Precursors to failure in a gel forming system

Cabriolu R.,[1,*] Bouzid M.,[2] Nagazi M.Y.,[3] Martens K.,[4] Del Gado E.,[2] and Cipelletti L.[3]

[1] *Department of Applied Chemistry, Norwegian University of Science and Technology, Trondheim*

[2] *Department of Physics, Georgetown University, Washington DC, USA.*

[3] *Laboratoire Charles Coulomb, Université de Montpellier, Montpellier, France.*

[4] *LIPhy, Université Grenoble Alpes, Saint Martin d'Hères, France*

Detecting precursors of failure in gels subjected to mechanical load is an interdisciplinary challenge with important applications in numerous fields including material science, medicine, engineering and geology, as well as food science and cosmetic.

It is well known that gels behave in a viscoelastic way, flowing like a viscous liquid or deforming like a solid according to the forces applied, but the mechanisms underlying the macroscopic failure in soft materials under load remain unclear. It has been shown that gels can be fragile [1] and local deformation and structural rearrangements may trigger catastrophic macroscopic failure. Hence, the detection of any dynamical precursor of failure would ensure a control of the conditions leading the material to fail. Despite the importance of the topic, little is known on the local dynamics [2–4], before the occurrence of such catastrophic events.

Dynamical light scattering experiments on PDMS samples by the group of L. Cipelletti in Montpellier have shown that a it is possible to observe a change in local dynamical features well before the macroscopic failure (to be published).

To detect precursors of failure at an atomistic level that are not easily accessible by experiments we chose to carry out atomistic molecular dynamic simulations. In particular, to gain insight in the microscopic dynamical precursors that lead to the macroscopic failure this work discusses the response of a gel model [5] to tensile strain step cycles. Each cycle consists of a strain step plus a subsequent long relaxation stage. Despite the idealized model system used for our investigations, the simulations are able to reproduce the dynamical change before failure, observed by experiments, suggesting this to be a very generic scenario. Within the simulations we are able to probe the reasons for this dynamical change at the molecular scale. We rationalize the experimentally observed precursors by studying in our simulations the broken bond statistics during the relaxation stages and the long range elastic consequences of individual bond breaking events. In this study we show that a powerful combination of experiments and simulations allows to make successful temporal and spatial predictions of macroscopic failure.

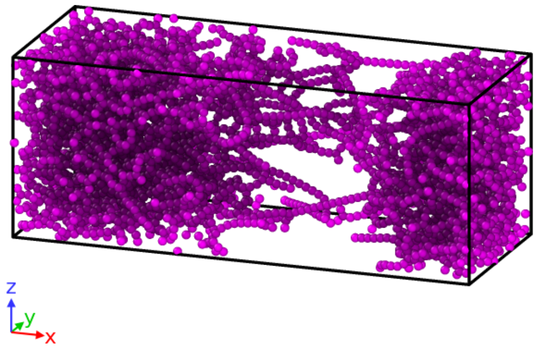

FIG. 1. Simulation snapshot of the gel system after several tensile step deformations leading to failure.

* Corresponding author: raffaela.cabriolu@ntnu.no

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