PhD subject

Multi-scale modelling of plasticity and damage in amorphous solids: from atomistic calculations to continuum 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, pedagogical qualities 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 of 2023. Applications will be considered until May 15. 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.

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Doctoral school : ED 391, Sciences mécaniques, acoustique, électronique et robotique de Paris
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CNRS UMR 7636 Physique et Mécanique des Milieux Hétérogènes – ESPCI Paris
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Keywords : Amorphous solids, atomistics, FTT, multi-scale, plasticity and damage

Description of the thesis

The deformation of amorphous materials at the continuous scale (>mm) is primarily based on a phenomenological description of the mesoscopic scale (~µm). This multidisciplinary project, at the interface between physics and mechanics, aims to better ground these approaches by achieving a rigorous passage between the atomic and mesoscopic scales.

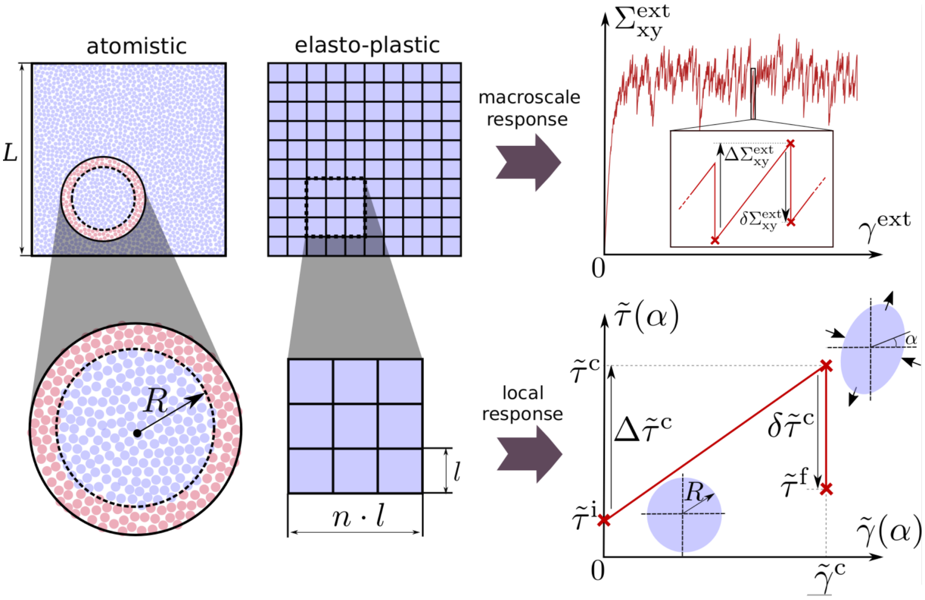

Figure 1: Multi-scale strategy in which macroscopic (top) and microscopic (bottom) mechanical responses are investigated in elasto-plastic and atomistic models.

For this, we will rely on our recent methodological advances both at the atomic scale (partner ESPCI) and mesoscopic by FFT methods (partner Mines). This approach has already been validated in the case of simple loading and plasticity. We propose to extend this study to complex and more realistic cases (non-monotonic loadings and different fictitious temperatures) and damage. For each protocol, mesoscopic and atomistic simulations will be compared quantitatively to identify the relevant parameters. The expected results will allow the derivation of physically justified constitutive equation for amorphous solids.

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).