Densification of amorphous silica obtained from different polymorphs

Aram Melkonyan*, Elena Kachan, Razvan Stoian, and Jean-Philippe Colombier

UJM Saint-Etienne, CNRS, Institute of Optics Graduate School, Laboratoire Hubert Curien UMR CNRS 5516, F-42023 St-Etienne, France

* Email: aram.melkonyan@univ-st-etienne.fr

Femtosecond laser irradiation can produce highly-localized changes of the physical properties inside dielectrics and, thus, efficiently tailor highly-resolved 3D nanostructures. For example, laser-induced super-dense phases have been observed recently in the bulk of sapphire and α-quartz [1,2]. In order to understand and better control such high local densification, we performed Molecular Dynamics simulations of amorphous silica under different thermodynamic conditions that can be possibly reproduced by a femtosecond laser pulse. Moreover, we explored different crystalline polymorphs of SiO_2 (α-quartz, β-quartz, α-cristobalite, keatite, coesite, stishovite) with the aim to produce amorphous silica with the highest possible density.

The influence of pressure, volume, heating rate and their combination on the densification of the amorphous silica in molecular dynamics was analyzed. It was shown that by using pressure of 100 GPa and ultrafast pressure relaxation the 40-50% density increase can be obtained (i.e. in case of α-quartz the density increases from 2.27 to 3.31 g/cm3). Additionally, we explored the possibility to recreate a density anomaly (density increase in liquid with the increase of temperature)[3] by ultrafast-laser-induced excitation.

Acknowledgements: The work is funded by EUR MANUTECH SLEIGHT project “Quicksilica”. The numerical calculations are performed using computer resources from GENCI, project gen7041.

References: [1] Vailionis, A. et al. Evidence of superdense aluminium synthesized by ultrafast microexplosion. Nat. Commun. 2:445 doi: 10.1038/ncomms1449 (2011); [2] H. D. Nguyen, A. Tsaturyan, S. Sao Joao, R. Dwivedi, A. Melkonyan et al. - Quantitative Mapping of Transient Thermodynamic States in Ultrafast Laser Nanostructuring of Quartz, Ultrafast Science, 2024, Vol 4, Article ID: 0056, DOI: 10.34133/ultrafastscience.005; [3] Cheng, S. The Origin of Anomalous Density Behavior of Silica Glass. Materials 2023, 16, 6218. https://doi.org/10.3390/ ma16186218