From Multiply-Twinned Particles to Epitaxial Nanocrystals: the crucial role of interface on the structure of Ag nanoparticles

BOQUAN LI, JIAN-MIN ZUO, University of Illinois at Urbana-Champaign — The effect of substrate on the structure of nanometer-sized metal particles is investigated for Ag on silicon surfaces. The nanometer-sized Ag particles, formed by vapor deposition of Ag on hydrogen-terminated Si (001) surfaces at room temperature, adopt multiply-twinned structures, while the Ag particles of similar sizes on H-Si (111) surfaces assume the face-centered cubic (fcc) crystal structure. Upon annealing, the multiply-twinned Ag nano-particles on H-Si (001) transform into fcc nanocrystals. The fcc Ag takes up the cube-on-cube epitaxy, with the orientation relationship of Ag (001)//Si (001) and Ag[110]///Si[110]. An energetic model is developed to account for the transition from multiply-twinned particles to fcc epitaxial crystals, in which the interface energy change on H-Si(001) due to hydrogen desorption plays a crucial role. A pair-correlation function study will also be presented in an effort to accurately determine the inter-atomic distances and strain in the multiply-twinned Ag nanoparticles.

Boquan Li
University of Illinois at Urbana-Champaign

Date submitted: 30 Nov 2004

Electronic form version 1.4