Analysis of crystal morphology of sulfamerazine (SMZ) based on the interfacial structure via molecular dynamics simulation

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The crystal morphology is important for industrial crystallization processes. The attachment energy (AE) was used to predict the crystal growth morphology of sulfamerazine (SMZ). The SMZ morphology predicted by AE is dominated by {0 2 0}, {1 0 1}, {2 1 0}, {2 0 0}, {0 1 1}, and {1 1 1} surfaces for phase I crystal and {1 1 1}, {0 0 2}, {0 2 1}, {0 2 0}, and {1 0 2} surfaces for phase II crystal. Based on these surfaces, molecular dynamics (MD) simulations have been performed on the interface between the SMZ crystal surfaces and acetonitrile (ACN) solvent to study the solvent effect on the crystalization by understanding the crystal growth and dissolution mechanisms in the solvent. Furthermore, we analyzed the interfacial structures of crystal surface, radial distribution function and diffusion coefficient of solvent, which heavily influenced the crystal growth behavior and morphology. This study showed the effects of solvent on crystal morphology and possible mechanisms of crystallization.