Postdoctoral Fellowship Proposal

Title: **Checking moLecular dynamics simUlations of fs-laser peening with a free Electron laser**

Host Institution: Hubert Curien Laboratory (LabHC) & Georges Friedel Laboratory (LGF) in Saint-Etienne, France – financed by EUR Manutech-SLEIGHT and in collaboration with Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany.

The Hubert Curien laboratory is a joint research unit (UMR CNRS 5516) of the Jean Monnet University, Saint-Etienne, the National Research Centre "CNRS" and the Institut d'Optique Graduate School. It is composed of 90 researchers, professors & assistant professors, 25 engineers & administrative staff, and around 110 PhD & post-PhD students. This total of approximately 230 staff makes the Hubert Curien laboratory the most important research structure in Saint-Etienne. Our activities are organized around two scientific departments: Optics, Photonics & Surfaces and Computer Science, Security & Image, and scientific projects are carried out by 6 main teams: Functional Materials and Surfaces, Materials for Optics and Photonics in Extreme Radiative Environments, Laser-Matter Interaction, Image Science & Computer Vision, Data Intelligence, and Secure Embedded Systems & Hardware Architectures. https://laboratoirehubertcurien.univ-st-etienne.fr/en/the-lab/edito.html

The Georges Friedel Laboratory - LGF (CNRS UMR 5307) is a joint research unit from INSIS-CNRS and École des Mines de Saint-Étienne, comprising 150 persons, dealing with activities in the fields of Materials Science, Mechanics and Process Engineering. LGF is an academic research player, in strong partnership with industry, addressing the durability and energy efficiency of components, from grain to material, from material to component and from component to factory. Research at LGF focuses on materials for application in the main fields of energy, transportation, chemistry. Competences are material science, physico-chemistry of solids (divided and massive), mechanics and chemical engineering. Scientists at LGF develop multiscale models from nano to macroscale, technological solutions for enriching knowledge and design of materials and processes with regard to their functional properties. https://www.mines-stetienne.fr/lgf/laboratoire/

Funding: EUR Manutech-SLEIGHT, ~4400 € gross/month salary, 18-month fellowship

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Subject:

Laser peening is a surface treatment technique that improves the mechanical performance of metals, increasing the material's resistance to crack initiation, extending the fatigue life and enhancing the fatigue strength [1]. In contrast to nanosecond lasers, commonly applied in the industry, femtosecond laser processing does not require a sacrificial coating layer to absorb the laser energy and to protect the work piece surface from melting and does not involve complex interaction with laser-induced plasma, thus, can be attractive for state-of-the-art applications [2-3]. High-quality laser peening, however, requires comprehensive understanding of multi-physical coupling between laser characteristics and the physical properties of the target which could be achieved only by theoretical-experimental synergy.

Understanding shock wave propagation under ultrashort laser peening conditions is critical for accurately describing the non-equilibrium dynamic response of metals, their exotic mechanical properties and unique phase transitions at high pressure and at extreme strain rates. Recently, the pressure wave dynamics has been in-situ probed by X-ray Free Electron Laser (XFEL) in DESY, Hamburg, Germany. The reconstruction of the measured phase images determines the shockwave velocity and the associated pressure as a function of time and the distance from the irradiated surface.

In this context, we propose to compare directly the XFEL measurements against molecular dynamics (MD) simulations with an appropriate ultrashort laser source that additionally uncover atomistic-scale processes that remain experimentally inaccessible. In particular, MD uniquely captures microscopic mechanisms such as non-equilibrium solid–solid phase transitions, the nucleation and evolution of defects (including dislocation slip and deformation twinning), but also allows to distinguish between elastic and plastic deformation regimes during shock loading. By resolving these processes in both space and time, MD simulations offer a powerful framework to interpret and extend XFEL observations of shock wave propagation. This combined computational–experimental effort presents a rare opportunity to rigorously test and refine the equation of state under extreme pressure, compression, and tensile conditions.

The postdoctoral fellow will be involved in the analysis of the experimental data for two metal targets (Al and Ti) with a short 3 month-stay in DESY, Hamburg, Germany and then, in the development/application of a multi-physical approach in Laboratoire Hubert Curien, Saint-Etienne, France to simulate the shock wave propagation, to compare with the XFEL measurements and to summarize the results of this study for a peer-reviewed publication. Such an approach, combining continuum two-temperature electron-phonon model (TTM) and MD within an open source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), was previously applied to subsurface hardening and defect generation in metals [4]. The postdoctoral fellow will benefit from the laboratory's strong expertise, spanning from ab initio quantum and atomistic to continuum modeling of ultrashort laser-matter interactions.

[1] K. Ding, and L. Ye, "Laser shock peening: performance and process simulations", Woodhead Publishing (2006).

[2] T. Sano et al., "Femtosecond laser peening of 2024 aluminium alloy without a sacrificial overlay under atmospheric conditions", J. Laser Appl. 29, 021005 (2016).

[3] A. Nakhoul et al., "Energy feedthrough and microstructure evolution during direct laser peening of aluminum in femtosecond and picosecond regimes", J. Appl. Phys. 130(1), 015104 (2021).

[4] L. Rousseau et al., “Subsurface hardening of Al irradiated with ultrafast infrared laser”, Scripta Mater. 255, 116404 (2025).

Keywords:

Laser-matter interaction; Laser peening; Molecular Dynamics; Ultrashort Laser; X-ray Free Electron Laser; Shockwave Propagation; Elastic & Plastic Deformations; Dislocations; Equation of state

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Candidate Profile:

The ideal candidate holds PhD in Physics, Chemistry, Materials Science, or related fields. The following skills and background are expected:

- Strong expertise & publication record in computational molecular dynamics
- Solid background in laser-solid interactions and thermodynamics; having strong expertise in ultrashort laser-matter interaction and/or non-equilibrium phase transitions modeling is a plus
- Experience with programming languages (Python, MATLAB, or C++), big data analysis (Python), and performing atomistic simulations LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)
- Proficiency in written and spoken English
- Familiarity with machine learning and parallel programming (OpenMP, MPI, or GPU) is a plus
- Motivated to work in a multidisciplinary environment and to collaborate with international experimental partners, including willing to stay up to 3 months in DESY, Hamburg, Germany for experimental XFEL data analysis
- Experience in writing/editing/preparing the manuscripts for a publication in high-impact journals

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The interested candidates should provide (1) an updated CV with the detailed education background, work experience and professional skills and a full list of peer-reviewed publications with references, (2) an optional short motivation letter, (3) three professional/academic references.
