Observation of the Nucleation of an Aggregation Induced Emission (AIE) Molecule in a Microfluidic System by Fluorescence Lifetime Video (FLIM)

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Polymorphism control of organic molecules has been under keen investigation for decades. Nucleation is the first step to control the polymorphs of crystals. Despite the Classic Nucleation Theory has been well developed and widely applied since 1950s, it has purposely avoided the difficulty of the structure of the nuclei. This thus needs further experimental investigations. So far, however, observation of nucleation encountered great difficulties, mainly because it is a small, random and rare event.[1, 2] The aim of this research is to developed a novel approach to control crystallization and probe the structure and kinetics of nucleation by fluorescence.

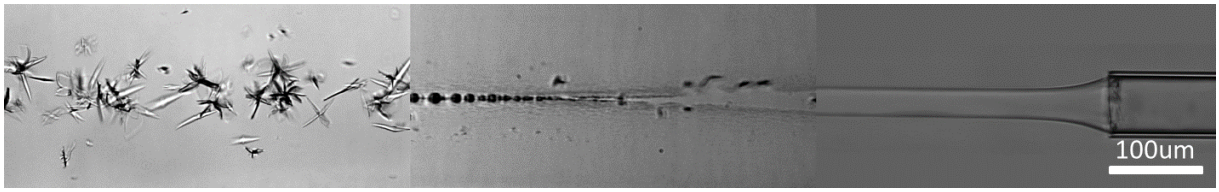

Figure 1. Crystallization of DBDCS in the microfluidic system.

Therefore, a new microfluidic system was built (Fig. 1) to control the crystallization of DBDCS, a molecule that is not fluorescent in solution, but becomes fluorescent after aggregation. A UV laser is focused at different places along the flow through a microscope, enabling an in-situ detection of nucleation by FLIM. The transit time of a particle moving flow through the field of view, depending on the velocity, is usually less than 40ms, wherein we can record its intensity, lifetime and shape. From the number of crystals detected at different positions of the same flow for the same duration, we can measure the nucleation rate. From their average sizes, we can deduce the growth rate. From their lifetimes, we can infer the polymorph. Real-time FLIM video of the moving particles were recorded for the first time. By changing microfluidic parameters, two types of crystallization processes have been observed: nucleation in the mixed solvents or liquid-liquid phase separation followed droplet formation and crystallization in the droplets. Depending on the composition of the anti-solvent, three different polymorphs were observed. A DBDCS/good solvent/bad solvent ternary phase diagram is partially built to explain the phenomenon.

We shall soon try to use fluorescence to detect the nuclei associated with the different polymorphs of DBDCS.

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References:

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[2] Vu-Long Tran et al., *New J. Chem.*, **2016,** 40, 4601-4605