Electronic Supplementary Material (ESI) for Soft Matter.
This journal is © The Royal Society of Chemistry 2018

Supplementary Information

Solid-Phase Nucleation Free-energy Barriers in Truncated Cubes: Interplay of Localized Orientational Order and Facet Alignment

Abhishek K. Sharma, Vikram Thapar, and Fernando A. Escobedo

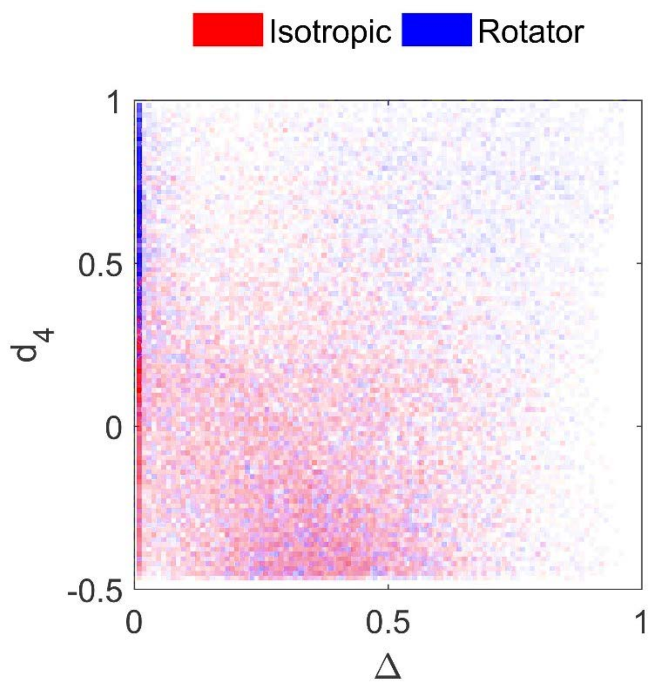
School of Chemical and Biomolecular Engineering, Cornell University, Ithaca, NY 14853

1 Calculation of Facet Alignment Measure

Here we describe the methodology used to implement facet alignment (Δ) for convex particles with convex facets (this can conveniently be generalized for concave cases). For two particles, say particle 1 and particle 2, the facet alignment measure is defined in the following steps:

1. Search for a pair of facets (belonging to either particles) F_{1n} and F_{2n} that have the shortest centroid-to-centroid distance.
   1.1. Centroid of a face is defined as the arithmetic mean of individual Cartesian coordinates all vertices of the face.
2. Project F_{1n} to the plane of F_{2n}.
   2.1. Create a 2×3 transformation matrix T to map vertices of F_{1n} onto a 2-D coordinate system defined in the plane of F_{2n}.
      2.1.1. In order to define the transformation matrix, we need two orthogonal unit vectors that lie in the plane of F_{2n}. Arbitrarily choose one edge vector of the face as the first unit vector. To obtain the second unit vector, use the cross product of the first unit vector with the cross product of itself and another non-parallel edge vector.
   2.2. Multiply T with each of the vertices ($3 \times 1\ matrix$) of F_{1n} to obtain the projected face F_{1n}^{p} in the plane of F_{2n}. Repeat the same for the vertices of F_{2n} to obtain its description in the 2-D coordinate system F_{2n}^{p}
3. Find the intersection area A_{12} between F_{1n}^{p} and F_{2n}^{p}.
   3.1. For all edges belonging to face F_{1n}^{p}, find their intersections with all the edges of F_{2n}^{p}. Call the set of intersections *I*.
   3.2. Find all the vertices that belong inside both F_{1n}^{p} and F_{2n}^{p}. This can be done using *inpolygon* MATLAB built-in function. Call this set of vertices *C*.
   3.3. Take the union of *C* and *I* and evaluate the area A_{12} of the resulting polygon.
4. Repeat steps 2 & 3 by projecting F_{2n} to the plane of F_{1n} and obtain area A_{21}.
5. Find $A_m = \max(A_{12}, A_{21})$.
6. Evaluate $\Delta = A_m / A_l$, where A_l is the area of the largest facet present on the particle.

2 d_4 $vs.$ Δ Histogram for s=0.667



It is noted that there is no significant range of Δ that is not accessed by the rotator phase, thus the hindrance due to incompatible facet matching is minimal.