Prediction and verifying of the spiral growth model of adipic acid crystal morphology in aqueous solution

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In this study, adipic crystal morphology grown from aqueous solution under low supersaturation condition was accurately predicted by simulation with that of experimental results. Previous models like BFDH (Bravais-Friedel-Donnay-Harker) model and AE (attachment energy) model only considers internal factors; crystal structure. Better prediction was achieved by including two external habit-controlling parameters, surface scaling factor and molecular orientation. Experimental data of adipic acid crystal morphology grown from aqueous solution features hexagonal plate with dominant face (100). Molecular dynamics simulation reproduced the experimental results by using spiral growth model assuming kink integration to be the time limiting step. Kink integration was taken into account by two external parameters, anisotropic local concentration at the surface (surface scaling factor) and free energy barrier for the reorientation (molecular orientation factor). Differences between the results can be explained by two external factors mentioned above with molecular bond energetics at the interfaces.