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Exploring epitaxial relationships between InAs nanowires and shaped Au nanoparticles DEBOSRUTI DUTTA, University of South Florida, R. MOHAN SANKARAN, XUAN GAO, Case Western Reserve University, VENKAT R. BHETHANABOTLA, University of South Florida — 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.

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