PhD subject

Toward realistic and systematic atomistic modelling of amorphous solids

Laboratory PMMH, ESPCI, Paris, France

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, david.richard@espci.fr and damien.vandembroucq@espci.fr: 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, David Richard and Damien Vandembroucq
Doctoral school : ED 391, Sciences mécaniques, acoustique, électronique et robotique de Paris
Laboratory : CNRS UMR 7636 Physique et Mécanique des Milieux Hétérogènes – ESPCI Paris
Websites : PMMH and Sylvain Patinet's web pages.
Keywords : Amorphous solids, dynamics, atomistic simulations, mechanics, statistical physics

Thesis summary

Amorphous solids encompass a broad class of materials that lack long-range order at the particle scale. Their structural disorder leads to mechanical properties distinct from those of crystalline solids, making their behavior difficult to predict and model. This PhD thesis aims to develop a robust methodological framework for investigating the mechanical properties of amorphous materials through atomistic simulations. The first objective is to construct a comprehensive database covering a wide range of force fields: machine-learning potentials, models of polymers, amorphous silicon, and metallic glass. A key challenge is to generate systems with fictive temperatures spanning a sufficiently broad range to capture the brittle-ductile transition. The project will employ the Swap Monte Carlo method to efficiently equilibrate liquids at low temperatures. The synthesized systems will be characterized using advanced techniques. All results will be openly shared via GitHub under a CC BY 4.0 license, ensuring data integrity, reproducibility, and accessibility. By developing and disseminating high-quality datasets and methodologies, this research will not only advance the understanding of amorphous solids but also accelerate discoveries and foster collaboration within the scientific community.

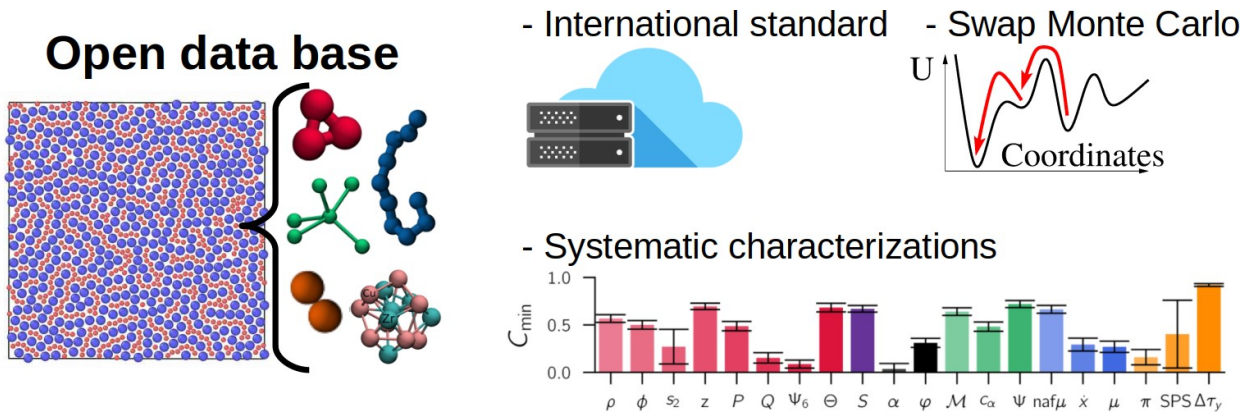

Figure 1: The tasks of the general methodology: open database construction, tuning the disorder with efficient preparation protocols, systematic characterization and reproducibility.

Scientific Context - Amorphous solids, ranging from structural glasses to biological networks, are ubiquitous in nature. Their properties differ so significantly from crystalline solids that many fundamental questions remain unresolved, often relying on crude empirical models. Key challenges include developing an atomistic understanding of their structural, mechanical, and dynamical properties, as well as distinguishing between a slowly cooled liquid and a solid glass. One major technical limitation is the short timescales accessible in classical molecular dynamics, which can only achieve quench rates several orders of magnitude faster than experiments. Additionally, mechanical properties are highly sensitive to particle interactions, as seen in microalloying effects on damage resistance, crack propagation, cavitation, shear banding, glass formability, and elastic moduli. Despite extensive research, studies often focus on specific model systems rather than providing generalized insights. Moreover, advanced structural analyses are required to characterize these disordered solids, making quantitative reproduction of literature results challenging.
At the interface of physics and mechanics, our group has developed multiscale numerical methods to study amorphous materials. A key achievement is an extensive international collaboration that systematically compares the predictive power of different structural indicators for plastic activity [1,2]. These methods have been applied to a wide range of preparation protocols, including systems with relaxation times extending to geological scales. While previous research focused on a few model systems and plasticity, this project aims to extend these approaches to more realistic materials and fracture mechanics. The goal is to develop a general methodological tool, providing a microscopic foundation for a mechanical theory of amorphous solids.

Thesis Description - To generalize our findings, the first step will be to systematically explore force field effects by constructing a database covering a wide range of interaction models, including two-dimensional polydisperse systems with soft repulsive, smoothed Lennard-Jones, and Hertzian potentials. The study will then extend to three-dimensional simulations of these systems, alongside amorphous polymer, silicon, and metallic glass models using multibody potentials. Initially, we will focus on model systems where interaction parameters can be easily adjusted at a modest computational cost. In the long term, for quantitative experimental comparisons, silicon and metallic glass will be studied using quantum-accuracy machine-learning potentials. A broad range of glassy mechanical stabilities will be investigated by generating solids through rapid quenches of supercooled liquids equilibrated at different temperatures. A key challenge is achieving systems with fictive temperatures spanning a wide enough range to observe the brittle-ductile transition. To overcome this, we will implement the Swap Monte Carlo method, which efficiently equilibrates liquids in low-temperature regimes inaccessible to classical molecular dynamics. All synthesized systems will undergo systematic characterization through geometric analysis of local atomic environments. To capture fluctuations, order parameters based on geometry will be complemented by local physical properties, such as atomic shear non-affinity, elastic moduli, thermal expansion, vibrational modes, and local yield stress. An integrated program will be developed to compute these indicators in real-time. For system preparation, LAMMPS—a widely adopted molecular dynamics software—will be used, with developed scripts shared via GitHub.
The amorphous configurations and characterization data will be structured into a coherent, interpretable, and openly accessible database under a CC BY 4.0 license. This resource will accelerate discoveries, foster collaborations, prevent redundant simulations, and promote data reuse, ensuring integrity, transparency, and reproducibility of the project results.

References

[1] D. Richard, M. Ozawa, S. Patinet, E. Stanifer, B. Shang, S. A. Ridout, B. Xu, G. Zhang, P. K. Morse, J.-L. Barrat, L. Berthier, M. L. Falk, P. Guan, A. J. Liu, K. Martens, S. Sastry, D. Vandembroucq, E. Lerner, and M. L. Manning, *Predicting plasticity in disordered solids from structural indicators*, Phys. Rev. Mater. **4**, 113609 (2020)
[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)