

Analysis of the experimental parameters impacting Non-Photochemical Laser-Induced nucleation of glycine in water

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Non-Photochemical Laser-Induced nucleation (NPLIN) is a promising nucleation technique [1] for which more than eighty papers have been published. In an NPLIN experiment, a supersaturated solution of a molecule is irradiated by a laser (pulsed or continuous, focused or non-focused) that induces the molecule's nucleation. Even though glycine nucleation constitutes almost one-quarter of these research activities reported in the literature, the impact of different experimental conditions on its nucleation is still not fully understood [2]. NPLIN of glycine in water has been demonstrated at different molarities and different energy densities induced using a non-focalized pulsed laser (532 nm) at 290 K. A new index (Ind50), allowing easy comparison with the literature, was used to characterize the impact of molarities and energy densities on the nucleation efficiency. A threshold index (Ind_{Thrs}()) indicating the minimum energy density required to obtain in a given experimental condition one crystal *per* vials in average has been determined. The impact of the circular or linear polarization of the laser beam on the glycine polymorphism (- or -glycine) has been studied and characterized using a third new index named NPLIN determinant. The experimental interface (glass-solution or air-solution) gives the opposite polymorphism behavior. The relationship between devices, solution, and experimental conditions and observable such as nucleation efficiency, nucleation site, induction time, crystal counting, and polymorphism have been modeled in a mind-map (figure 1). Within this context, this work is a contribution towards a better understanding of the impact of experimental conditions on NPLIN nucleation that will permit a better design and control of NPLIN experimental setups.

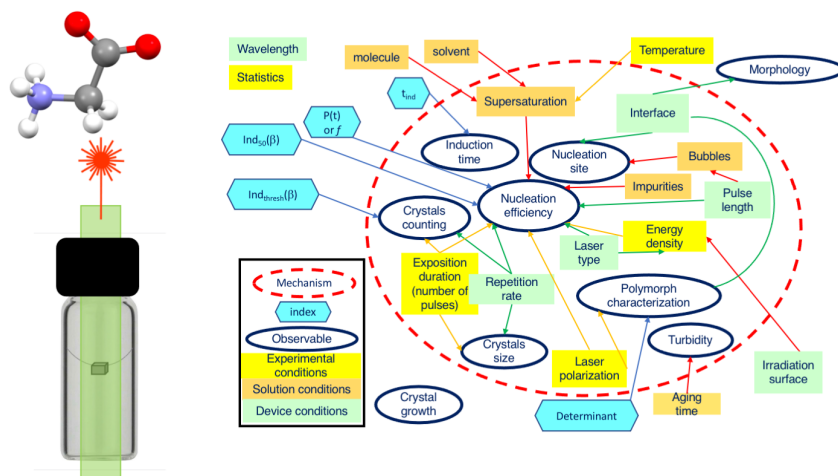


Figure 1. NPLIN mind-map parameters. Parameters inside the red dashed circles has a significant influence on the mechanism.

[1] Garetz, B. A.; Aber, J. E.; Goddard, N. L.; Young, R. G.; Myerson, A. S. (1996) Phys. Rev. Lett. **77**, 3475–3476.

[2] Clair, B.; Ikni, A.; Li, W.; Scoufflaire, P.; Quemener, V.; Spasojević-de Biré, A. (2014) J. Appl. Crystallogr., **47**, 1252–1260

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