LABORATOIRE HUBERT CURIEN
UMR • CNRS • 5516 • SAINT-ETIENNE

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UNIVERSITÉ DE LYON

Atomistic simulations of ultrafast laser-induced devitrification of metallic glasses

Ph.D. offer: This 3-year scholarship is available at Laboratoire Hubert Curien (LabHC) of Université Jean Monnet in Saint-Étienne, France. The PhD will be performed in the framework of the French proposal ANR "MEGALIT". In addition to LabHC, part of the work will be carried out at the MATEIS laboratory (MATErials engIneering and Science) of the INSA school (Lyon) for part of the Molecular Dynamics simulation. LabHC is a mixed research unit (UMR CNRS 5516), jointly run by the CNRS (Centre National de la Recherche Scientifique) and University Jean Monnet, which is part of University of Lyon.

Ph.D. objectives: This PhD thesis aims at understanding the routes of metallic glass phase transition from initial amorphous state to a crystalline state upon femtosecond laser irradiation. The theoretical investigation will rely on multi-scale modelling tools, on a molecular scale with Molecular Dynamics (MD), on atomic scale by ab initio calculations and on the microscale with fluid computing codes. The results will be directly compared with laser-matter experiments where surface functionalization is targeting for biomedical and mechanical applications by enhancing wettability and mechanical properties of metallic glasses.

Context: Bulk metallic glasses are elaborated by fast quenching of a melted metal alloy (10^6 K/s down to 1K/s depending on the composition), which inhibits the crystallization process during the cooling stage and results in a metastable "amorphous" phase. This fast cooling step and the necessity to work under very inert atmosphere remains the main drawback for the large industrialization of metallic glasses, along with brittleness and insufficient fatigue resistance issues. The scientific originality of the proposal is based on the use of ultrafast laser (< 100fs) to address both the surface texturing and materials modifications by local devitrification, through very high heating rate (10^{15} K/s) and quenching rates (10^{13} K/s), and involving strong undercooling conditions by appropriate choices of laser processing parameters.

The Ph.D. program is based on two computing strategies to interpret and guide experiments:
Atomistic simulations: Molecular Dynamics will be performed via the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to reveal the processes responsible for the formation of crystal domains in the amorphous matrix of a binary Zr-Cu metallic glass upon laser irradiation. The simulation will require specific developments of the hybrid atomistic–continuum model, combining the atomistic MD representation of laser-induced structural and phase transformations with a continuum-level description of the electron sub-system, the two-temperature model (TTM). The interatomic interactions are described by the embedded atom method (EAM) potential parametrized for the specific material. Ab initio (ABINIT code) calculations could also been performed for designing pseudo-potential in nonequilibrium regimes.

Laser-induced surface modification and self-organization: Simulation of light-matter interaction will support experiments, specifically for predicting inhomogeneous energy distribution, heat rate and out-of-equilibrium thermodynamic conditions favoring structural transformations. These studies will also rely on fluid models as hydrodynamics (ESTHER code) and electromagnetics (3D FDTD) approaches already mastered at LabHC. The main goal consists of predicting and understanding the surface structures formation within the irradiated surface depending on the laser parameters (spatial intensity distribution, polarization, wavelength, etc.), as well as the temporary surface roughness, in connection with the atomistic simulations.

Keywords*: Molecular Dynamics, Ultrashort laser, Phase transition, Metallic glasses, Simulation*

Qualifications*:* We are seeking a highly motivated candidate for working at the interface between physics, material science and photonics. The candidate should hold a master degree (or equivalent) in physics or closely related field no later than July 2019. The candidate must have sound knowledge in the field of material science, solid state physics and thermodynamics. Additional programming skills (C, Python, matlab, etc.) will be requested.

How to apply*:* Interested candidate should send a short cover letter and a resume to:
Prof. Jean-Philippe Colombier - Hubert Curien Laboratory (Jean.philippe.colombier@univ-st-etienne.fr)
Prof. Florence Garrelie - Hubert Curien Laboratory (florence.Garrelie@univ-st-etienne.fr)
Dr Jonathan Amodeo – INSA Lyon (jonathan.amodeo@insa-lyon.fr)Dr Claudio Fusco – INSA Lyon (claudio.fusco@insa-lyon.fr)
Salary conditions: The gross salary is around 20200 euros/year with potential extension for teaching position.
Application deadline*:* July 1, 2019.