ESPCI PARIS | PSL

Gulliver
UMR 7083 CNRS
ESPCI, PSL

Nanoscopic probes of mechanical and dynamical properties of amorphous solids

Directeurs de thèse :

Ludovic Berthier (Gulliver ESPCI, Paris)
https://ludovicberthier.github.io/
Sylvain Patinet (PMMH, ESPCI, Paris)
https://blog.espci.fr/spatinet/

Scientific context: Amorphous solids represent a broad class of materials with physical properties that differ so drastically from crystalline solids that most basic questions about their physical properties are only understood at some crude empirical level. A major challenge is to develop an atomistic understanding of the structural, mechanical, and dynamical properties for this large class of disordered systems, and of the nature of the phase transformation between a slowly cooled liquid and a solid glass.

In particular, close to the experimental glass transition temperature the structure of a viscous liquid relaxes using very complex dynamic pathways characterized by non-trivial spatio-temporal correlations at the atomic scale. The physical mystery stems from the fact that these non-trivial dynamic correlations seem to emerge from a fully homogeneous and completely featureless atomic structure, suggesting that information about the dynamics is encoded in the atomic structure in a manner that is not easy to decode. Understanding the origin of this apparent decoupling between structure and dynamics in dense glassy liquids is currently at the heart of glass transition studies [1].

Computer simulations represent a central tool to study amorphous solids as they grant access to detailed information about the microscopic structure and molecular dynamics at the atomic scale. Very recently, two independent lines of work have emerged, which we propose to combine in this project. First, we developed a computational method to probe at the nanoscale the heterogeneity in the mechanical response of amorphous solids [2]. Ultimately this provides a way to measure the spatial variation and the heterogeneity of the non-linear mechanical response of glass. A very recent study suggests that these nanoscopic mechanical heterogeneities may be linked to the heterogeneous relaxation of the liquid at finite temperature [3]. Second, we developed a swap Monte Carlo algorithm to considerably speedup the equilibration of dense supercooled liquids near the experimental glass transition [4]. Recent work shows that this algorithm can be used to access for the first time a temperature regime that is relevant to understand the dynamics of liquids over experimentally relevant timescales [4].

Description of the thesis: The central objective is to combine these two computational methods to separately characterize local mechanical and dynamical properties of deeply supercooled liquids using computer simulations and understand if and how nanoscopic mechanical inhomogeneity can explain the relaxation dynamics of these materials.

The first task will be to develop and generalize the nanoscopic mechanical probe proposed in Ref. [2] to make it readily applicable to a wide variety of glass-forming models in both two and three dimensions. The second task is to combine the swap Monte Carlo algorithm to the efficient characterization of the structural relaxation dynamics of deeply supercooled liquids. In particular, a novel method to locally probe these dynamics will be developed to characterize nanoscopic fluctuations in the relaxation behavior of glassy materials. Finally, armed with these two methods it will become possible to understand if and how the local mechanical properties of the material locally control the long-time dynamics. The ultimate goal of the project is to develop a predictive computational method from which the dynamical properties of a supercooled liquid can be directly inferred by a detailed characterization of its microstructure, thereby fully solving a long-lasting problem in the field of disordered materials.

Supervision: The thesis could take place at Gulliver (ESPCI UMR 7083 CNRS) and be supervised by L. Berthier (DR1, CNRS, HDR). The lab has developed well-known expertise for the study of disordered and non-equilibrium materials, and has a large experience regarding the numerical simulations of these systems. Another possible location is the Physique et Mécanique des Milieux Hétérogènes laboratory (PMMH, UMR 7636), a multidisciplinary research unit within the École Supérieure de Physique et de Chimie Industrielles de Paris, where S. Patinet (CRCN) develops his research activities. His work lies at the interface of physics and mechanics and focuses primarily on the study of dissipative processes, such as plasticity and fracture, induced by mechanical loading in heterogeneous materials. L. Berthier and S. Patinet have collaborated in the past [5], have conceived the present PhD project together, and will be both actively involved in the research whatever the chosen location.

Références :

[1] L. Berthier and G. Biroli, Theoretical perspective on the glass transition and amorphous materials, Rev. Mod. Phys. 83, 587 (2011)

[2] S. Patinet, D. Vandembroucq and M. L. Falk, Connecting Local Yield Stresses with Plastic Activity in Amorphous Solids, Phys. Rev. Lett. 117, 045501 (2016)

[3] M. Lerbinger, A. Barbot, D. Vandembroucq and S. Patinet, On the relevance of shear transformations in the relaxation of supercooled liquids, Phys. Rev. Lett. 129, 195501 (2022)

[3] A. Ninarello, L. Berthier, and D. Coslovich, Models and algorithms for the next generation of glass transition studies, Phys. Rev. X 7, 021039 (2017)

[4] B. Guiselin, C. Scalliet, and L. Berthier, Microscopic origin of excess wings in relaxation spectra of deeply supercooled liquids, Nature Phys. 18, 468 (2022)

[5] P. Richard et al., Predicting plasticity in disordered solids from structural indicators, Phys. Rev. Mater. 4, 113609 (2020)