Kinetic Monte Carlo Simulations for Twinned Nanoparticles Growth

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The growth of face-centered cubic (fcc) metal nanoparticles in solution is often governed by kinetic effects rather than equilibrium thermodynamics, giving rise to stacking faults and twin boundaries. Owing to their low formation barriers, these defects promote the emergence of multiply-twinned particles (MTPs), including decahedral and icosahedral morphologies. Such structures are distinguished by nonuniform strain fields and defect-rich interiors, which are widely associated with enhanced catalytic and functional properties. Although successive twinning has been proposed as a dominant mechanism for their growth, the atomic-scale pathways- remain unresolved. Here, we employ kinetic Monte Carlo simulations to explore the defect-mediated growth of twinned metal nanoparticles and to resolve the kinetic origins of morphological diversity. By modeling their formation, we reveal how subtle variations in kinetic barriers redirect growth trajectories, producing distinct nanoparticle shapes under otherwise identical conditions.

Keywords:
Nanocrystal growth, Multiply Twinned Particles(MTPs), Stacking Faults, Twin Boundaries, Anti-Mackey Cluster, pent-twinned nanorods

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