The Crystallography of Nanparticles (particularly pentagonal ones)

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Traditionally crystallography focuses upon the atomic structure of materials, but in many respects it can be traced back to the study of crystals before the Christian era. The two combine when one considers the structure of nanoparticles where due to finite size effects such as large surface energy contributions, the shape and internal arrangement of atoms can be coupled. This is well known for icosahedral and decahedral (or pentagonal) ones which contain disclinations and are commonly found in fcc metals. Up to now it has been believed that these are special structures that are only thermodynamically stable below a critical size, and then undergo a first-order phase transition to single crystals. After a general introduction, this talk will focus upon a re-examination of this conclusion based upon recent results which indicate that instead of a first-order phase transition, there is a continuous transition associated with migration of the disclination from the center of the particles. It appears that there are still many unknowns in the combined crystallography of atoms and shape in nanoparticles.