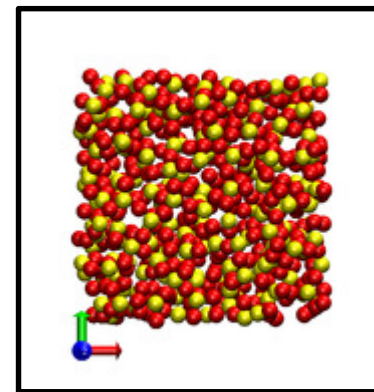
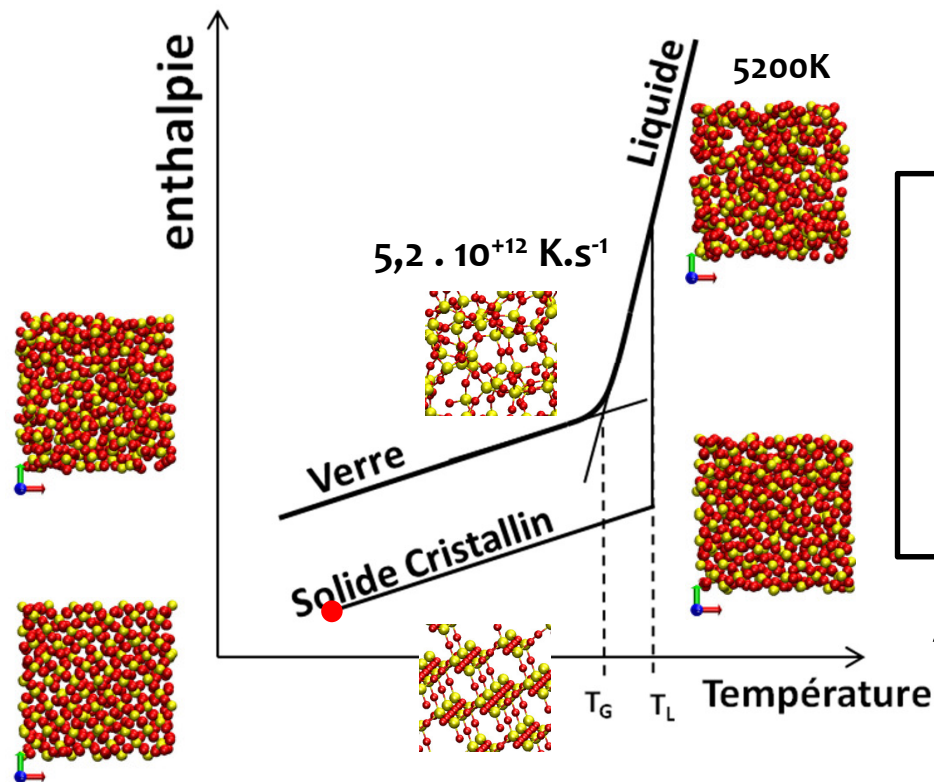
Exemple: obtention d'un verre de silice

Cristal de départ:
Cristobalite

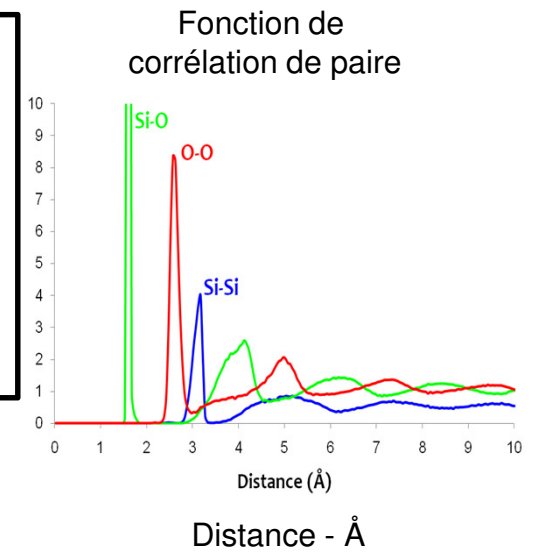
Thermostat de Nosé-Hoover:
300°K → 5200°K

Passage à l'état liquide:
Création du désordre.

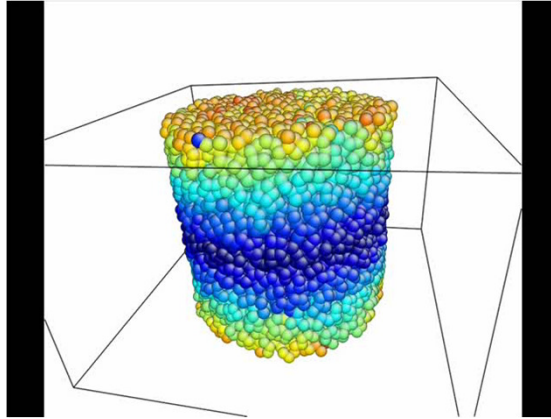
Trempe:
Obtention du verre



Animation



Quelques propriétés des matériaux amorphes: élasto-plasticité



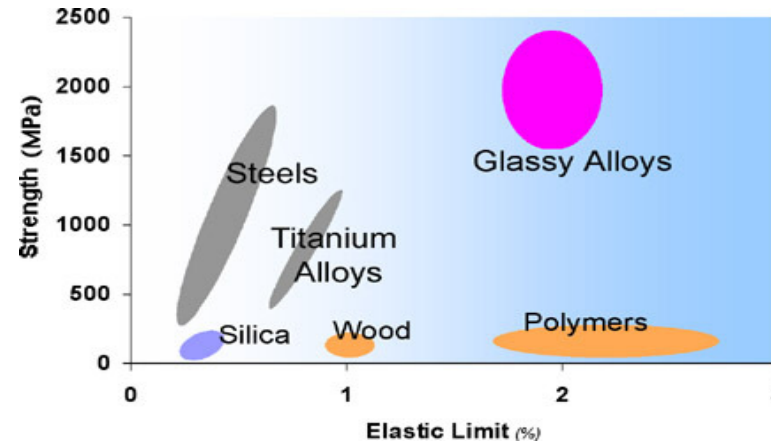
Faible rigidité:

Tableau II.-Module d'Young (E), coefficient de température ($\frac{1}{E} \cdot \frac{dE}{dT}$) et rapport de E à l'état cristallisé à E à l'état amorphe ($E_{crist.}/E_{am}$) mesurés à 20°C pour différents verres métalliques.

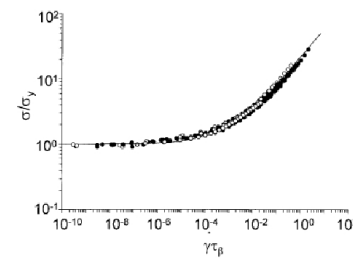
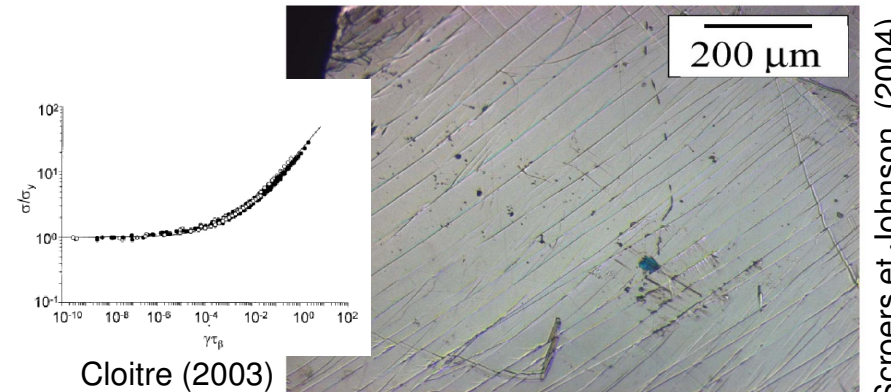
ALLIAGE	E(GPa)	$\frac{1}{E} \cdot \frac{dE}{dT} / ^\circ C (X10^4)$	$E_{crist.} / E_{am}$	Réf.
Pd ₈₂ Si ₁₈	78	- 2,9	1,28	(3)
Pd ₈₀ Si ₂₀	65	- 7,3	1,24	(26)
Fe ₈₀ P ₁₅ C ₅	124	- 3,4		(1)
Fe ₇₅ P ₁₅ C ₁₀				
- désaimanté	128	- 0,6	1,45	(3)
- aimanté à saturation	150	- 2,6	1,23	
Fe ₈₃ B ₁₄ Si _{1,5} C _{1,5}				
- brut d'hyper-trempe	130	- 0,7	1,37	
- état relaxé	91	+ 12,5	1,75	(23)
Co ₈₀ P ₂₀	105	- 2,8	1,23	(3)
Ni ₇₆ P ₂₄	95	- 9,2	1,32	(27)

$$E_{amorphe} \approx E_{crist.} / 1.3 < E_{crist}$$

Dureté très élevée:

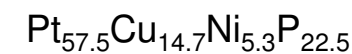


Bandes de cisaillement:



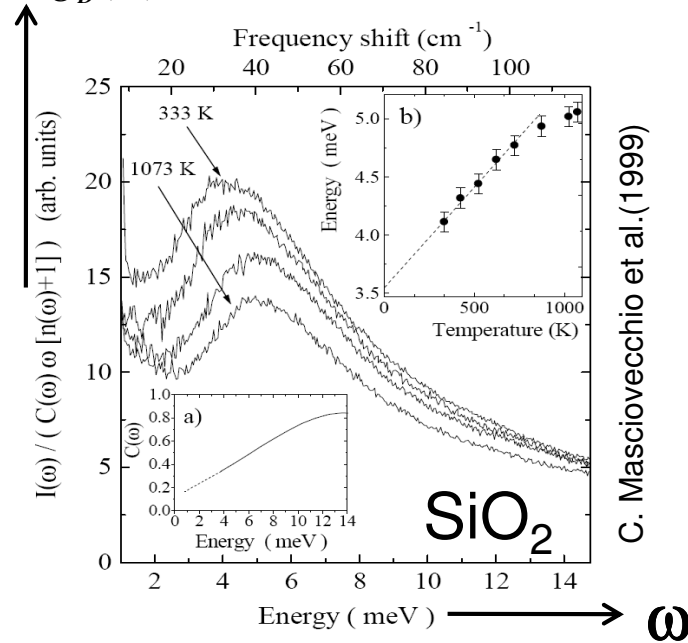
Cloitre (2003)

Scroers et Johnson (2004)



Quelques propriétés des matériaux amorphes: propagation du son

$$\frac{g(\omega)}{\omega^2} \propto \frac{g(\omega)}{g_D(\omega)}$$

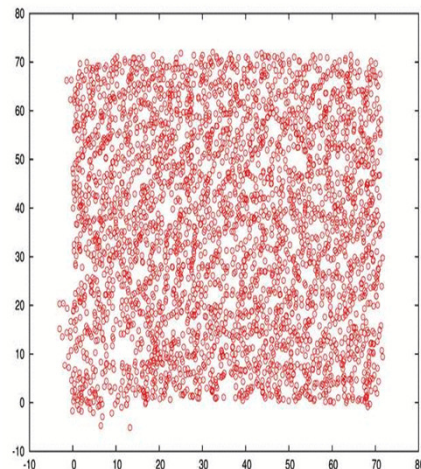
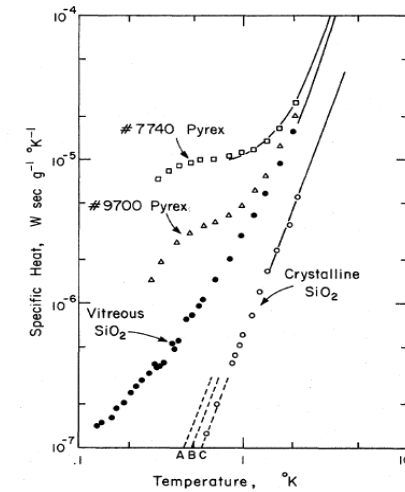


C. Masciovecchio et al. (1999)

Capacité calorifique élevée:

$$\delta Q = C_v \cdot dT$$

(densité élevée)



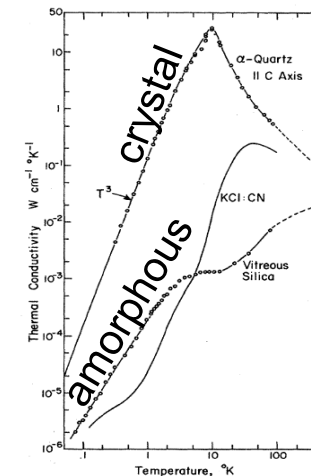
B. Mantisi et al. (2010)

Faible Conductivité thermique:

$$du / dSdt$$

$$= -\lambda \cdot dT / dx$$

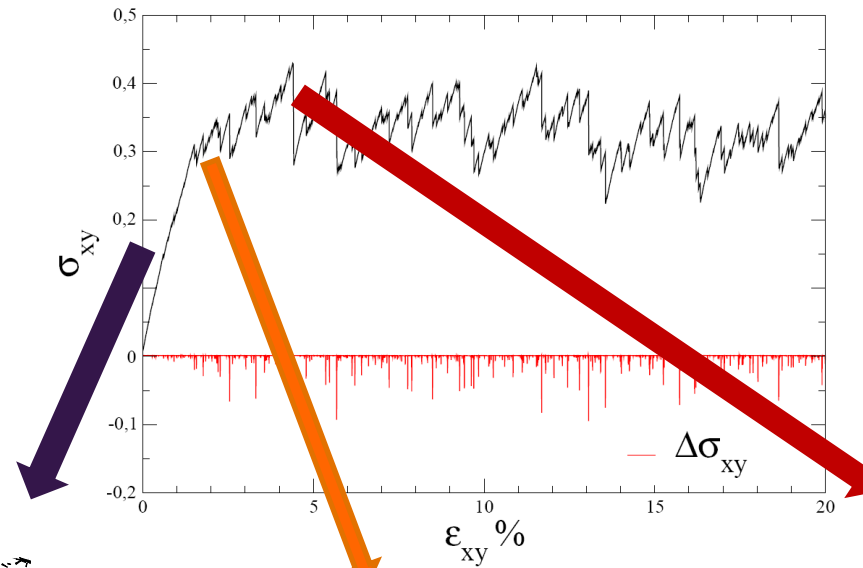
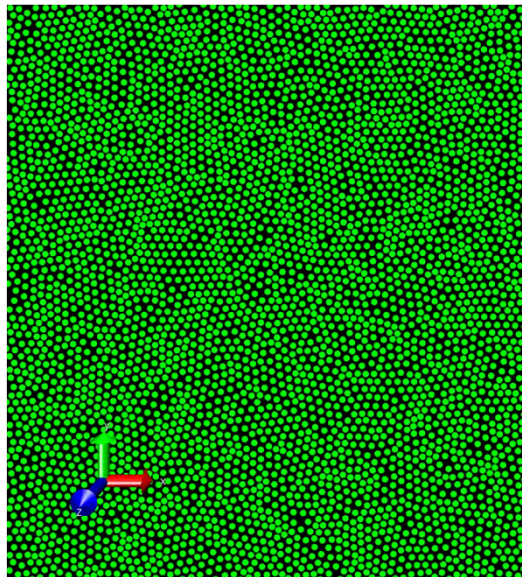
(libre parcours moyen)



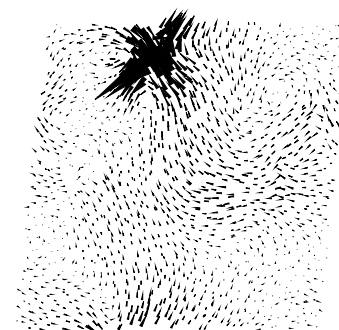
R. Zeller et R. Pohl (1971)

Verre de Lennard-Jones: Elasticité Locale

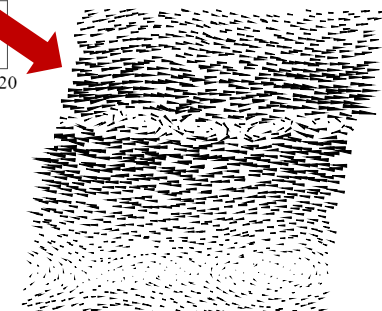
Réponse sous cisaillement d'un verre de Lennard-Jones:



Non-affine **reversible** displacements ($\times 10^3$)



Local shear **irreversible** ($\times 40$) quadrupolar event



Elementary Shear band ($\times 0.4$)

Calcul des modules d'élasticité locaux:

Cas 2D: contraintes *coarse-grained*

$$\begin{pmatrix} \delta\sigma_{xx} \\ \delta\sigma_{yy} \\ \sqrt{2}\delta\sigma_{xy} \end{pmatrix} = \begin{pmatrix} \hat{C}_{xxxx} & \hat{C}_{xxyy} & \hat{C}_{xxxy} \\ \hat{C}_{xxyy} & \hat{C}_{yyyy} & \hat{C}_{yyxy} \\ \hat{C}_{xxxy} & \hat{C}_{yyxy} & \hat{C}_{xyxy} \end{pmatrix} \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \sqrt{2}\epsilon_{xy} \end{pmatrix}$$

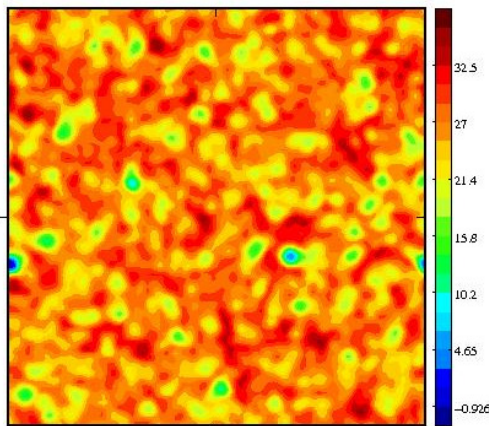
déformations

• **Isotropic case:**

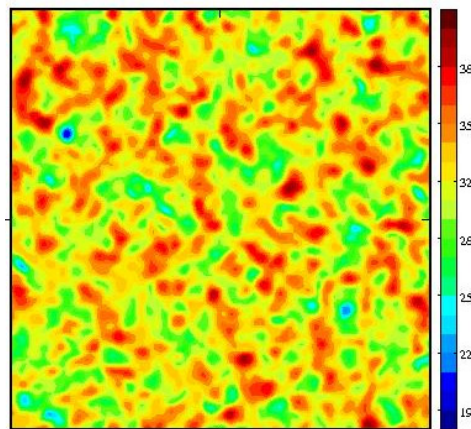
$$\hat{C} = \begin{pmatrix} \lambda + 2\mu & \lambda & 0 \\ \lambda & \lambda + 2\mu & 0 \\ 0 & 0 & 2\mu \end{pmatrix} \Rightarrow \begin{matrix} \Lambda_1 = \Lambda_2 = 2\mu \\ \Lambda_3 = 2(\lambda + \mu) \end{matrix}$$

6 inconnues $C_{\alpha\beta\gamma\delta}$ déterminées grâce à 3 déformations (**9 équations**)

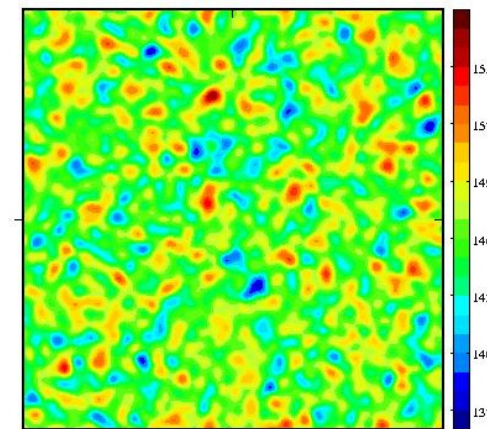
C. Goldenberg (2007)



$C_1 \sim 2\mu_1$



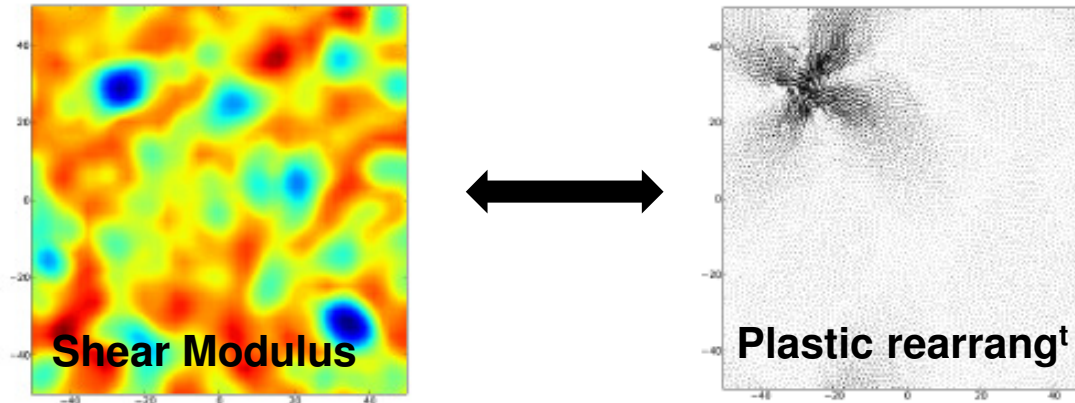
$C_2 \sim 2\mu_2$



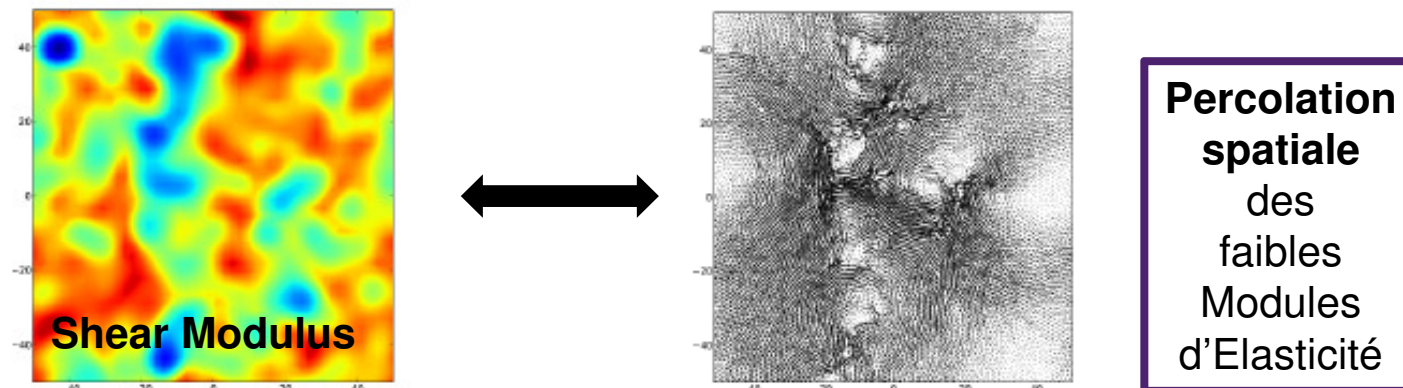
$C_3 \sim 2(\lambda + \mu)$

Modules d'élasticité locaux comme prédicteurs de la plasticité:

Réarrangement localisé (zone de cisaillement):

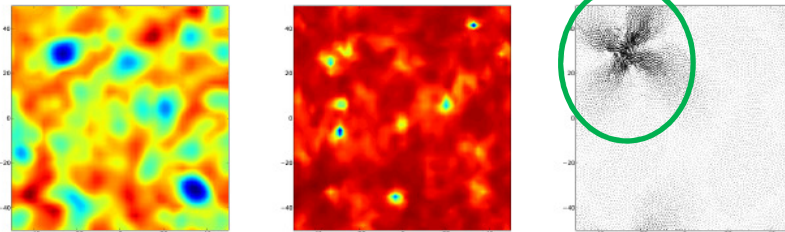


Bande de Cisaillement Élémentaire:

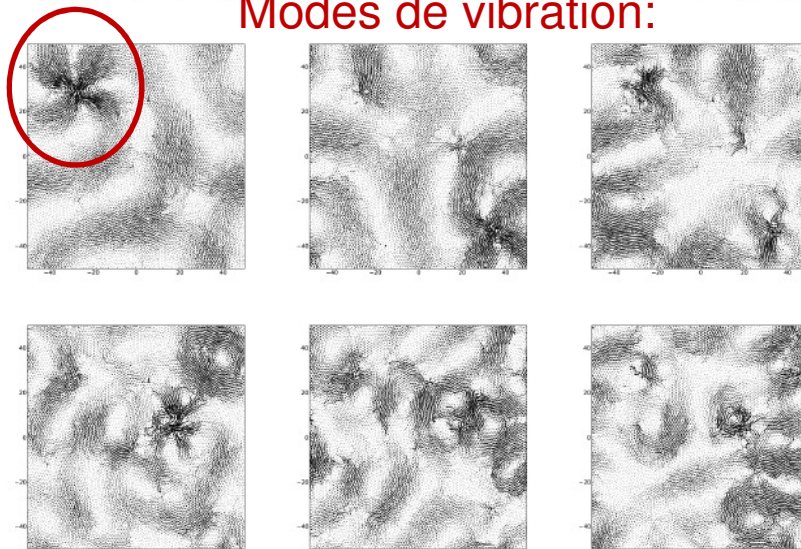


Modes de Vibration prédicteurs de la plasticité:

Réarrangement localisé:

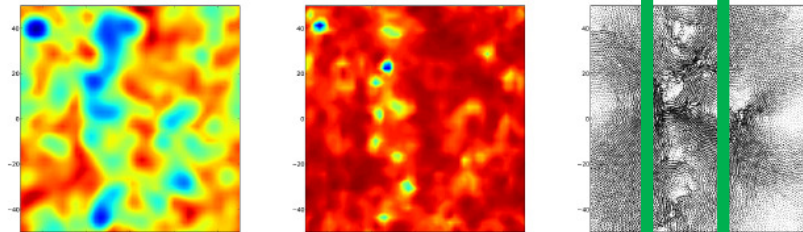


Modes de vibration:

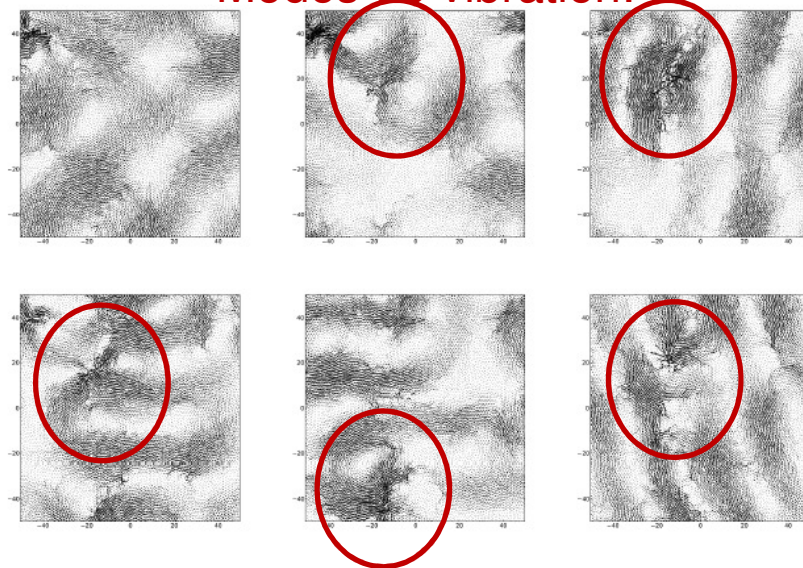


Un unique mode localisé

Bande de Cisaillement:

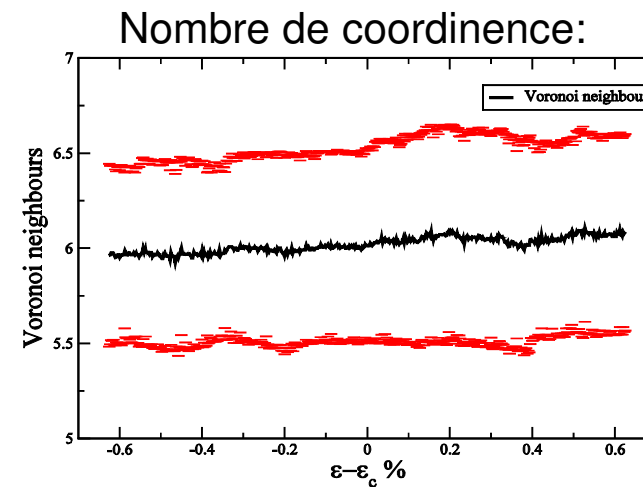
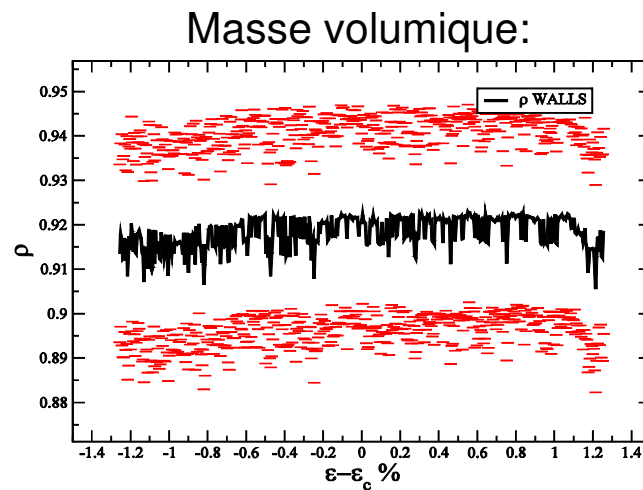
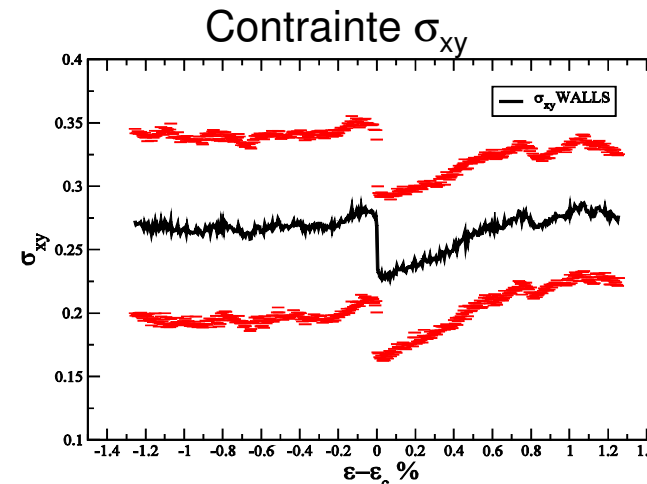
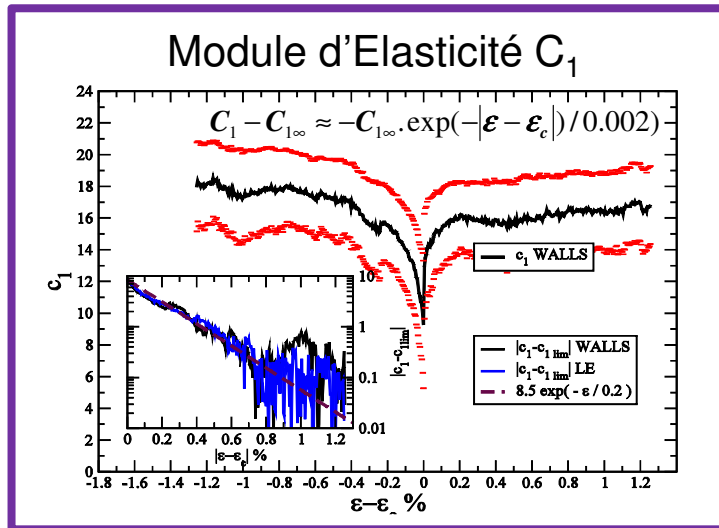


Modes de vibration:



Superposition de modes localisés

Autres prédicteurs de la plasticité (paramètres de contrôle)

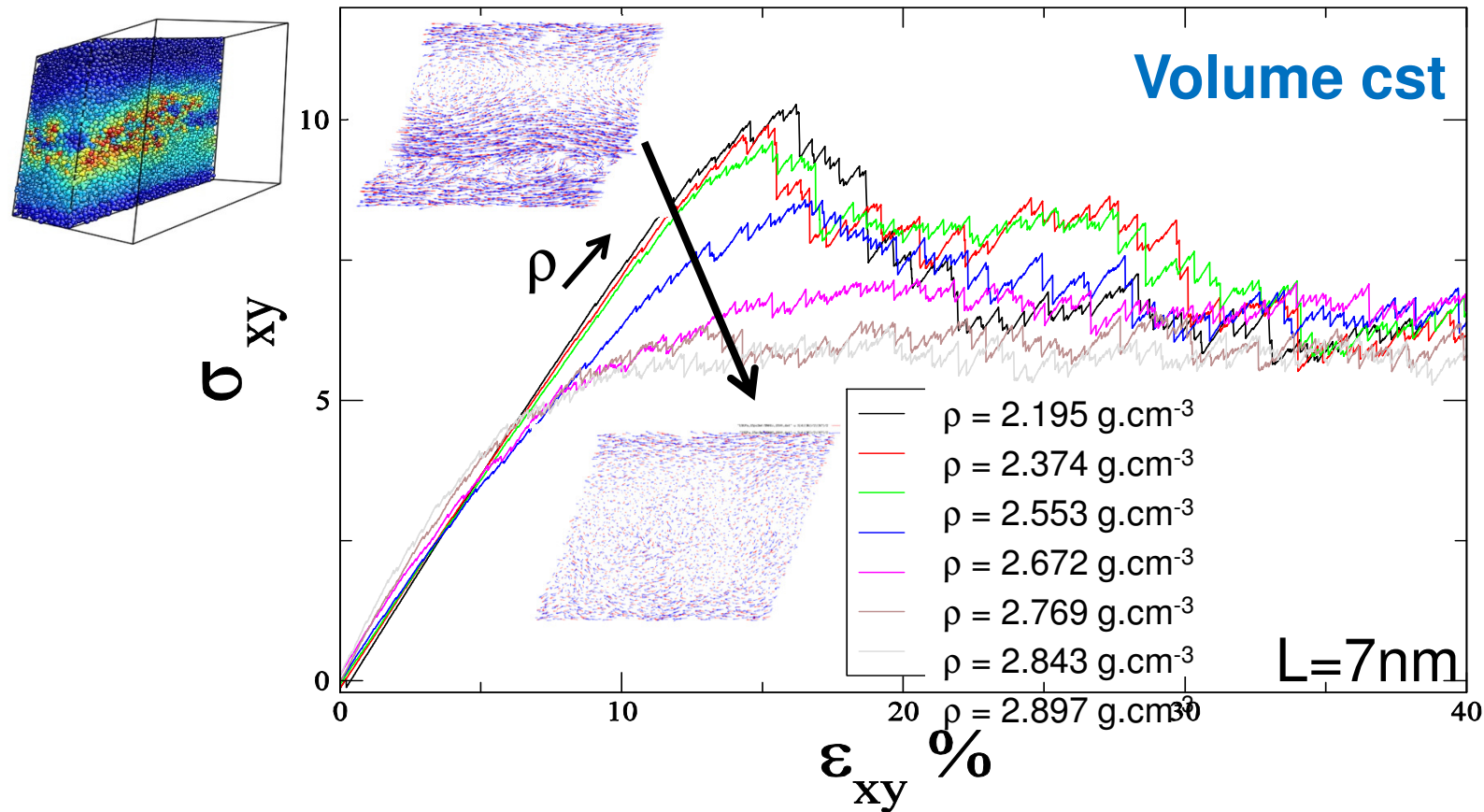


Le plus faible module d'élasticité local C_1 permet de prédire l'activité plastique

Silice SiO_2 : Effet de la pression

Cas de la silice: Effet de la pression

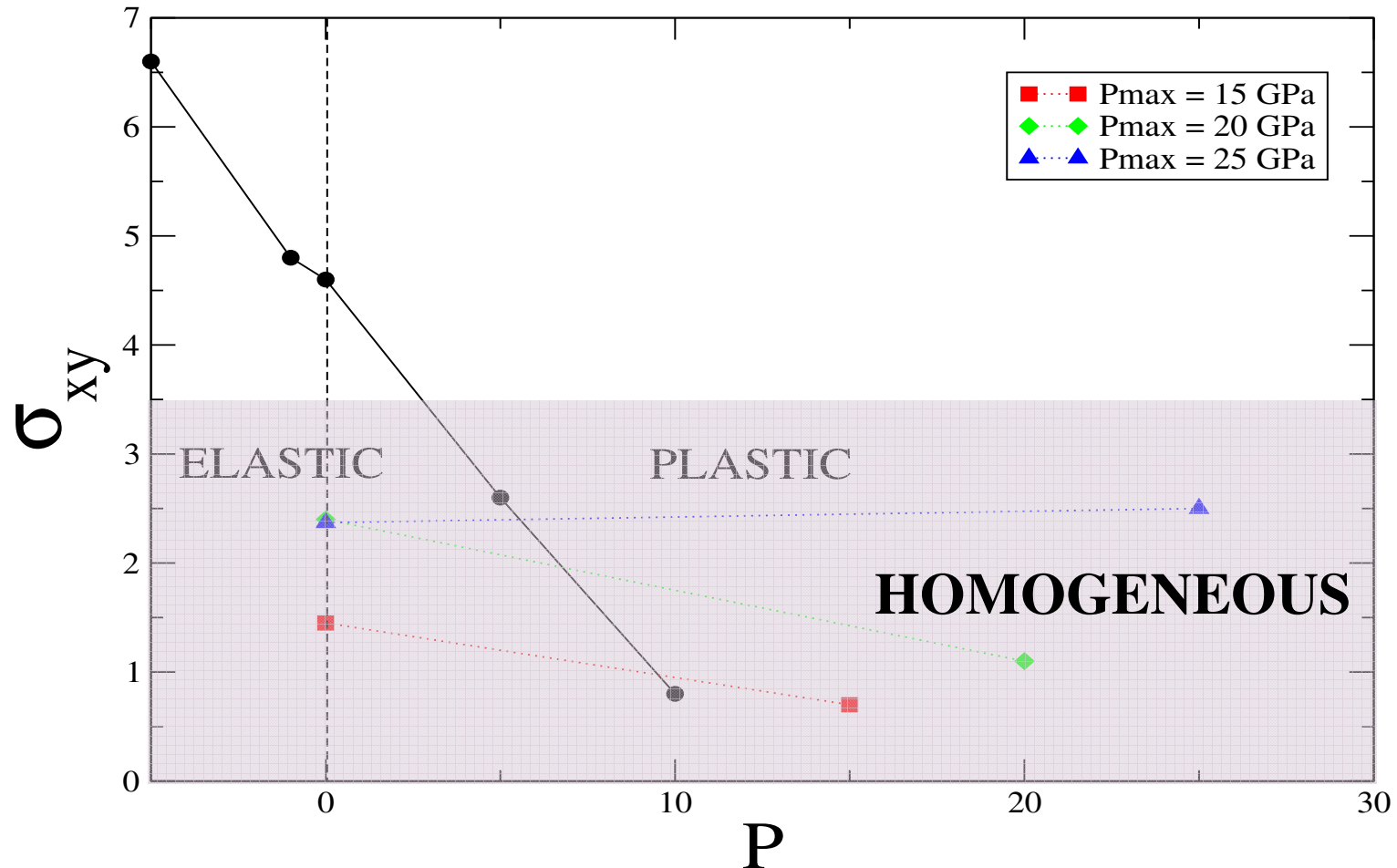
SiO₂: effet d'une densification permanente



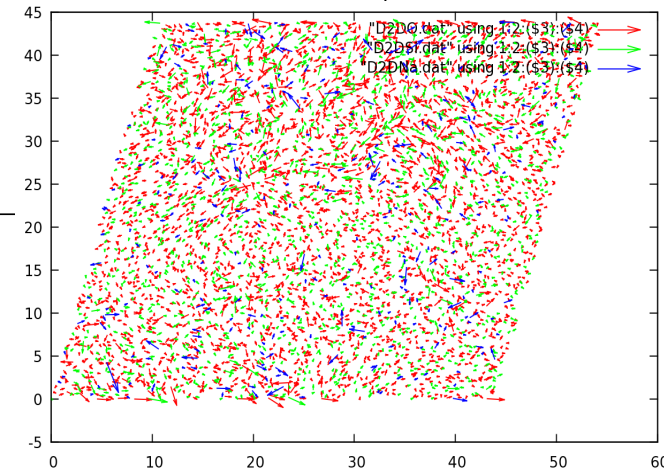
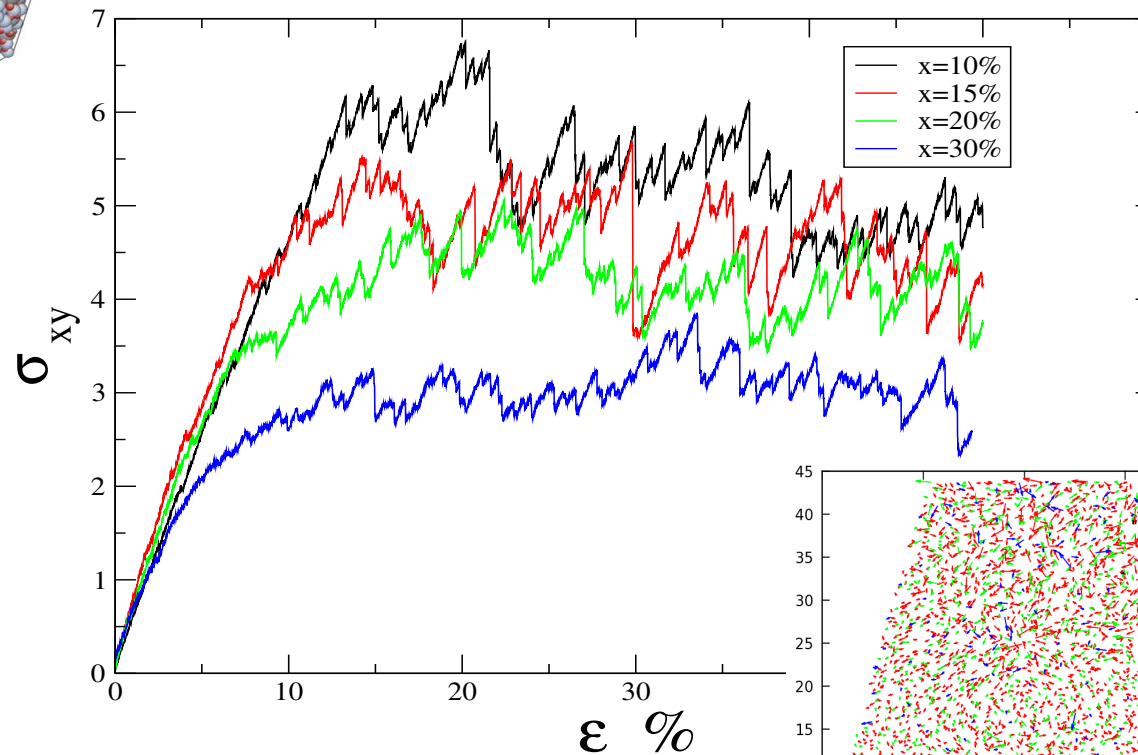
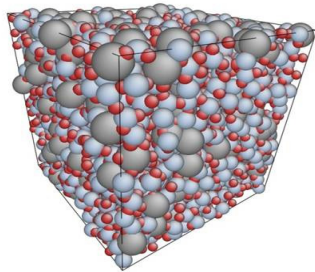
La décroissance de la **contrainte** peut être reliée à l'**inhomogénéité** de la réponse.

Courbe de charge de SiO₂:

SiO₂: Courbe de Charge

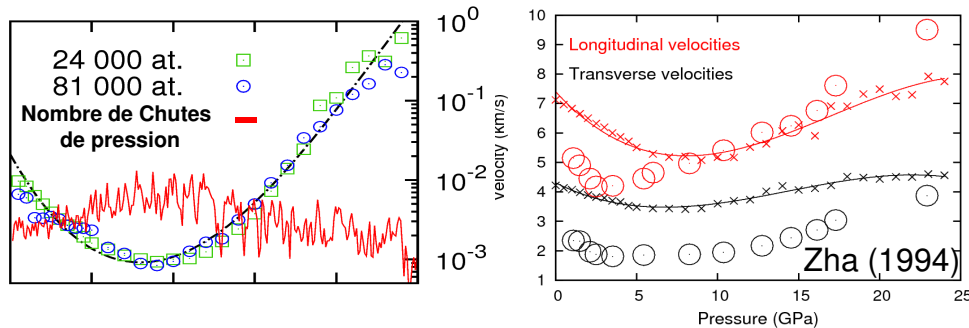
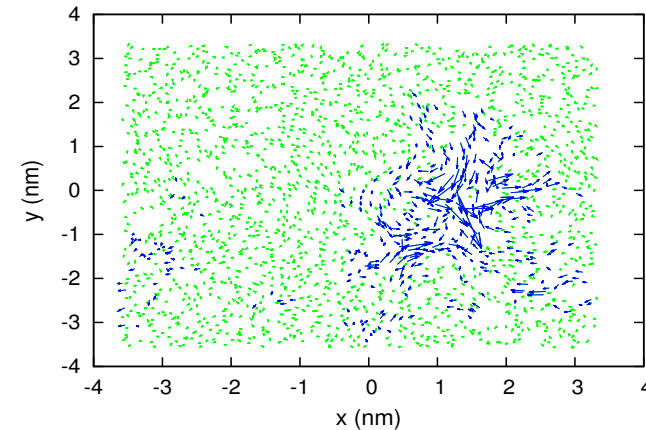
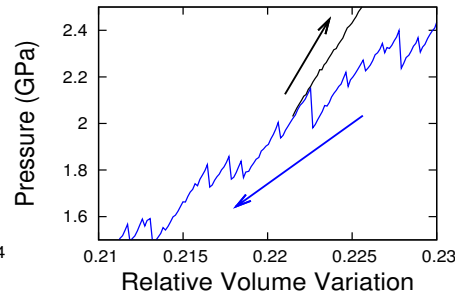
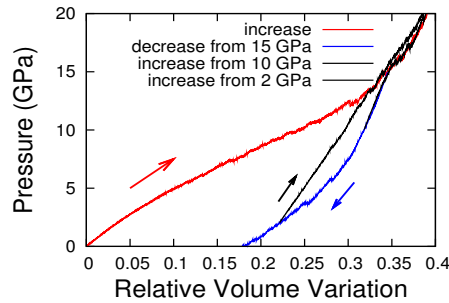
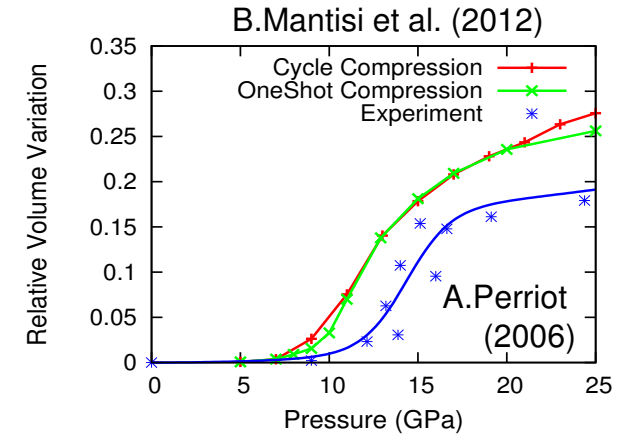
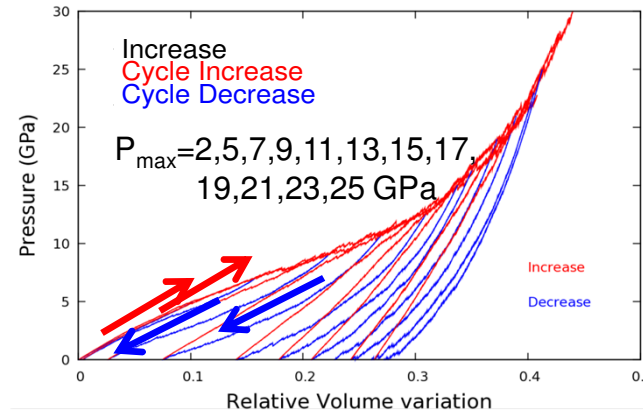
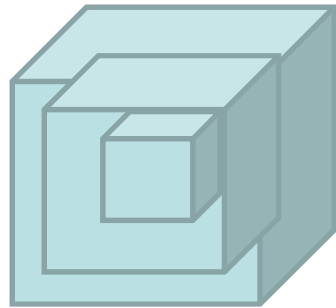


Cas des silicates: Effet de la composition



Les ions Na⁺ supportent la déformation **non-affine** de façon **homogène**.

Compression Hydrostatique de SiO₂:



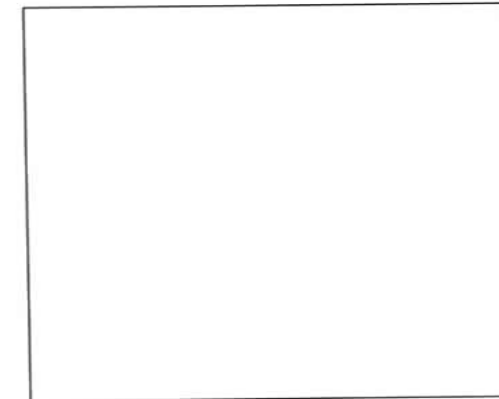
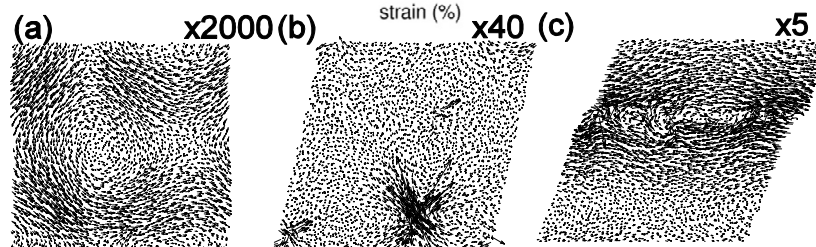
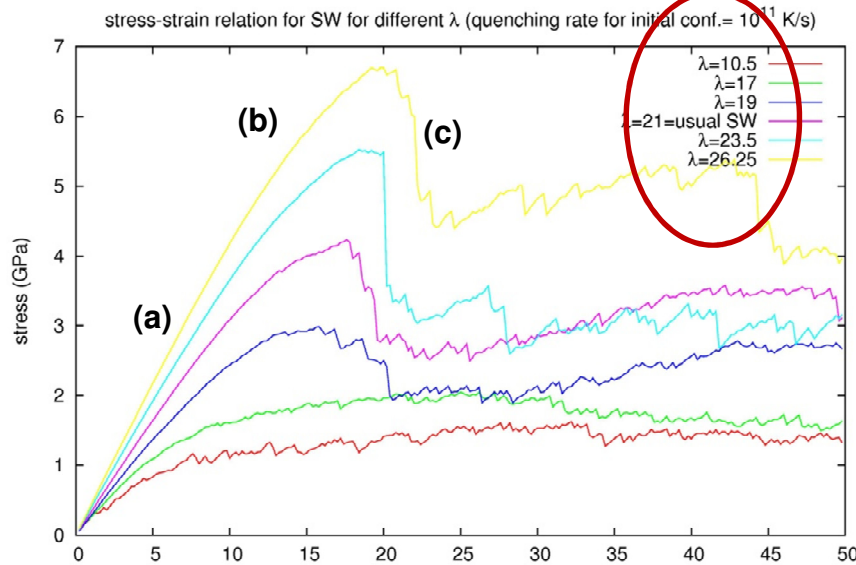
« L'anomalie élastique »
du verre SiO₂ trouve son origine
dans la micro-plasticité

Silicium Si (Stillinger-Weber): Rôle de la directionnalité des liaisons

Cas du « silicium amorphe » : effet de la directionnalité des liaisons.

a-Silicon

$$E_{SW}(1,2,\dots,N) = \sum_{(i,j)} (A \cdot r_{ij}^{-4} - B) \cdot e^{-(r_{ij}-a)^{-1}} + \sum_{i,j,k} \lambda_{ijk} \left(\cos \theta_{jik} + \frac{1}{3} \right) e^{\gamma \cdot (r_{ij}-a)^{-1} + \gamma' \cdot (r_{ik}-a)^{-1}}$$



T. Albaret (2013)

C. Fusco et al. (2010)

Cas du « silicium amorphe »: effet de la directionnalité des liaisons.

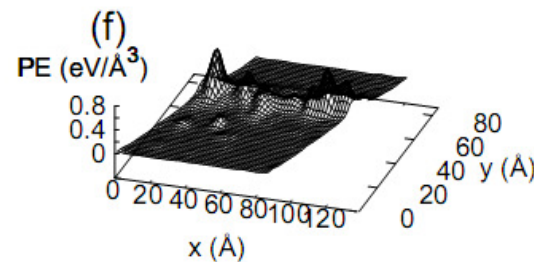
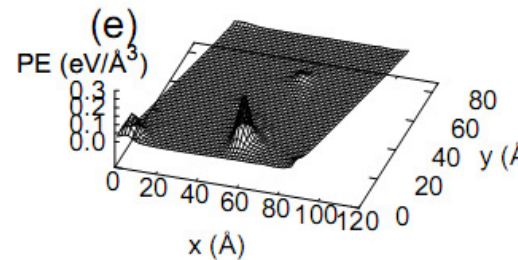
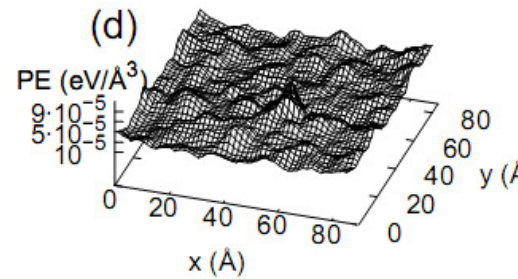
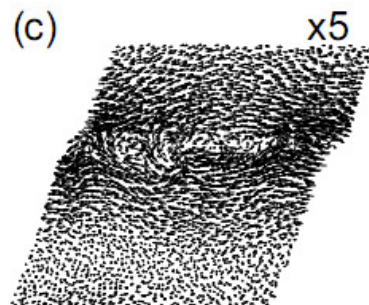
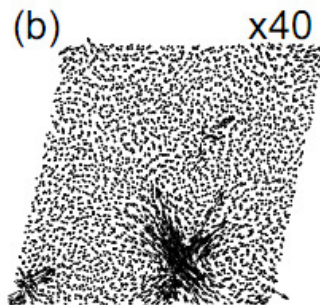
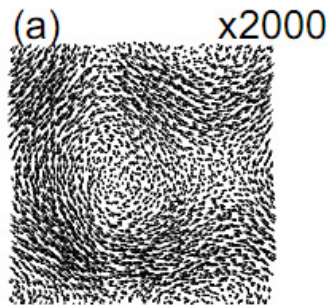


TABLE III: Yield stresses σ_Y , width of the plastic event at the yield point W and corresponding values of b obtained by using Eq. (5) for different values of λ for a A-Si system prepared with a quenching rate of 10^{11} K/s, and for different values of the quenching rate at $\lambda = 21$.

λ	ν	W (Å)	σ_Y (GPa)	$2\pi^{-1}b$ (Å)
17	0.389	6.11	2.01	1.64
19	0.365	6.11	2.80	1.75
21	0.347	5.63	4.23	1.75
23.5	0.347	5.13	5.47	1.67
26.25	0.331	4.73	6.64	1.59
40	0.318	4.57	10.13	1.59
quench. rat	0.273	W (Å)	σ_Y (GPa)	b (Å)
10^{11} K/s		5.63	4.23	1.75
10^{12} K/s		5.39	3.53	1.61
10^{13} K/s		5.39	3.0	1.56
10^{14} K/s		5.30	2.32	1.45

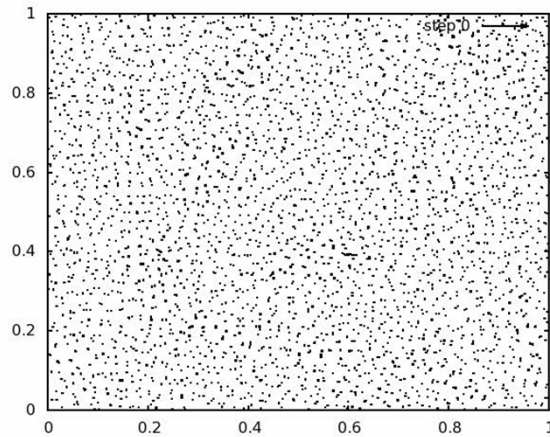
width

Contrainte de Peierls:

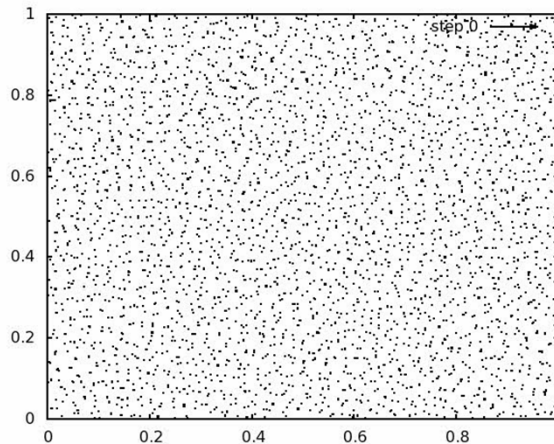
$$\sigma_{xy}^* = A e^{-2\pi W/b}$$

where $A = 2C_{44}/(1 - \nu)$

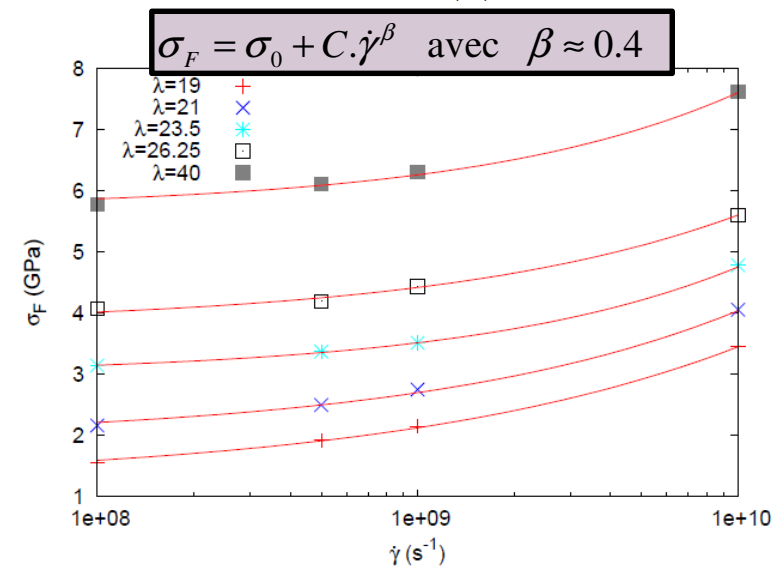
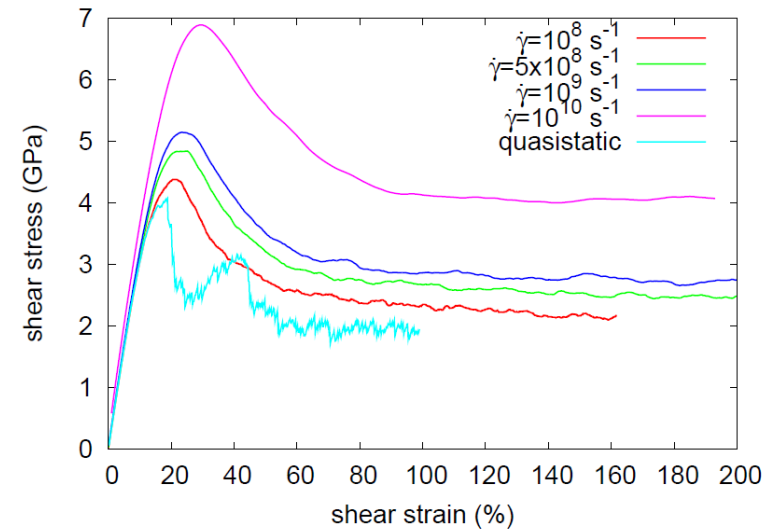
Cas du « silicium amorphe » : Effet du taux de cisaillement.



10^{+8}s^{-1}



10^{+10}s^{-1}

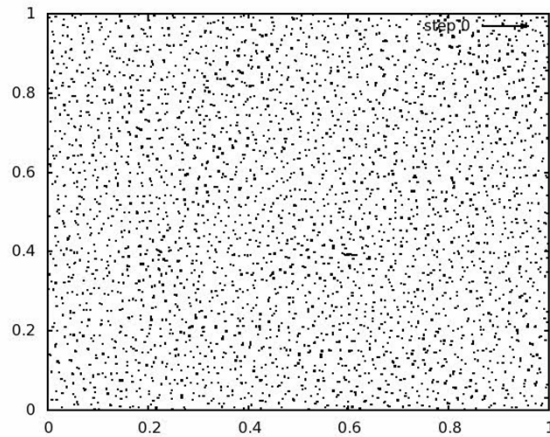


Cas du « silicium amorphe » : Effet du taux de cisaillement.

$$\sigma_F = \sigma_0 + C \cdot \dot{\gamma}^\beta \quad \text{avec } \beta \approx 0.4$$

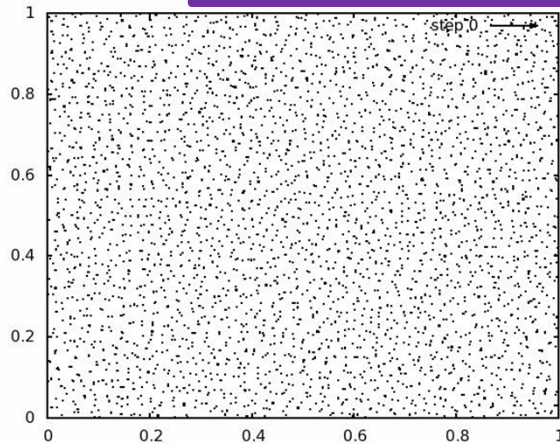
Incoherent Intermediate Scattering Function:

$$F_s(\vec{q}, t) = \frac{1}{N} \sum_j \langle \exp[i\vec{q} \cdot [\vec{r}_j(0) - \vec{r}_j(t)]] \rangle \sim \exp(-(t/t_{rel}(\dot{\gamma}))^{b(T)})$$

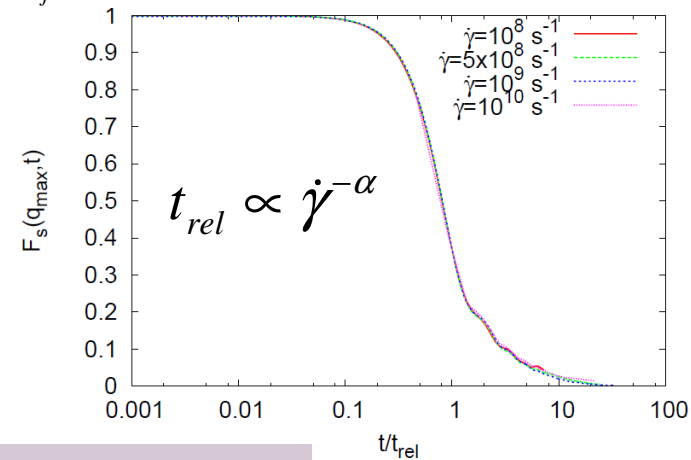


10^{+8} s^{-1}

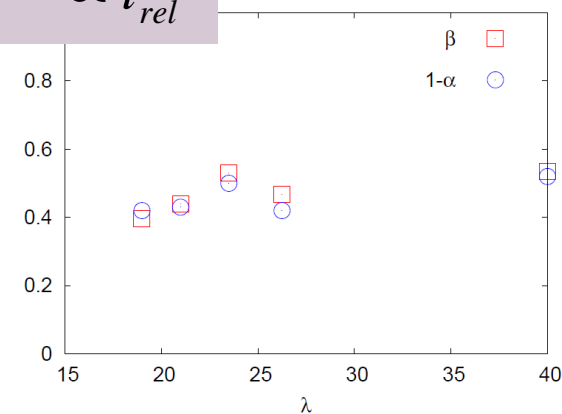
La viscosité anormale résulte de la dynamique locale.



10^{+10} s^{-1}

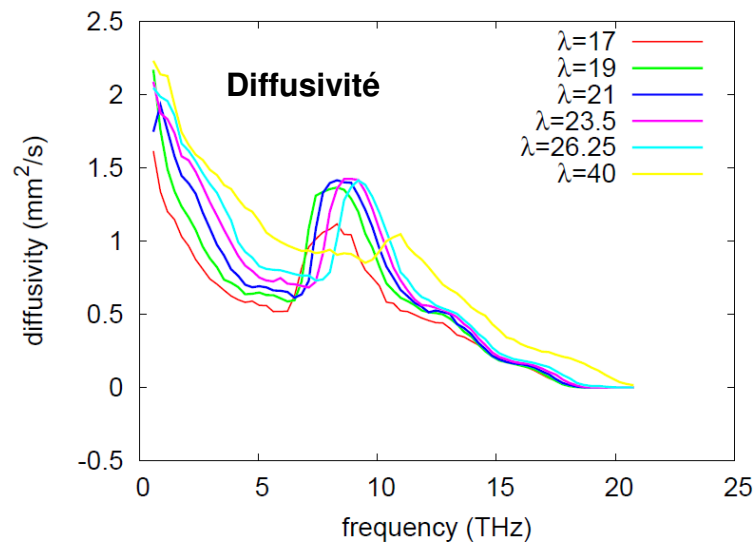
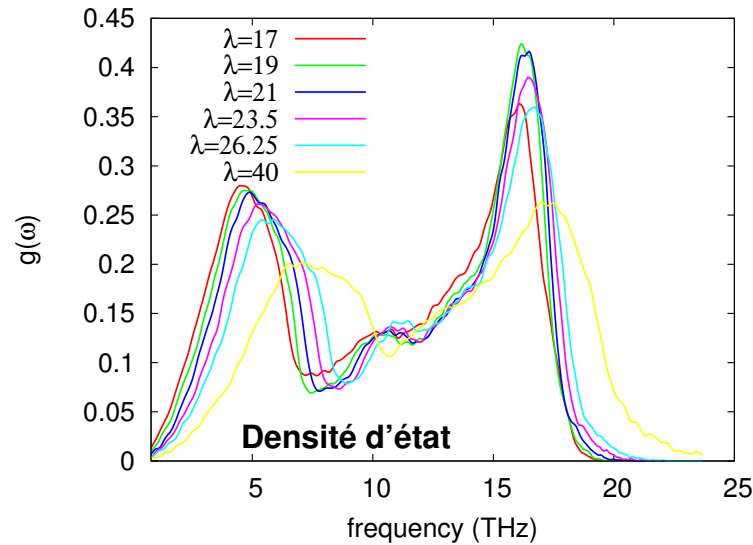


$$\eta \propto \sigma_F / \dot{\gamma} \propto \dot{\gamma}^{\beta-1} \propto t_{rel}$$

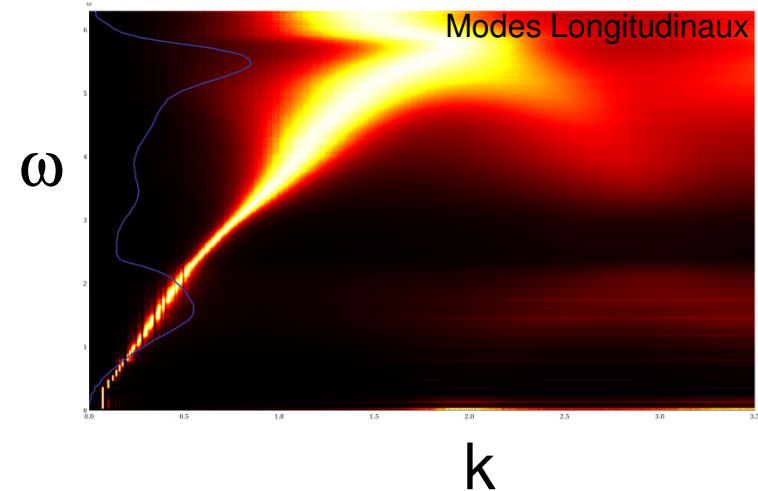
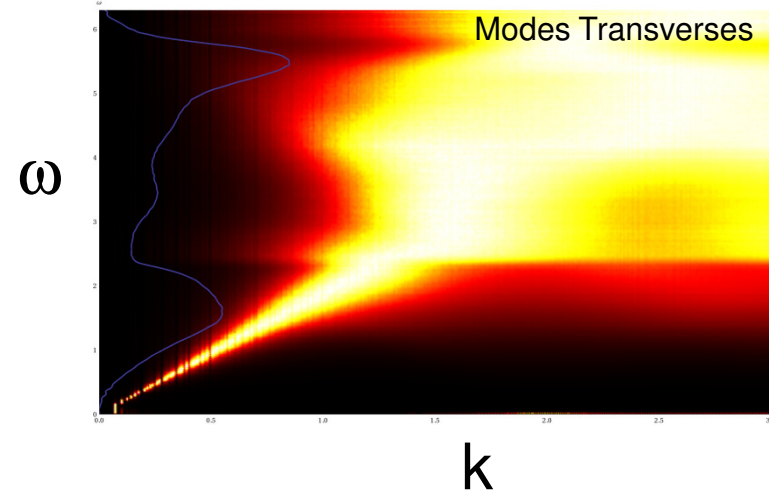


Cas du « silicium amorphe »:

Modes de Vibration.

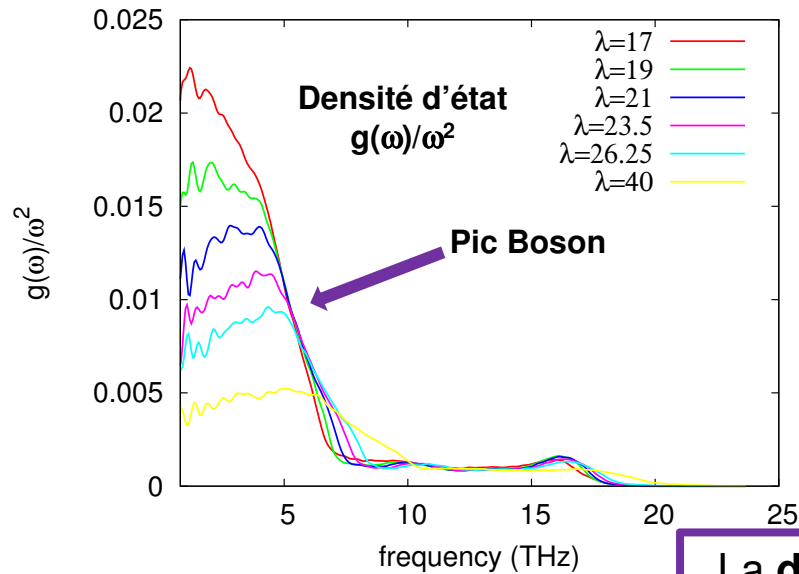


$$S(\mathbf{q}, \omega) = \frac{2}{NT} \left| \sum_{i=1}^N e^{-i\mathbf{q}\mathbf{r}_i} \int_0^T u(\mathbf{r}_i, t) e^{i\omega t} dt \right|^2$$

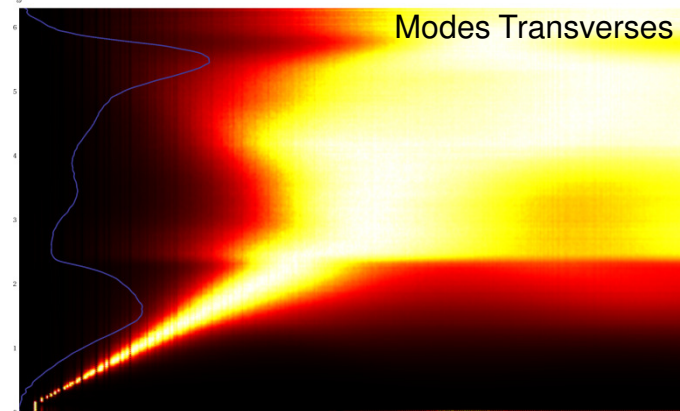


Cas du « silicium amorphe »:

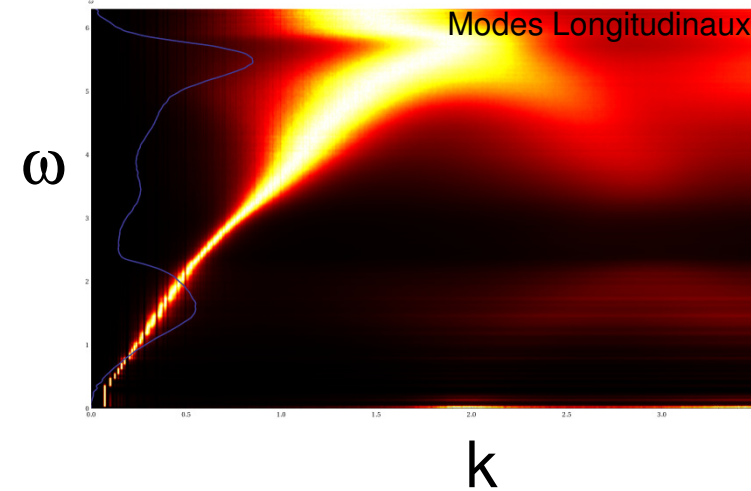
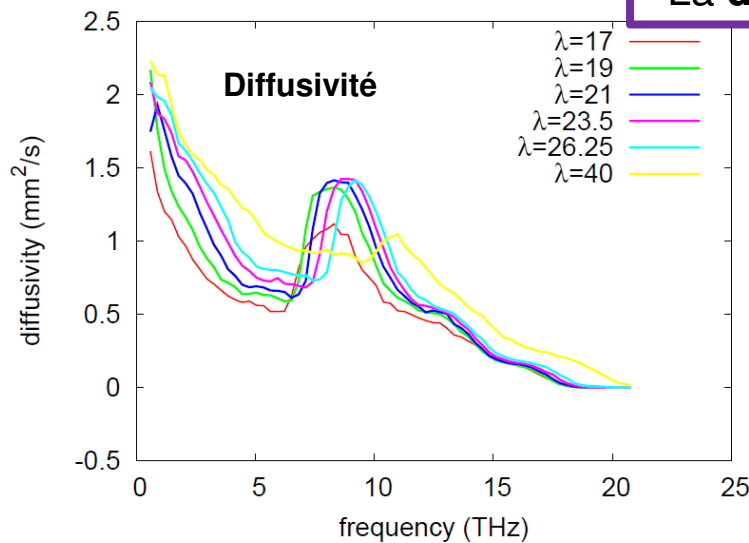
Modes de Vibration.



$$S(\mathbf{q}, \omega) = \frac{2}{NT} \left| \sum_{i=1}^N e^{-i\mathbf{q}\mathbf{r}_i} \int_0^T u(\mathbf{r}_i, t) e^{i\omega t} dt \right|^2$$



La densité d'état reflète la diversité des modes.



Conclusion

Analyse du comportement **mécanique** vs. **dynamique locale**

Importance des **hétérogénéités** de déformation.

Identification des **réarrangements** caractéristiques.

Organisation **spatiale** des modules d'élasticité locaux.

Sensibilité à la **contrainte extérieure** (pression, cisaillement..)

Réponse acoustique dépendant des **interactions**.

Modes de vibration **quasi-localisés**. Diffusons.

Prédiction de l'endommagement plastique.

Le rôle des **défauts structuraux** dépend des interactions.

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