Exploring epitaxial relationships between InAs nanowires and shaped Au nanoparticles

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The high electron mobility and strong spin-orbit interactions make InAs nanowires (NWs) an excellent material for the micro-electronics industry. However, our inability to precisely control their structural properties like defects, crystalline orientation, etc pose a significant obstacle to their widespread usage. Recent evidence in the literature suggests an epitaxial relationship exists between the structural properties of a NW and the size and shape of the metal seed nanoparticle (NP) from which it is grown. In this work, we have explored the epitaxial relationship between H-terminated [111] zinc blende (ZB) and [0001] wurtzite (WZ) InAs NW fragments with the (111) & (100) facets of Au NP using density functional theory calculations. The binding energies suggest greater stability of ZB [111] over WZ [0001] fragments on Au surface facets with both fragments being more stabilized by Au (111) than Au (100) surface. This suggests that shaped Au NPs with a higher number of Au (111) facets should produce higher yields of InAs NWs, with (111) growth directions. A chemical potential based Arrhenius model that takes into account these binding strengths, is used to compare the relative thermodynamic stability of these NW-NP interactions.