Elastic Strain Energy Effects in Faceted Decahedral Nanoparticles

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Decahedral morphology, with re-entrant surface modifications, is one of the common structures observed in nanoparticles. These motifs, although thermodynamically stable only at very small size ranges, have been experimentally observed to grow up to much larger sizes (100 nm to several micrometers). Whereas the surface energy plays an important role, the contributions of the elastic strain energy are non-negligible at larger sizes and the effect of stress relaxation due to re-entrant surface faceting is poorly understood. We compute the volumetric strain energy due to the disclination defect using finite element analysis and show the relaxation due to the formation of re-entrant surfaces. Contrary to conventional wisdom, the disclination strain energy is shown to be a nontrivial function of the geometry and in general increases with increasing aspect ratio. The computed strain energies also result in approximately 50% increase in the stability regime than the previously reported results obtained using thermodynamical analysis. Finally, finite element analyses are utilized to explain the commonly observed defect configurations and compute the internal rigid body rotations in these particles.

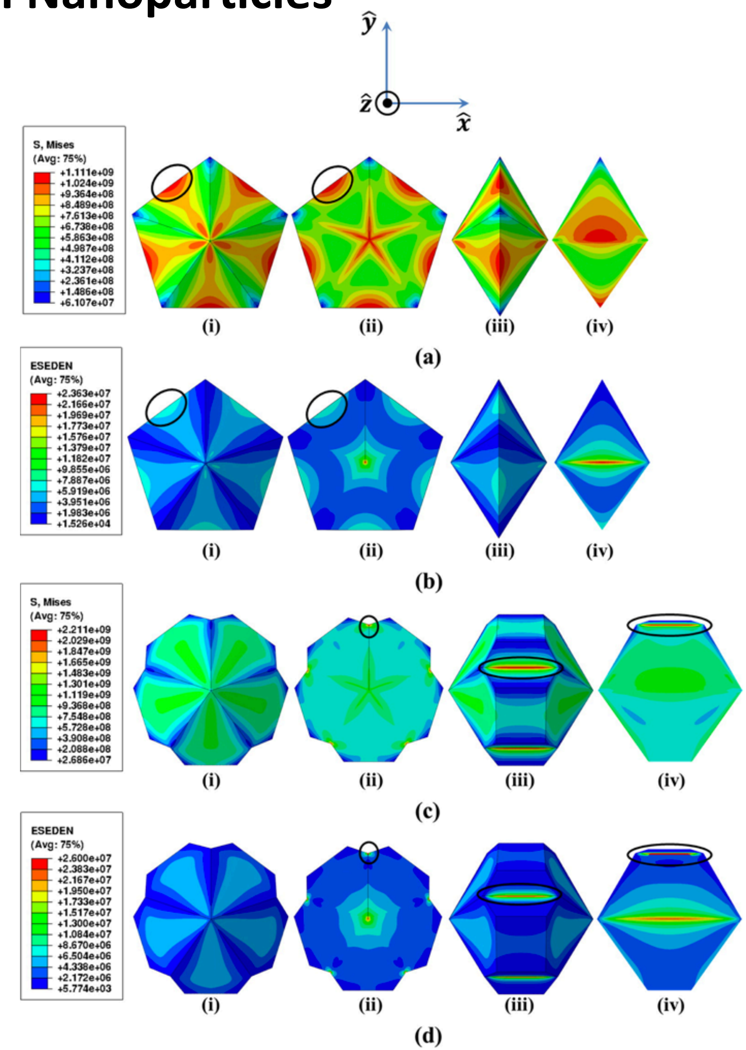

Figure: (a,c) Von Mises stress concentration and (b,d) strain energy density profiles in decahedral nanoparticles with geometric parameters: (a,b) β = 1, h_r = 1, and (c,d) β= 0.5, h_r = 1.5. In (i) and (ii), the nanoparticle is viewed along the z-axis direction (i.e., along the disclination axis). The section showed in (ii) represents a cut along the center of the nanoparticle (i.e., along the plane z = 0). Shown in (iii) and (iv) is a side view of the nanoparticle along the x-axis and the cut in (iv) is made along the x = 0 plane. The stress concentrators and regions of high strain energy density where defects are likely to nucleate are highlighted.

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