Gold bipyramidal (GBP) nanoparticles show significantly higher field enhancement than nanorods, being promising candidates for sensing applications involving enhanced Raman and fluorescence spectroscopy techniques [1,2]. The plasmon resonance spectral range and the optical enhancement can be tuned through shape and size of GBP nanoparticles. However, full shape and size control during the growth is challenging since the aspect of the final nano-object depends on various factors including initial seed geometry, surfactant type and ions concentrations [3]. Here, we have investigated the role of the cetyl trimethylammonium bromide (CTAB) surfactant, as its use is crucial for GBP nanoparticle formation and stability, using atomistic molecular dynamics simulations. The surface coverage of CTAB (positively charged) heads and (bromide) counterions has been investigated on various exposed surfaces of the gold seeds, showing different behavior on side, bridge and tip facets. This difference in coverage partially explains the anisotropic growth of GBP nanoparticles, which differentiates from that of nanorods since high index facets, such as Au(113), Au(115) and Au(117), can be stabilized on the side of the nanoparticles, providing different aspect ratios of the final object[4,5]. We found that CTAB surfactant forms micellar structures also on stepped high index surfaces, with inter-micelles channels similar to those observed on nanorods [6]. However, the presence of higher CTAB coverage and narrower inter-micelles channels in GBP nanoparticles as compared to nanorods, explains the formation GBP nano-objects and their remarkable stability.