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Modelling of Plasticity in Amorphous Solids: From atomic simulations to discrete lattice models

How to describe physically, i.e. without phenomenological assumption, the plastic deformation of amorphous solids? The topics of this internship aims to answer this open question using the new method developed by our research group that allows us to systematically measure the local yield stresses, down to atomic scale. On the basis of this innovative measure, making it possible for the first time to quantify the relation between structure and plasticity, we want to transfer this new information to upper scales by using discrete mesoscopic models. These models have already been used successfully for different systems and manage to reproduce the essential characteristics of plasticity with relative simplicity. The expected results will be a real scientific breakthrough needed for multi-scale modelling of the mechanical properties of amorphous solids.

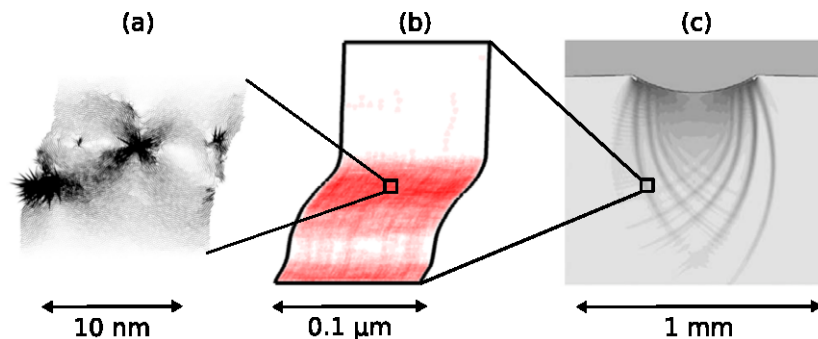


Figure 1: Multi-scale modelling strategy [1]. The plasticity of amorphous materials is studied at different scales: (a) atomic, (b) mesoscopic and (c) continuous. So far, the absence of quantitative link between local structure and plasticity at the atomic scale has confined this approach to a qualitative description. A new method developed by our research group has just addressed this scientific challenge, opening the way to a better understanding of the mechanical properties of glassy materials.

[1] D. Rodney, A. Tanguy and D. Vandembroucq, Modeling the mechanics of amorphous solids at different length scale and time scale, *Model. Simul. Mater. Sci. Eng.*, 19 083001 (2011).

[2] S. Patinet, D. Vandembroucq and M.L. Falk, Connecting local yield stresses with plastic activity in a model amorphous solid, *Phys. Rev. Lett.* 117, 045501 (2016)