HRTEM and image simulations of icosahedral nanoparticles: A detailed analysis of images and their power spectra.

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Icosahedral multiply twinned nanoparticles of Ni, Cu and Au were studied by HRTEM, concentrating on particles oriented along the 3-, 2- and 5-fold axes. Due to multiple superposition of differently oriented tetrahedral subunits the images show complex contrast patterns. In the power spectra (PS) of the images frequently a splitting of diffraction spots can be observed. Mostly this splitting was attibuted to an angular misalignment of twinned tetrahedra since regular tetrahedra cannot form an icosahedron without spatial dicontinuities. A perfect icosahedron consists of 20 homogeneously deformed tetrahedra (rhombohedral point group symmetry, angle ≈ 63.4°) with preserved close packing but two different nearest neighbour distances. For such icosahedra image simulations were performed for the main orientations. The related PS show the typical spot splitting as well, clearly indicating that angular misalignment is not the reason for this phenomenon. Further simulated images were calculated for selected pairs and groups of tetrahedral subunits. Analysis of their PS reveals that the spot splitting has its origin in interference effects (in analogy to Young's interference fringes) of diffraction patterns from tetrahedral units arranged diametrically opposite and contributing to the same diffraction spot. Detailed analysis of images and PS from real icosahedral particles shows which modifications of the principal interference pattern can be introduced by spatial/angular misalignment.