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Interaction of Nanometer-Sized Gold Nanocrystals with Rutile (110) Surface Steps Revealed at Atomic Resolution[1] WENPEI GAO, ANN SE CHOI, JIAN-MIN ZUO, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — We show that progress in atomic resolution Z-contrast imaging now enables a detailed understanding of nanocrystal (NC) interactions with surface steps. The interaction is studied based on the shape, orientation, strain and interfacial energy of Au NCs supported on surface steps of TiO_2 (110) surfaces with a small miscut angle. Au NCs with the approximate $Au(111)_{[-110]} \| TiO_2\ (110)_{[001]}$ epitaxial relationship observed as it is on flat surfaces are selected for study. The presence of surface steps induces a small rotation in the NC in an amount less than the surface miscut angle. From the recorded images, we measured the atomic displacement around the surface steps. It shows that there is significant strain near the surface step inside Au NC. Experimental measurements of NC geometry on low miscut surfaces, however, reveal an approximate similarity in NC shapes. From this, an analysis of the average NC shape is performed using the modified Wulff-Kaishew theorem. Compared to NCs on flat surfaces, the measurements show a large height/width ratio, lowered interfacial energy and increased triple line energy for NCs observed on vicinal rutile (TiO_2) surfaces.

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