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Nucleation in the Anatase-to-Rutile Transformation of Nanocrystalline Anatase[1] YA ZHOU, KRISTEN FICHTHORN, Penn State University — We use molecular dynamics (MD) simulations to investigate the anatase-to-rutile transformation of titania nanocrystals in vacuum. By comparing energies of various Wulff-shaped nanocrystals, we find that rutile becomes favored over anatase past a critical size that is significantly smaller than that predicted by thermodynamic models based on surface energies, indicating that edges play a profound role in the energetics of nanocrystals. We develop a local order parameter to distinguish anatase from rutile and intermediate anatase (112) twins at the resolution of a single TiO_2 unit and we apply it in direct MD simulations of spherical and Wulff-shaped anatase nanocrystals, as well as nanocrystal aggregates. To further characterize the transformation, we simulate X-ray diffraction of the nanoparticles. The anatase-to-rutile transformation originates at surfaces and interfaces, where alternating anatase (112) twin planes form. Rutile nuclei form via transformation of anatase (112) twins and they grow rapidly when they reach a critical size that can be as small as 10 TiO_2 units. Rutile nucleii tend to have planar structures bounded by (101) surfaces and the ease with which they form is dependent on the structure of the nanocrystal.

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