Stress response of 2D silica under quasi-static tension

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We use classical molecular dynamics simulations to generate topologically different models of vitreous 2D silica, all of which are subjected to quasi-static tensile loading until fracture occurs. We demonstrate the effects of structural disorder on the material behaviour of 2D silica. For each sample, we determine the network structure by identifying the relative count of single rings and so-called ring triplets each of which composed of three adjacent rings that share a common corner. In each sample, we spatially detect the first local atomic-scale rearrangement during deformation and correlate it to the ring triplet involved.

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1 Introduction

The synthesis of vitreous two-dimensional (2D) silica and its imaging using scanning microscopy allowed for a clear picture of the structural characteristics of the random network model of glasses [1]. 2D silica consists of two identical layers whose elementary units are [SiO$_4$] tetrahedra, each of which has three common corners with adjacent tetrahedra in the same layer, while the fourth corner acts as a bridge between the top and bottom layer, as depicted in Figure 1a. In each layer, the variable inter-tetrahedral angle introduces structural disorder resulting in rings of different sizes. The size of a ring denotes the number of Si atoms the ring is composed of, e.g. a six-membered ring contains six Si atoms. Ring triplets are defined as three rings, sharing a common Si atom. The network topology is, thus, characterised by the count of single rings of particular size and the ring triplet statistics.

Considerable efforts have been devoted to analyse 2D silica and provide further steps towards the understanding of the structural and mechanical properties that paves the way for possible applications [1]. From both experiments and molecular dynamics studies it is well known that the deformation and fracture behaviour of glasses strongly depend on the underlying network topology [2–4]. Atomic-scale rearrangements are, generally, accepted as the elementary events for plastic deformation in glasses [5]. Using the concept of the potential energy landscape (PEL), the relationship between structural features and the deformation behaviour of glasses can effectively be illustrated. It terms of the PEL, the initially relaxed and undeformed glass is trapped inside a basin (local minimum). When applying external load the glass is forced to jump into another basin involving dissipative localised atomic rearrangements, as shown in Figure 1b.

In the present study we investigate the plastic deformation of 2D silica under athermal quasi-static deformation. Our main objective is to address the correlation between structural rearrangements and the network topology determined by the ring and triplet statistics.

2 Computational details

In this work, we use classical molecular dynamic simulations in the absence of thermal effects. We prepare a set of vitreous 2D silica models starting from a hexagonal monolayer. Using a Monte Carlo bond-switching algorithm, randomly selected Si-O-Si bonds in the hexagonal lattice are rotated by 90 degrees around the centre O atom. After each bond switch the system energy is minimised. This method generates a periodic vitreous monolayer consisting of fully coordinated atoms. The monolayer Si bonds in the hexagonal lattice are rotated by 90 degrees around the centre O atom. After each bond switch the system energy is minimised. This method generates a periodic vitreous monolayer consisting of fully coordinated atoms. The monolayer is built using a Yukawa-type potential function employed by Roy et al. [6] in order to simulate the network formation of silica in two dimensions. Finally, the switched monolayer is duplicated and the Si atoms of the upper and lower layers are bridged via O atoms yielding a vitreous silica bilayer. For the subsequent mechanical loading in three dimensions we use a Stillinger-Weber type potential function that has been used widely, and, shown to reproduce the structural arrangement and mechanical behaviour of both bulk [2–4] and 2D silica [5].

We perform the mechanical deformation in the athermal quasi-static (AQS) regime. The AQS deformation protocol consists of incremental application of uniaxial tensile deformation and energy minimisation between the increments in order to remove all thermal fluctuations. Thus, we investigate the effects of pure structural disorder in the network. We consider 100 topologically different samples, each of which contains 2016 atoms. Tensile deformation is applied in small strain increments of $10^{-4}$ followed by energy minimisation using the conjugate gradient algorithm with an energy tolerance of $10^{-17}$ eV.

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3 Results and discussion

In order to investigate the effects of structural disorder in 2D silica under mechanical loading, we apply AQS deformation via energy minimisation at constant volume after each deformation increment. For two representative samples A and B, the corresponding stress response is shown in Figure 1c. The stress-strain curves show different regimes. They are made of elastic segments intersected by discontinuous stress drops that correspond localised atomic rearrangements and are referred to as avalanches.

For both samples the stress increases to a maximum value (tensile strength) followed by gradual decrease, and, finally, drops to zero. However, belonging to different network topologies, the stress response of sample A and B exhibit clear differences. Both the number of rearrangements and the strain at which they occur vary. Furthermore, the maximum stress and the maximum strain for each sample are different. The above results are all in line with studies on bulk silica, whose stress-strain relation has been shown to significantly depend on the network structure [2].

For each sample, we now focus on the first rearrangement associated with dissipative behaviour. We identify the site of each first rearrangement, more precisely, we count the respective triplet that are involved in the first rearrangement. The corresponding count of each triplet is given in Table 1. It is apparent that triplets composed of medium-sized rings are involved more frequently in the first rearrangement. In comparison, triplets that include large rings, i.e. eight- or nine-membered rings, are less involved.

Table 1: Count of ring triplets that are involved in the first rearrangement for a total number of 100 samples. The label 567, for instance, describes a triplet that is made of a five-, six- and seven-membered ring.

| Triplet | 568 | 567 | 667 | 577 | 677 | 678 | 888 | 688 | 569 | 668 |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Count [%] | 17.2 | 15.6 | 15.6 | 14.1 | 10.9 | 9.4 | 4.7 | 4.7 | 4.7 | 3.1 |

In conclusion, we used of a Monte Carlo bond-switching algorithm to generate samples of vitreous two-dimensional silica with different network topologies. We imposed mechanical loading in the athermal quasi-static regime and demonstrated that topologically different samples show different stress-strain relation. We determined the ring and triplet counts in each sample. We identified that, under deformation, triplets composed of large rings are rarely involved during the first rearrangement. However, further studies should focus on a more comprehensive and systematic investigation of possible correlations between triplet energies and rearrangements.

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