Atomistic simulations of ultrafast laser-induced devitrification of metallic glasses

Contact: Dr. Claudio Fusco (claudio.fusco@insa-lyon.fr), Dr. Jonathan Amodeo (jonathan.amodeo@insa-lyon.fr)

Laboratory: MATEIS laboratory, Univ. Lyon , INSA-Lyon, CNRS

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Bulk metallic glasses are used in a variety of applications for their exceptional mechanical properties, e. g. high toughness and mechanical strength. On other hand, due to their amorphous nature, the processability of this kind of materials is not always straightforward, and moreover their brittleness can be an important issue. In fact, in some applications materials modifications and surface texturing are required for better functionalization and this can be successfully achieved by local devitrification.

This thesis aims at understanding the routes of metallic glass phase transition from initial amorphous state to a crystalline state upon femtosecond laser irradiation.

During the Master thesis, theoretical investigations at the molecular scale using Molecular Dynamics (MD) and continuum (TTM) simulations will help to understand the devitrification, mimicking the femtosecond laser irradiation. 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.
Hybrid atomistic-continuum simulations 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.

We are seeking a highly motivated candidate for working at the interface between physics, material science and photonics. The candidate should prepare a master degree (or equivalent) in physics or closely related field. The candidate must have sound knowledge in the field of material science, solid state physics and thermodynamics. Additional programming skills (C, Python, matlab, etc.) are welcome.

The Master thesis will be prepared in the context of the ANR Megalit funding hold by the Hubert Curien and MATEIS laboratories of Univ. Lyon, respectively in Saint-Etienne and Lyon. The project will fund a PhD thesis on the same topic starting October 2019.

If interested, please send CV/letter/questions to claudio.fusco@insa-lyon.fr and jonathan.amodeo@insa-lyon.fr.