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 ($\Delta$) 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 $2 \times 3$ 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 $\text{inpolygon}$ 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.
It is noted that there is no significant range of $\Delta$ that is not accessed by the rotator phase, thus the hindrance due to incompatible facet matching is minimal.