Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Crystal growth: an anisotropic mass transfer process at interface

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Application of Equation (17) to calculate the anisotropic growth rates can help use to obtain the anisotropic growth geometry for the single crystal. As shown in Figure S1, thermodynamic morphologies of rutile-TiO_2, anatase-TiO_2, and brookite-TiO_2 have been successfully predicted.

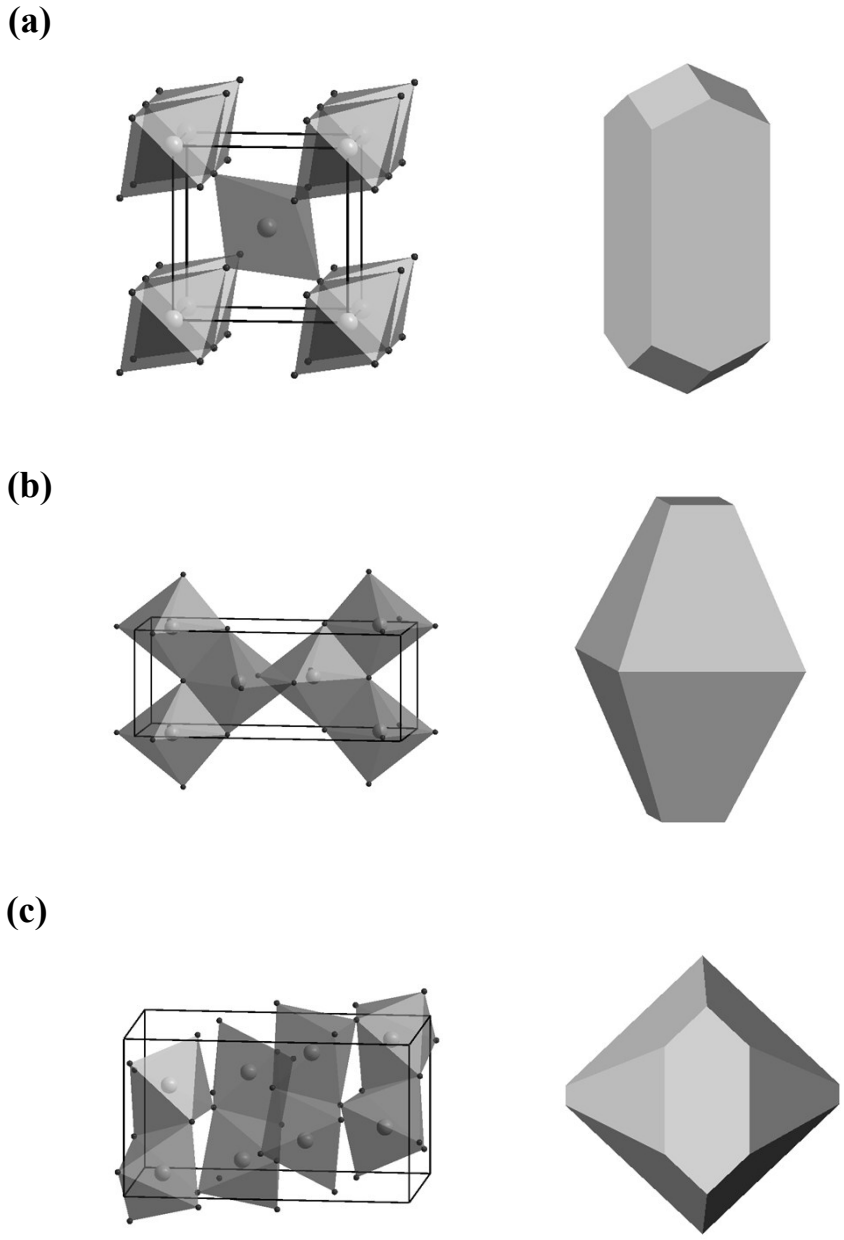

Fig. S1 Crystallographic structures and thermodynamic morphologies of TiO_2 single crystals. (a) Rutile-TiO_2, (b) Anatase-TiO_2, (c) Brookite-TiO_2.

Table S1 Different crystal growth models

Crystal growth model	Model description	Characteristics
Gibbs-Wulff model	The equilibrium shape of single crystal growth is constructed by the minimum surface energy.[S1]	By calculating the surface energy under different surface conditions, several morphologies can be obtained. However, the crystal surface is not growth active.[S2,S3]
BFDH theory	Crystal growth rate is proportional to $1/d_{hkl}$, where d_{hkl}, is the interplanar distance of $\{hkl\}$ crystalline faces.[S4]	Only one equilibrium shape of single crystal will obtained by this model.
Attachment energy (AE) model	Crystal growth rate is proportional to its attachment energy. [S5]	Morphology of organic single crystals will obtained by this model.
BCF theory	The curvature of the spiral near its origin was related to the spacing of successive turns and the level of supersaturation.[S6]	Some critical physical parameters are assumed without experiential values.
Surface area limited model	It combines surface diffusion, step growth rate and surface site availability to describe anisotropic coarsening of faceted nanoparticles.[S7]	The effective number of sites available for monomers to adsorb determines nanoparticle shape evolution.
Present model	*The chemical bonding architecture is used to regulate the mass transfer process of a compound in a straightforward manner.*	*Multiple morphologies that may be exhibited for a single crystal by identifying all possible chemical bonding architectures at [uvw] growing interface, enclosing the origin of various geometries of a multicomponent crystal.*

References

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