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ReaxFF Reactive Force Field Study of Oriented Attachment of TiO_2 Nanocrystals in Vacuum and Humid Environments MURALIKRISHNA RAJU, Dept of Physics, The Pennsylvania State University, KRISTEN FICHTHORN, Dept of Chemical Engineering, Dept of Physics, The Pennsylvania State University, ADRI VAN DUIN, Dept of Mechanical and Nuclear Engineering, The Pennsylvania State University — We use a ReaxFF reactive force field to study the aggregation of various titanium dioxide (anatase) nanocrystals in vacuum and humid environments. The nanocrystals are in the 2-6nm size range, with shapes dictated by the Wulff construction. In vacuum, the nanocrystals tend to merge along their direction of approach, resulting in a polycrystal. By contrast, in the presence of water vapor, the nanocrystals tend to reorient themselves and aggregate via the oriented attachment mechanism to form a single or twinned crystal. We find that adsorbed water molecules and hydroxyl groups play multiple roles in oriented attachment. As the nanocrystals approach one another closely, adsorbed water molecules and surface hydroxyls prevent their immediate aggregation. These adsorbed species create a hydrogen bonding network, which aligns the nanoparticles in registry. Upon the eventual elimination of these species, the nanoparticles fuse into a single-crystal or twinned aggregate. We observe this aggregation mechanism for anatase(101), anatase(112), and anatase(001) surfaces, as is also seen experimentally. This indicates the important role that solvent plays in nanocrystal aggregation and how solvent can be a powerful tool for directing and controlling nanocrystal growth.

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