

Template induced targeted crystallisation of computationally predicted polymorphs.

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Polymorphism is defined as the ability of a compound to exist in different crystal packing arrangements. Different polymorphs possess different physical and chemical properties and are therefore of high commercial interest across a range of industries including pharmaceuticals, dyes, pigments, food industries. Whilst polymorph screening is routinely performed, they are generally a trial and error processes without a targeted outcome. We recently reported a new robust template induced crystallisation method for the targeted crystallisation of carbamazepine form-V (CBZ-V)¹. The generality of the method (figure 1(a)) was demonstrated by producing novel polymorphic forms of cyheptamide (CYH-III). The studies of the growth of CBZ-V and CYH-III on the surface of dihydrocarbamazepine form-II (DHC-II) indicate that crystals grow both laterally and vertically on the template surface without any face selectivity (figure 1(b)), indicating epitaxial induced two-dimensional preferential nucleation as the mechanism. Analysis of the template surface at different time points of vapor deposition from the nano-micro scale indicates Stranski-Krastanov growth mode². Utilizing the robust templating method, following crystal structure prediction studies, we have been able to target and crystallize novel polymorphic forms of organic compounds of pharmaceutical relevance. Based on the results, we propose a set of templating rules and show that template induced crystallisation can be used as a one-step synthetic route for the targeted crystallisation of certain thermodynamically plausible computationally predicted polymorphs.

1. Vijay K Srirambhata, Rui Guo, Sarah L. Price and Alastair J. Florence, (2016). Chem. Commun., 52, 7384-7386.
2. Arvind Baskaran and Peter Smereka, (2012). J. Appl. Phys., 111, 044321.

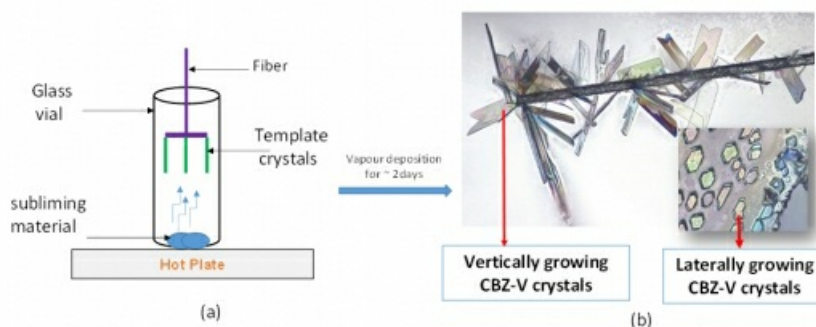


Figure 1: (a) Templating method. (b) Optical microscope images of CBZ-V on DHC-II surface.

Keywords: [Polymorphism](#), [Template induced crystallisation](#), [Homo- and hetero-molecular epitaxial growth mechanism](#).