PhD subject

Enhanced and efficient Multi-Scale Modelling of Plasticity and Damage in Amorphous Solids: From Atomistic to Emergent Mesoscopic Mechanics

Profile

Master of Science — excellent level in science and general culture. A good level of English is required. The essential skills sought for this doctorate are: human qualities, communication, creativity, autonomy and adaptation, pedagogy and a strong motivation for research. A good level of programming, data analysis, physics and mechanics of materials is particularly appreciated.

Application

The doctoral contract is scheduled for three years, starting in the fall. Please send your application to sylvain.patinet@espci.fr and francois.willot@minesparis.psl.eu: a detailed CV, cover letter, detailed exam results, master's notes, names and contact details of professors and supervisors who have followed your work, letters of recommendation, master's thesis, journal and conference articles or any other document establishing your skills for this doctorate.

Thesis supervisors : Sylvain Patinet and François Willot

Doctoral school : ED 391, Sciences mécaniques, acoustique, électronique et robotique de Paris

Laboratories : CNRS UMR 7636 Physique et Mécanique des Milieux Hétérogènes – ESPCI Paris
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Websites : PMMH, Sylvain Patinet and François Willot's web pages.

Keywords : Amorphous solids, atomistic, FTT, multi-scale, plasticity and damage

Description of the thesis

The deformation of amorphous materials at the continuum scale (>mm) is predominantly described through phenomenological models at the mesoscopic scale (~μm). This multidisciplinary project, at the intersection of physics and mechanics, aims to provide a more rigorous foundation for these approaches by bridging the gap between atomic and mesoscopic scales. To achieve this, we will leverage our recent methodological advances at both the atomic scale and the mesoscopic scale using FFT-based methods. This approach has already been successfully validated for simple loading conditions and plasticity. We propose to extend it to more complex and realistic scenarios, including non-monotonic loadings, variations in fictitious temperature, and damage mechanisms. The expected outcomes will facilitate the development of physically justified constitutive equations for amorphous solids, significantly improving the predictive accuracy of existing models.

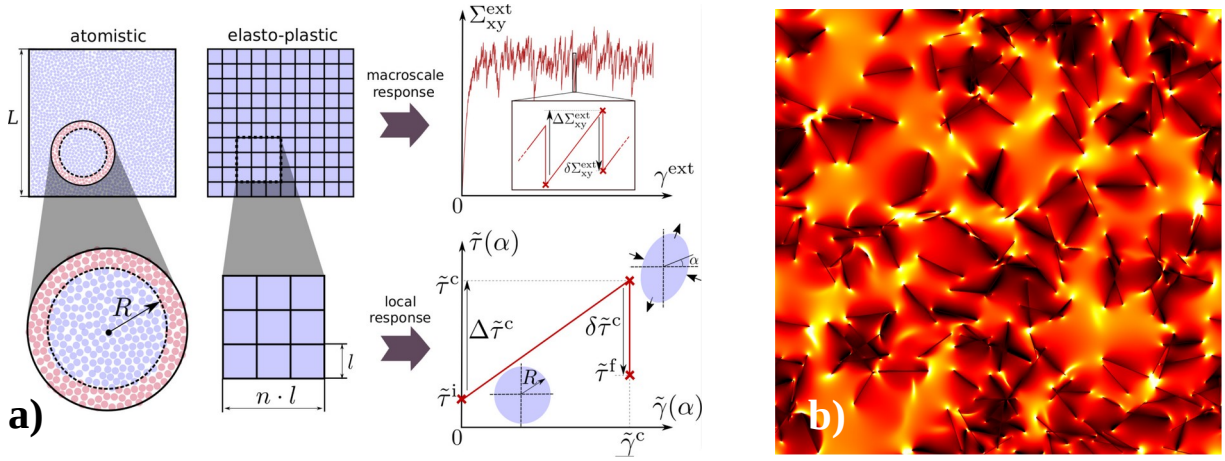

Figure 1: (a) Quantitative multiscale strategy of macro and microscopic responses of elastoplastic and atomistic models [1]. b) We propose to apply this approach to FFT methods [2] for the first time by efficiently treating elastic heterogeneities, damage and cracks.

Scientific Problems and Objectives - Amorphous solids are ubiquitous in nature and play a critical role in numerous industrial applications, including glass, gels, and granular materials. However, their mechanical behavior remains poorly understood at a fundamental level. Unlike crystalline materials, where topological defects can be readily identified, amorphous solids exhibit a universal mechanical response. The disordered nature of these materials makes it difficult to pinpoint specific flow defects at the particle scale arise from irreversible rearrangements. These shear transformations can manifest as avalanches or shear bands, spanning multiple spatial scales. Additionally, the mechanical response of these non-equilibrium systems is highly dependent on their thermomechanical history. While continuum-scale elastoplastic models successfully capture some of these behaviors, they often rely on highly simplifying assumptions, such as scalar descriptions, homogeneous, and properties statistics that do not evolve with plasticity and damage. Furthermore, most of these models neglect pressure dependence, contradicting recent findings from microscopic simulations. Given the inherent softening behavior of amorphous solids, which leads to localization, classical homogenization techniques are unsuitable. Instead, enriched kinematic models incorporating internal length scales are necessary. Several fundamental questions remain unresolved within this framework: What is the microscopic origin of nonlocal rheology when transitioning from discrete mesoscopic models to continuous descriptions? How can internal length scales be derived from first principles? How can fracture in amorphous solids, particularly in heterogeneous systems, be effectively modeled alongside plasticity and damage?

Approaches and Methods - To address these challenges, this project will build upon recent methodological advances developed by the research team. Specifically, we have pioneered innovative numerical techniques that enable: 1. The systematic measurement of local yield stresses in amorphous solids at the atomic scale. 2. The resolution of full continuum mechanical problems, including plasticity and damage, in heterogeneous solids using high-performance FFT-based methods. Leveraging these breakthroughs, this study aims to establish a rigorous multiscale framework for modeling the mechanical behavior of amorphous materials. First, we will extract key information from atomistic simulations and transfer it to discrete mesoscopic models, which can handle significantly larger systems while focusing on essential physical parameters. Second, we will quantitatively compare atomistic and mesoscopic approaches, ensuring that our models accurately capture the impact of thermomechanical history on material behavior.

Expected Results - In an ideal scenario, this research will lead to a structural understanding of amorphous solid mechanics. By deciphering the micromechanics of discretized instabilities, we aim to lay the groundwork for a physical theory of deformation in amorphous materials. Furthermore, this project will identify the fundamental ingredients required for a rigorous multiscale approach, bridging the gap between atomistic and continuum descriptions. Additionally, this multiscale strategy will guide the development of physically justified constitutive laws, moving beyond ad hoc modeling approaches. In the long term, the insights gained from this study will serve as a foundation for the rational design of novel amorphous materials with tailored properties, including memory effects. By providing a predictive framework for their mechanical response, this work could pave the way for a more systematic and less empirical approach to the engineering of advanced amorphous materials.

References

[1] D. Fernández Castellanos, S. Roux, S. Patinet, *Insights from the quantitative calibration of an elasto-plastic model from a Lennard-Jones atomic glass*, Comptes Rendus Physique de l'académie des sciences, Special Issue: Plasticity and Solid State Physics **22** (S3), 1 (2021).

[2] F. Willot, *Fourier-based schemes for computing the mechanical response of composites with accurate local fields*, C. R. Meca. **343** (3), 232-245 (2015).