Département Mécanique et Verres
Institut de Physique de Rennes – Université de Rennes, CNRS

Research project (Master's thesis)

2025-2026

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Molecular dynamics simulations of shocks in metallic glasses

Since their appearance in the 1960s [1], metallic glasses have been the subject of numerous studies highlighting mechanical properties that are often superior to those of their crystallised counterparts (yield strength, hardness and fracture resistance) [2-3]. Although the compositions of these amorphous alloys have expanded in terms of the elements present (Zr, Ti, Al, Cu, Ni, Fe, etc.), their industrialisation is currently limited to a few niche markets (luxury watchmaking and jewellery, cutting-edge medical applications, aeronautics, defence, and high-end leisure goods). In the field of shock and impact applications, the potential of metallic glasses is largely untapped, for example in golf clubs or the armouring of space structures against hypervelocity impacts [4]... with studies on their dynamic behaviour initiated in the early 2000s still in their infancy.

In the literature, studies have established the Hugoniot curve (location of shock-induced states) for certain compositions [5-9]. These data from the literature cover a limited range in terms of pressure (up to 120 GPa) and deformation rates (up to 5x105 s-1). The Rennes team is the only one to have studied the response of metallic glasses to stresses representative of a hypervelocity impact, thanks to the use of laser-generated shocks on three national facilities (GCLT at the CEA, HERA and LULI2000 at the LULI laboratory). We have thus achieved deformation speeds of 105 to 108 s-1 and pressures of 100 GPa (corresponding to an impact of a millimetre-sized object at 7 km.s-1) [10].

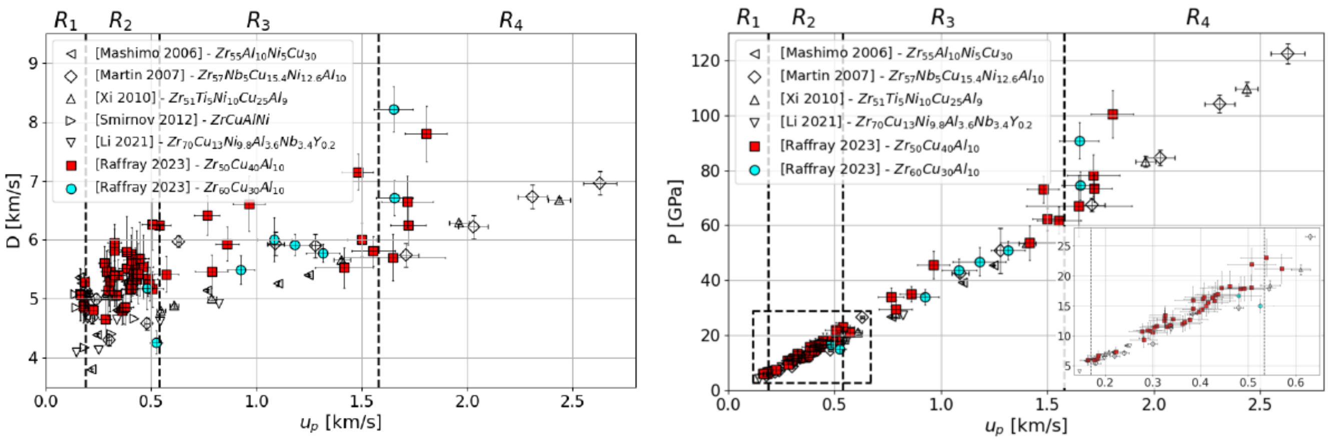

Figure – Thermodynamic states reached by shocking the material, in a range of pressures up to 100 GPa [10]

Below 100 GPa, the literature [7] suggests phase changes starting at certain shock pressures depending on the composition. The implementation of laser shock campaigns instrumented by in situ X-ray diffraction enabled us to identify the nature of the transition, namely crystallisation around 70 GPa for a Zr50Cu40Al10 metallic glass [11]. During loading, the shock pressure is then relaxed until tensile stress appears, which can cause spalling (dynamic fracture) of the target. Monitoring the evolution of the microstructure during the relaxation phase by molecular simulation will allow us to study: the origin of the high fracture limits [10], the mechanism of cone and cup formation [3] and the phenomenon of atomic segregation leading to an overconcentration of zirconium at the tip of the cone on the flake and its defect at the bottom of the cup on the rest of the target [12].

The results already obtained on Zr50Cu40Al10 glasses at the macroscopic scale (change of state, plasticity, fracture) originate at the microscopic scale in the modification of the organisation and local composition of the material at the atomic scale. It is therefore also at this scale that the behaviour of different metallic glasses under laser shock must be studied. To analyse behaviour at this scale, we will use molecular dynamics simulations with the LAMMPS code. Once validated in our stress range, the EAM potentials from the literature [13-14] will enable us to account for the evolution of the atomic organisation of metallic glasses under dynamic stress (crystallisation under shock, deformation mechanism leading to the formation of cones and cups, atomic segregation).

Beyond this project, the validated potentials can be used to explore the ZrCuAl glass family in order to find an optimal composition in terms of species concentration (mass proportion of each species) and initial atomic organisation (depending on the manufacturing process and any heat treatments) with a view to optimising the performance required for the application.

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Methods: LAMMPS, molecular dynamics, high-performance computing.

Preferred skills: materials science, statistical physics, physical chemistry, numerical methods.

The subject allows a candidate with one of the skills listed to learn about the other skills, as well as to express himself and develop the subject in one of the directions envisaged.

Compensation: approximately 600€/month

Possibility to pursue a PhD thesis: yes