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Claudio Fusco

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# Small-scale mechanical response and vibrational properties of amorphous silicon

C. Fusco<sup>a</sup>, A. Tanguy<sup>a</sup>, T. Albaret<sup>a</sup>, Y. M. Beltukov<sup>b</sup>, D. A. Parshin<sup>c</sup>

a. Institut Lumière Matière, UMR 5306, Université Lyon 1-CNRS, 69622 Villeurbanne cedex, France

b. Ioffe Physical Technical Institute, 194021 St Petersburg, Russian Federation

c. Saint Petersburg State Polytechnical University, 195251 Saint Petersburg, Russian Federation

## Résumé :

Nous présentons une étude numérique de la réponse mécanique du silicium amorphe par des simulations de dynamique moléculaire à la fois dans le régime de cisaillement quasi-statique et à des taux de cisaillement finis. Nous considérons l'influence de l'ordre local sur la réponse plastique du système en faisant varier le poids relatif du terme à 3 corps de l'interaction locale. Dans le cas quasi-statique, nous constatons que la loi de comportement est fortement affectée par l'ordre local. A taux de cisaillement finis, nous observons que la contrainte d'écoulement dans le régime plastique suit une réponse Herschel-Bulkley : un comportement en loi de puissance en fonction du taux de cisaillement. L'exposant de cette loi de puissance ne dépend guère de l'ordre local. Enfin, nous analysons la densité d'états vibrationnels (VDOS). On observe un pic de boson, i. e. une augmentation de la VDOS à basse fréquence, surtout pour les systèmes ayant un faible degré d'ordre local.

## Abstract :

We present a numerical study of the mechanical response of amorphous silicon through Molecular Dynamics simulations both in the quasi-static shear regime and at finite shear rates. We consider the influence of the local order on the plastic response of the system by varying the relative weight of the 3-body term of the local interaction. In the quasi-static case we find that the global stress-strain behaviour is strongly affected by the local order. At finite shear rates we observe that the average flow stress in the plastic regime follows a Herschel-Bulkley response, i. e. a power-law behaviour as a function of the shear rate. The exponent of this power law only slightly depends on the local order. Finally we analyze the vibrational density of states (VDOS). A boson peak, i. e. an enhancement of the low-frequency VDOS, is observed, especially for the systems with a lower degree of local order.

**Mots clefs :** amorphous materials ; plasticity ; vibrational properties

## 1 Introduction

The microscopic origin of plastic deformation in amorphous solids is not so well understood as plasticity in crystals. While in crystals it can be described in terms of dislocations, for amorphous materials the nature of defects, their spatial organization and their interaction is still a matter of debate. The aim of this study is to examine the elasto-plastic response of a model glass in the athermal limit, with the help of classical simulations both in the quasi-static regime and at finite shear rate. We analyze the effect of the local order on the plastic response and on the vibrational density of states of the system.

## 2 Plastic response

We consider a model amorphous silicon consisting of 32768 atoms contained in a cubic box with lengths  $L_x = L_y = L_z$  of approximately 87 Å. It is described through empirical interactions with 2 and 3-body interactions, and is submitted to an external shear. Tuning the prefactor  $\lambda$  of the 3-body

contribution in the interatomic interaction allows us to study the systematic effect of local order and directionality of the bonds on the mechanical response of the system. The shear is applied both in a quasi-static manner and with a finite shear rate and we perform Molecular Dynamics simulations. More details about the model and the preparation of the amorphous state can be found in Ref. [1].

The stress-strain relationship is shown in Fig. 2(a) for the quasi-static case. We can see that the local order has a strong influence on the elastic and plastic response. The global behaviour is very smooth for low  $\lambda$  and tends to be rather erratic with a very pronounced yield point by increasing  $\lambda$ . The stress drops correspond to localized particle rearrangements (plastic events) and the large jumps in the stress-strain curve are often associated to the occurrence of shear bands. The shear modulus, corresponding to the slope of the linear part at low stresses, increases with  $\lambda$ .

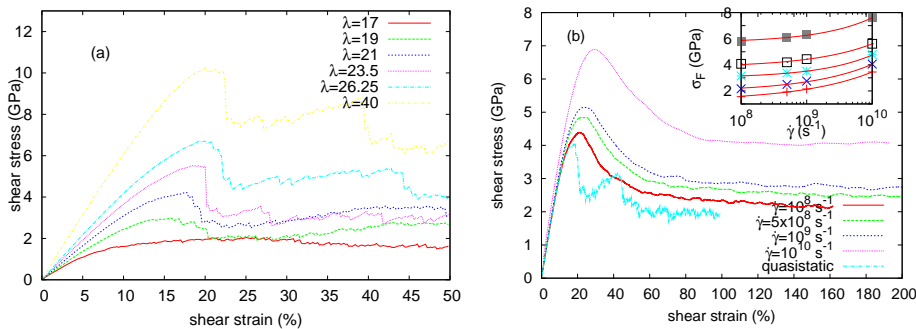


FIGURE 1 – Stress strain relationship for (a) the quasi-static for different values of  $\lambda$  and (b) for different shear rates with  $\lambda = 21$ . The inset in (b) represents the flow stress as a function of the shear rate for different values of  $\lambda$  ( $\lambda = 19, 21, 23.5, 26.25, 40$ ), where the lines are fits according to the Herschel-Bulkley law.

The behaviour at finite shear rates at a fixed value of  $\lambda$  is much smoother than for the quasi-static case, as it can be seen in Fig. 2(b), since in the latter the effects due to plastic collective rearrangements of atoms are more pronounced. In order to quantify the effect of the shear rate  $\dot{\gamma}$  on the flow behaviour of the system we plot the flow stress  $\sigma_F$ , defined as the average of the macroscopic stress in the plastic plateau, as a function of the shear rate  $\dot{\gamma}$  in Fig. 2(b) for different values of  $\lambda$ . A typical nonlinear flow curve following a Herschel-Bulkley behaviour, of the type  $\sigma_F = \sigma_0 + C\dot{\gamma}^\beta$ , is observed.

### 3 Vibrational density of states

In order to characterize the vibrational properties of the system we have calculated the vibrational density of states  $g(\omega)$  by using the Kernel Polynomial Method [2]. Plotting  $g(\omega)/\omega^2$  we see deviations from the Debye behaviour, with the occurrence of a peak at  $\omega_0 \sim 1$  THz which is more pronounced for low values of  $\lambda$ . We observe a systematic increase of  $\omega_0$  with  $\lambda$ . This anomaly can be possibly associated to the so-called boson peak and its origin is currently under investigation.

### 4 Conclusions

We have shown that the mechanical response of a model amorphous system at small scales is strongly affected by the local order and that the global mechanical behaviour is connected to microscopic particle rearrangements. In particular, the nonlinear dependence of the flow stress on the shear rate is linked to local relaxation dynamics. Our results can also be of interest for colloidal systems and yield stress fluids.

### Références

- [1] Fusco, C., Albaret, T., Tanguy, A. 2010 *Phys. Rev. E* **82** 066116
- [2] Beltukov, I.M., Kozub, V.I., Parshin, D.A. 2013 *to be published in Phys. Rev. B*