Crystal Growth and Morphology Prediction of Two Quinacridone Polymorphs

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Quinacridone – a widely used organic pigment – is known to have three polymorphs. Two of them, the beta-polymorph and the gamma-polymorph, grow as very thin platelets.

Vapour growth starting from both polymorphs was performed by vacuum sublimation in a specially constructed furnace. During characterization of the polymorphic phases by DSC recrystallization was observed. This led to the formation of beta-crystals. The new polymorph was formed via the vapour phase.

To explain the observed morphology of the crystals computer simulation of crystal growth was performed. Both the attachment energy model and kinetic Monte Carlo simulations were used to predict the crystal morphology starting from the crystal structure. The crystal structure of the gamma-polymorph is known from the Cambridge Structural Database and the crystal structure of the betapolymorph was predicted using the Polymorph Predictor of Accelrys.

The attachment energy model based on the Hartman Perdok theory fails to predict the large aspect ratio of the platelet morphology for the polymorphs. The kinetic Monte Carlo simulations use the actual crystal structure and growth mechanism; they predict the morphology of both polymorphs successfully.

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