Thermodynamic Analysis of Multiply Twinned Particles: Surface Stress Effects

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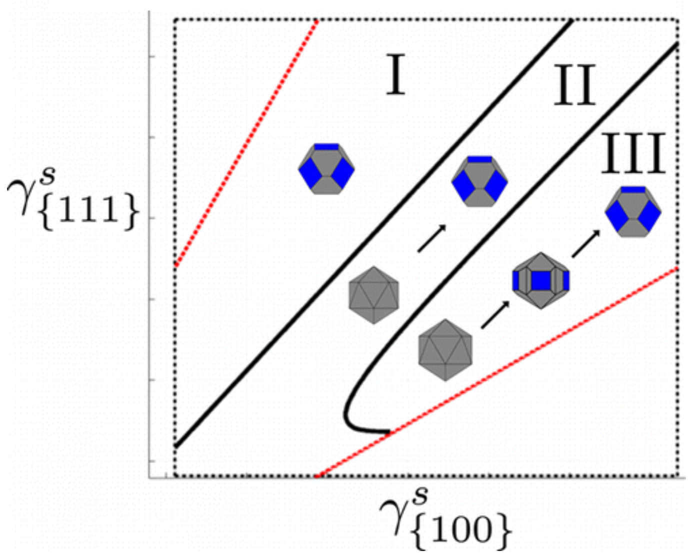
In nanoparticle technologies, such as SERS, fuel cell catalysis and data storage, icosahedral (Ic) and decahedral (Dh) nanoparticles, owing to their defect structure, provide higher functionality than their single-crystal Wulff counterparts. However, precise control on the yield of multiply twinned structures during solution synthesis has been challenging. In particular, it is difficult to synthesize icosahedral structures due to the high volumetric strain energy associated with the disclination defects and the transition to decahedral morphologies. We show the role of surface stresses in influencing the thermodynamic stability of multiply twinned particles. Increasing the surface stresses inhibits the formation of decahedral structures and increases the likelihood of synthesizing metastable icosahedral particles. Analogously, large decahedral particles may be stabilized by decreasing the surface stresses. Therefore, by tailoring the solution chemistry to influence the surface stresses, greater control over the synthesis of multiply twinned structures can be achieved.

- We compute the strain energy of the disclination line defects in the Ic morphology.
- We incorporate the effect of surface energies and stresses, and present the thermodynamic analysis of the stability regimes for MTPs.
- We observe that, in the region where MTPs are thermodynamically viable, higher surface stresses result in an increase in the likelihood of obtaining Ic nanoparticles and lower surface stresses stabilize the formation of Dh morphologies.
- This phenomena emphasizes the importance of measuring and controlling surface stresses in the solution synthesis of nanoparticles.



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