3D printing flow reactors for the synthesis of single crystal perovskites

Simone Marchetti [1], Diego Iglesias,[1] Cristopher Tinajero,[1] Jaume Luis-Gómez,[2] Raul Martinez Cuenca,[2] Marcileia Zanatta,[1] Victor Sans[1]

[1] Institute of Advanced Materials (INAM), Univesitat Jaume I, Avda Sos Baynat s/n, 12071 Castellón, Spain

[2] Department of Mechanical Engineering and Construction, Universitat Jaume I, 12071 Castellon, Spain

smarchet@uji.es

Keywords: Perovskites single crystal • crystallization • flow • 3D printing • reactor design

Abstract: Perovskite materials have garnered considerable attention for their exceptional electronic and optical properties, positioning them as promising candidates for diverse optoelectronic applications. However, the conventional batch-wise synthesis methods often struggle with limitations in control over reaction conditions, scalability, and reproducibility. Addressing these challenges, we propose a novel approach for the synthesis of defect-free single crystal perovskites using continuous-flow reactors fabricated via 3D printing technology. Our methodology leverages the advantages of continuous-flow platforms to overcome the shortcomings of batch protocols. By digitally designing reactors and employing low-cost stereolithography with commercially available resins, we establish tailored continuous-flow platforms for the synthesis of lead halide perovskites. The reactor chambers are meticulously crafted to enable the controlled, continuous addition of reagents, thereby ensuring consistent concentrations within the reactor. Through a combination of residence time distribution (RTD) and computational fluid dynamics (CFD) experiments, we optimize the reaction chamber design to achieve precise control over reactant concentrations, reaction times, and temperature profiles. This optimization process facilitates the synthesis of high-quality perovskite crystals with reproducibility and scalability. Our experimental results demonstrate the successful synthesis of high-quality single crystal perovskites under both seeding and seedless conditions. The obtained crystals exhibit excellent photoluminescence properties and optimal optoelectronic responses, surpassing those achieved through conventional batch synthesis methods. Moreover, our continuous-flow approach yields perovskite crystals with lower surface roughness compared to analogous batch synthesis conditions, showcasing the effectiveness and potential of this innovative technology in advancing perovskite materials for optoelectronic applications.[1]

Acknowledgements

This work was supported by FEDER/Ministerio de Ciencia e Innovación – Agencia Estatal de Investigación (PID2020-119628RB-C33), European Union's Horizon 2020 (GA no. 101026335), Generalitat Valenciana (CIDEGENT 2018/036 and CIGRIS/2021/075) and FPU21/03740.

References

[1] D. Iglesias *et al.*, '3D printed flow reactors for the synthesis of single crystal perovskites', *Materials Today Energy*, vol. 39, p. 101476, Jan. 2024, doi: 10.1016/j.mtener.2023.101476.