Molecular Dynamics of Oriented Attachment

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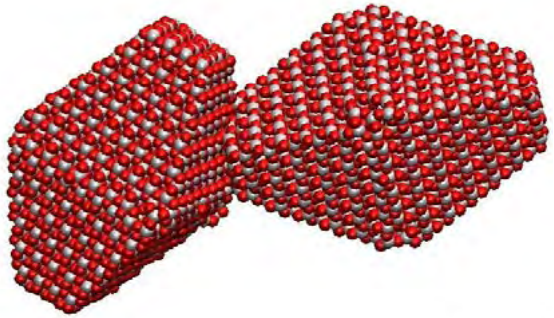
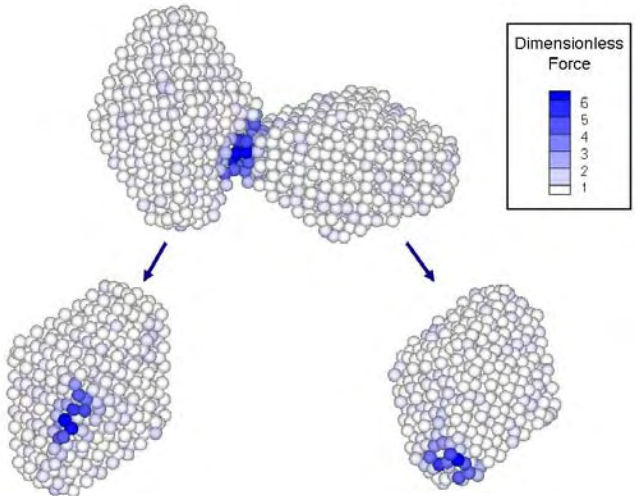
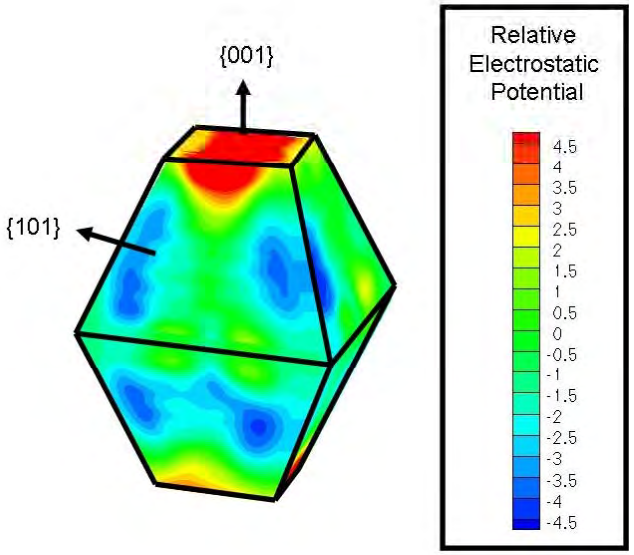


TiO_2 (anatase) nanoparticles aggregate preferentially on the edges of {001} facets and the edges between two {101} facets.



Electrostatic forces dominate and are the highest between aggregating edge atoms.



Electrostatic potential maps indicate regions of positive and negative charge associated with under-coordinated Ti and O edge atoms that create high-order multipole moments and drive aggregation.