An Experimental Verification of morphology of ibuprofen crystals from CAMD designed solvent

In our previous work [Karunanithi et al., 2006. A computer-aided molecular design framework for crystallization solvent design. Chemical Engineering Science 61, 1247-1260] we proposed a computer-aided molecular design (CAMD) framework to design solvents for crystallization processes. One of the important aspects of that work was the consideration of a qualitative property, namely crystal morphology, along with other physico-chemical properties (quantitative) of the solvents within the modeling framework. However, it is our view that consideration of any qualitative property, such as morphology of crystals formed from solvents, necessitates additional experimental verification steps. In this work we report the experimental verification of crystal morphology for the case study, solvent design for ibuprofen crystallization, presented in Karunanithi et al. [2006. A computer-aided molecular design framework for crystallization solvent design. Chemical Engineering Science 61, 1247-1260]. This we believe is an important step for the validation of the proposed solvent design model.