CORE-SHELL AND JANUS STRUCTURES IN NANOALLOYS

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Abstract

Binary metallic nanoparticles (often referred to as nanoalloys) present a wide variety of structures and properties, which make them suitable for many applications in catalysis, optics, magnetism and biomedicine. When the two components are weakly miscible, phase-separated arrangements, such as core-shell and Janus arrangements, are the expected to be the most favourable.

Here we consider a series of binary nanoparticles (Ag–Cu, Ag–Co, Ag–Ni, Au–Co, Cu-Ni) and computationally determine their most stable structures for different sizes and compositions. We single out transitions between core-shell and (quasi)-Janus arrangements, showing that they can be rationalized by a unifying concept, that is symmetry breaking caused by the accumulation of strain at the atomic level and its subsequent release. The computational results are compared to the experimental data with good agreement.

Keywords: Nanoparticles, alloys, computational methods

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