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, 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 david.richard@univ-grenoble-alpes.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.

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Keywords : Amorphous solids, dynamics, atomistic simulations, mechanics, statistical physics

Thesis summary

Amorphous solids correspond to a broad class of materials disordered at the particle scale. Their properties differ significantly from crystalline solids, making it challenging to understand their physical properties. This PhD thesis aims to develop a methodological tool for studying the mechanical properties of amorphous materials via atomistic simulations. The first task is to build a database covering an extensive range of force fields for two-dimensional and three-dimensional systems. The project will also use machine-learning potentials to study amorphous models of polymers, amorphous silicon and metallic glass. The challenge is to obtain systems whose fictive temperatures spread over a range large enough to observe the brittle-ductile transition. The project will use a Swap Monte Carlo method to equilibrate liquids in the low-temperature regime efficiently. The synthesized systems will be characterized by various methods, such as geometric analysis of local atomic environments and physical properties computed on the fly. The results will be shared via the GitHub platform with a CC-by 4.0 license for data reuse, integrity, and reproducibility of the project results. This project can accelerate discoveries and promote collaboration in the study of amorphous solids.

Scientific context

Ubiquitous in nature, amorphous solids represent a broad class of materials from structural glasses to biological networks. Their physical properties differ so drastically from crystalline solids that most basic questions about their physical properties are only understood at some crude empirical level. Major challenges encompass the development of an atomistic understanding of the structural, mechanical, and dynamical properties for this large class of disordered solids as well as to comprehend differences between a slowly cooled liquid and a solid glass. A first technical difficulty

lies in the small-time scales accessible via classical molecular dynamics. To obtain amorphous systems by direct simulations, one can expect, at best, a quench rate six orders of magnitude faster than in experiments. A second problem comes from the great sensitivity of the mechanical properties with the details of the particle interactions. This is illustrated by the significant property variations with microalloying on damage resistance, crack propagation, cavitation, shear banding, glass formability and elastic moduli. Despite significant efforts, the studies focus generally on model systems and address questions most often from a specific system. In addition, even if we know what we are looking for in the structure, the characterization of the solid requires advanced structural analyses. Hence, a scientist wishing to study the mechanical properties of amorphous materials via atomistic simulations must generally start by carrying out long and energy consuming simulations and faces difficulties in reproducing quantitatively the literature results.

At the interface between physics and mechanics, our group has developed in recent years multiscale numerical methods to study in depth amorphous materials. The most salient result is undoubtedly the development of a very large international collaboration bringing together the best specialists in the physics of glassy materials [1]. This study systematizes the methodology he developed to quantitatively compare the predictive powers of the plastic activity of different structural indicators [2]. This work has been carried out for a wide range of preparation protocols, including systems whose relaxation times ranged up to geological times. These recent works constitute the ground roots on which this project will be based. So far our previous line of research focused on few model systems and was restricted to plasticity. Here, the project's ambition is to systematize these approaches to more realistic systems and to fracture. It will give a general methodological tool providing a solid microscopic basis for a mechanical theory of amorphous solids. Ideas in this direction have already produced results by generalizing the methods to more realistic three-dimensional systems [3] or using a multiscale approach to study transient response from different non-equilibrium states [4].

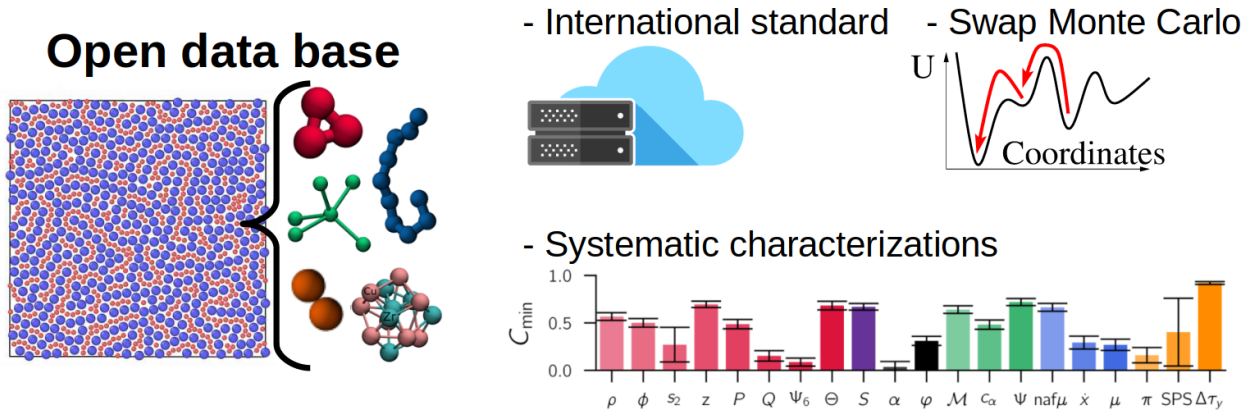

Figure 1: The tasks of the general methodology: open database construction, tuning the disorder with efficient preparation protocols, systematic characterization and reproducibility.

Description of the thesis

In order to generalize our results, the first task will consist in systematically exploring this effect by building a database covering an extensive range of force fields: two-dimensional polydisperse systems of particles interacting via soft repulsive potentials, smoothed Lennard-Jones potentials, and Hertzian contacts. In a second step, three-dimensional simulations will be implemented for the same polydisperse systems. They will be complemented by amorphous models of polymers, amorphous silicon and metallic glass (with multibody potential). The philosophy is to have first model systems where we can adjust the parameters by taking advantage of the analytical form of the interaction for a relatively modest computational cost. In the long term, with a view to a quantitative comparison with the experiment, two archetypal systems of silicon and metallic glass will be studied using quantum-accuracy machine-learning potentials. A wide range of glassy mechanical stabilities will be studied for each atomic system. The solids will be obtained from instantaneous quenches of supercooled liquids at thermodynamic equilibrium at different temperatures. The

challenge is to obtain systems whose fictive temperatures spread over a range large enough to observe the brittle-ductile transition. For this, we will implement a Swap Monte Carlo method which allows liquids to be equilibrated efficiently even in the low-temperature regime, unreachable by classical molecular dynamics methods [5]. All synthesized systems will be systematically characterized by structural identification methods based on the geometric analysis of local atomic environments. In order to analyze and identify fluctuations, order parameters based on the geometry will be complemented by local physical properties. Further analyses involving the system's response will give access to atomic shear non-affinity, elastic moduli, thermal expansion, vibrational modes and local yield stress. We plan to develop an integrated program to calculate all these indicators on the fly. As for the system preparation, the code will be a LAMMPS script, a program that tends to become an international standard for massively parallel molecular dynamics calculations. The source of the codes developed will be shared via the GitHub platform. The amorphous configurations and their characterizations will be aggregated and organized to form a coherent whole to be interpretable and publishable under CC-by 4.0 license. This database will aim to accelerate discoveries, encourage collaborations, avoid duplication of simulations, and promote data reuse. It will also ensure the integrity and reproducibility of the project results and the transparency of the implemented methodologies.

References

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