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Electronic Supplementary Material:

Reduced Hydrogen diffusion in strained amorphous SiO2: understanding ageing in MOSFET devices†

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Negative Bias Temperature Instability (NBTI) is one of the main ageing process in MOSFET devices, and it is related among others to the *H* diffusion within the SiO_2 dielectric layer of the device. In this work we use molecular simulations to study the underlying mechanism that governs diffusion of H within SiO_2, and suggest how to modify the material to decrease it. The computed diffusion activation energies are in excellent agreement with existing experi- mental data, and the analysis of the diffusion paths reveals a *H* hopping mechanism governed by the same orientational constraints as proton exchange in bulk water. Based on this mechanism, we test an hypothetical NBTI ageing retarding modification based on a mechanical deformation of the SiO_2 dielectric. Stretching the material induces a rearrangement of the silicate units, increasing the O-O distance, and consequently the activation energy required for *H* diffusion. Hence, stretching the semiconductor during the MOSFETs manufacturing process could reduce significantly the NBTI-based ageing of the devices.

Guttman's Ring Analyses

Ring analyses is a useful method to compare average topologies of amorphous three dimensional networks. In this work we have analysed our structures following the Guttman's criterion as implemented in the ISAACS software[1]. Figure S1(a) shows the ring size probability of the amorphous SiO_2 created with different cooling rates, and figure S1(b) the ring size probability of the unstrained and 10% strained samples. Below each plot, the probability difference is given for a better view of the dissimilarities. In the case of temperature, the difference corresponds to the highest and lowest cooling rates, 10^{14} K and 10^{13} K.

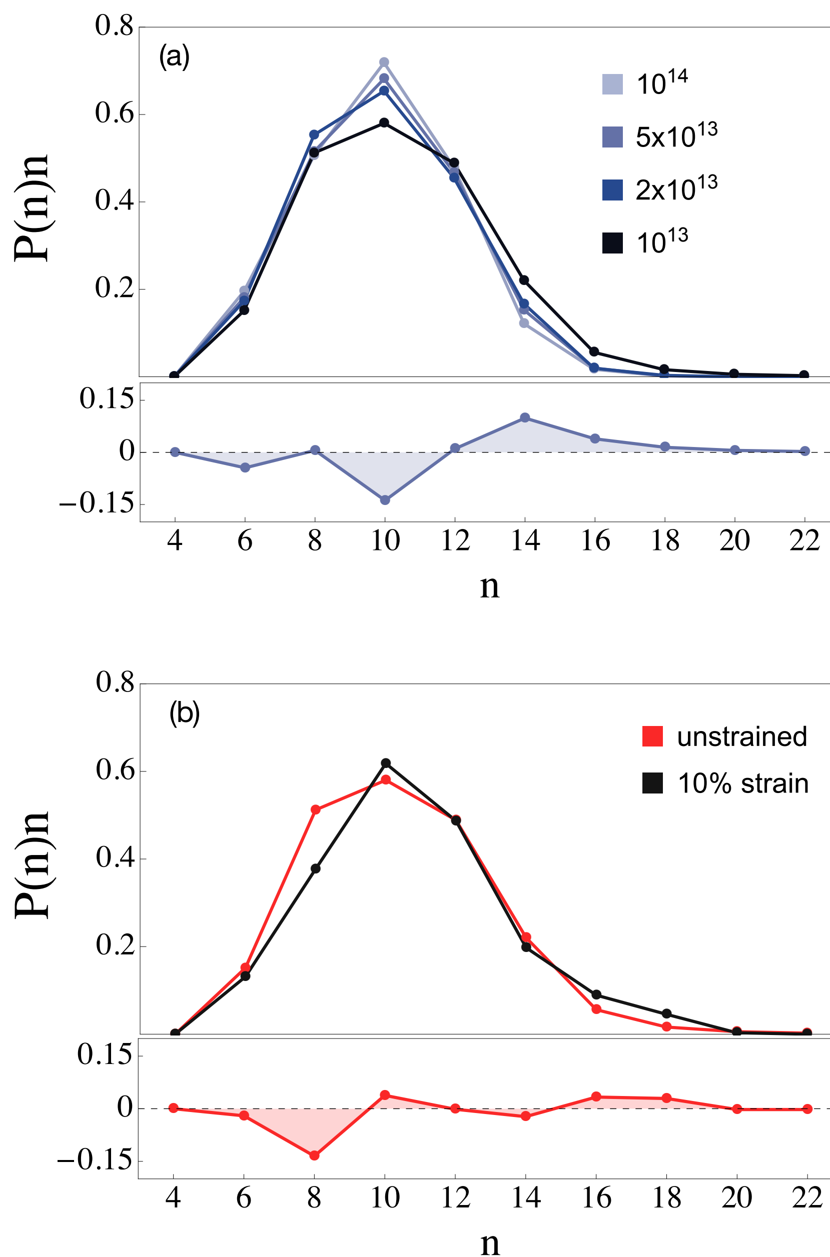

Figure S1. Guttman's ring distribution. (a) Amorphous SiO_2 models built using different cooling rates. (b) SiO_2 model without external strain and after applying a 10% tensile strain.

Stress-strain behaviour

In the manuscript we focused on the impact of strain on the short range structural order, more precisely, on how the strain modifies the the cross-ring O-O distance in the silicate network, as we found that it the key factor that governs proton diffusion. For a more detailed analysis

of the effect of strain on the structure, we present here the stress-strain curve obtained from our simulations.

The results are in good agreement with previous simulations performing MD at different temperatures and different strain rates[2]. It must be noted that our faster strain rate is one order of magnitude faster than the reported in ref [2], but the stress built up is still in very good agreement. From the linear fit of the data we can estimate the Young's modulus in the applied strain direction, which in a glass should be equivalent in any direction due to the structural isotropy. We obtain E = 67 GPa, again in good agreement with previous simulations (73 GPa) [2], and room temperature compression and tension experiments (72 GPa)[3]. Both experiment and theory determine the failure strain between 12% and 16% depending on the sample (bulk or fibers) and temperature [2,3]. Our maximum strain guaranties that the structural changes do not correspond to a fracture processes, just to a elastic/plastic rearrangements of the silicate network.

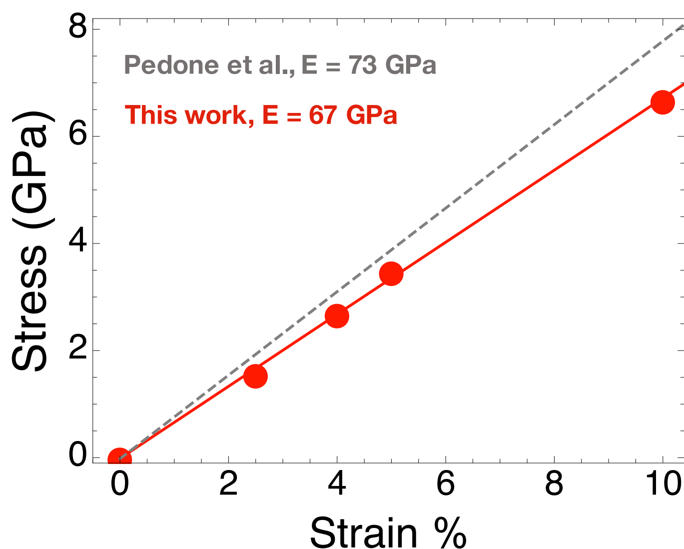

Figure S2. Tensile stress-strain curve for amorphous SiO_2 computed in this work. The dashed line represents the data from Pedone et al.[2] The Young modulus obtained from a linear fit of the data is also included for comparison with the experimental value (72 GPa)

Supplementary Bibliography

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