PhD thesis at ESPCI and Mines Paris

Multiscale Modeling of Plasticity and Damage in Amorphous Solids: from atomistic computations to continuum mechanics

Thesis directors:
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Doctoral school:
ED 621 Systems, Engineering, Materials, Mechanics and Energy (ISMME)

Research labs:
CNRS UMR 7636 Physics and Mechanics of Heterogeneous Media (PMMH) – ESPCI Paris
Centre for Mathematical Morphology (CMM) – Mines Paris

Location:
The PMMH lab is located in Paris. The CMM lab is located in Fontainebleau, south of Paris.

Funding:
The PhD thesis is funded by a grant from PSL's "Programme Gradué" on "Ingénierie, Sciences Appliquées, Innovation (ISAI)".

Dates:
The PhD thesis will start on Oct. 1, 2025 (or around that date) and end on Sep. 30, 2028.

Websites:
https://www.pmmh.espci.fr/
https://www2.cmm.minesparis.psl.eu/nous-rejoindre/

Keywords:
Atomistic simulations; Fourier-based methods; multi-scale; plasticity; damage

Summary:
The deformation of amorphous materials at the continuum scale (>mm) is largely based on a phenomenological description of the mesoscopic scale (~µm). The present multidisciplinary PhD thesis, at the interface between physics and mechanics, aims to understand how atomistic simulations and micro-mechanical approaches may be combined in order to deal with plasticity and damage, and how a rigorous passage between the atomic and mesoscopic scales may be achieved. To do this, we rely on our recent methodological advances both at the atomic scale (ESPCI partner) and mesoscopic by FFT methods (Mines partner). 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 to damage. For each protocol, mesoscopic and atomistic simulations will be compared quantitatively in order to identify the relevant parameters. The expected results will allow the derivation of physically justified behavior laws of amorphous materials.

References:

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

Profile:

Engineer and / or Master of Science – excellent level in science and general culture. A good level of English is required. Essential qualities sought for for this PhD are: human qualities, communication, creativity, autonomy and adaptation, but also teaching skills, and a strong motivation for research. A good level in programming, optimization methods and data analysis and the mechanics of materials is especially appreciated.
Students may supply the following documents with their application:
a detailed resume, a covering letter explaining the motivation for doing a PhD, detailed exam results, master grades, the name(s) and contact details of professors who followed your work, recommendation letters, master thesis, journal or conference articles and any other document establishing your qualities for this PhD.

Please send your application by email to:
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