A fournir au format WORD exclusivement

Titre : First-principles molecular dynamics simulations of atomic-scale processes involved in laser welding of glassy materials

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Établissement de rattachement : Université de Strasbourg

Collaboration(s) (s'il y a lieu) : IPP team, ADynMat consortium (https://adynmat.cnrs.fr)

Rattachement à un programme (s'il y a lieu) : ICube transversal research program IMEE

Résumé **(1500 caractères au maximum)** :

The pulsed femtosecond laser welding is used to get an accurate and local melt the interface between two materials. This technique has shown promising outcomes in the case of interfaces between two glasses or glass and metal. However, its application, as demonstrated by ICube's IPP team, requires a fine control of both the power and timing of the pulses. To this aim, finite element multi-physics modelling is currently used. Nonetheless, the predictive power is still limited by a lack of atomic-scale knowledge. The aim of this thesis is to resort to first-principles molecular dynamics (FPMD) to get a quantitative insight into the phenomena occurring in the glass upon laser excitation. The modeling methods proposed here, based on the density functional formulation of quantum mechanics, allow to simulate the evolution in time and temperature of materials providing a quantitative description of these processes. Specifically, the melt/quench technique will be used to construct glass models of silica and borosilicate, as in the IPP team's experiments. Then, Free Energy Molecular Dynamics (FEMD) will expand the FPMD to high electronic temperatures reached upon laser irradiation.
These methods are available in the CPMD code (https://github.com/OpenCPMD), and the HPC mesocentre of the University of Strasbourg will provide the needed facilities. The PhD student will work in a stimulating environment and interact with experts in atomic-scale methods and advanced microlaser processes.

Descriptif du sujet (en complément, au format Word ou pdf)

Experiments using the heating method termed "pulsed femtosecond laser welding" [1] have paved the route to a precise and well localized melting of specific regions at the interface between two different materials or between different phases (e.g. crystal and vitreous) of the same compound. Within this context, atomic-scale simulation will be conducted aiming at unraveling the underlying mechanism responsible for these phenomena.

The candidate will be formed to the use and exploitation of advanced first principles methods and related codes.

The methodologies will be based on the combination of density functional theory (DFT) and molecular dynamics [2] to study the finite temperature evolution of the system undergoing fast heating. Extension to the free energy molecular dynamics (FEMD) [3] will be used to simulate electronic excitation as occurring upon femtosecond laser pulse irradiation, an approach already well benchmarked and used for analogous problems in the formation of pure Si in a matrix of silica (SiO_2) [4,5].

The CPMD code [6], complemented by the CP2k [7] if needed, will be used. These worldwide used codes, for which we are co-developers, are available on the massive parallel high-performance computing (HPC) architectures available at the local Mesocenter of the University of Strasbourg (https://hpc.pages.unistra.fr/) and at national HC centers under the GENCI grants.

We emphasize the fact that this doctoral project will be conducted as a collaboration between the researchers active in atomic scale modeling of ICube (members of the consortium ADynMat, https://adynmat.cnrs.fr) and the experimental colleagues of the team Photonics Instrumentation and Processes (IPP) at the same institute. The PhD student will the experience a stimulating synergy et the multidisciplinary crossroad among physics/chemistry of innovative materials, their applications and future engineering applications.

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[2] R. Car, M. Parrinello, Phys. Rev. Lett. **55**, 2471 (1985) DOI: 10.1103/PhysRevLett.55.2471

[3] A. Alavi et al. Phys. Rev. Lett. **73**, 2599 (1994) DOI : 10.1103/PhysRevLett.73.2599

[4] M. Boero et al. Appl. Phys. Lett. **86**, 201910 (2005). DOI: 10.1063/1.1929879

[5] M. Boero et al. Physica B **376-377**, 945 (2006). DOI: 10.1016/j.physb.2005.12.235

[6] CPMD © 1990-2023 IBM Corp. and © 1994-2001 Max Planck Institute, Stuttgart. Available on GitHub under the MIT License (https://github.com/OpenCPMD)

[7] CP2k, https://www.cp2k.org/