

Self-assembled supported Co nanocrystals: The adhesion energy

of face-centered-cubic Co on SrTiO₃(001)-(2X2)

Fabien Silly^a and Martin R. Castell

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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We have investigated the structure and morphology of self-assembled cobalt nanocrystals supported on a SrTiO₃(001)-(2X2) substrate using scanning tunneling microscopy. Nanocrystals with a truncated pyramid shape were imaged, allowing crystallographic identification of the cluster facets. These nanocrystals result from the epitaxial growth of fcc Co on SrTiO₃(001). The dimension of the nanocrystal facets at equilibrium and an energy minimization calculation result in $\gamma_{\text{adh}}=(3.96\pm 0.37)\text{J/m}^2$ for the adhesion energy of face-centered-cubic Co/SrTiO₃(001)-(2X2) APPLIED PHYSICS LETTERS **87**, 053106 (2005)

Fe nanocrystal growth on SrTiO₃(001)

Fabien Silly and Martin R. Castell^a

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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We have investigated the structure and morphology of self-assembled iron nanocrystals supported on a SrTiO₃(001)-c(4X2) substrate using scanning tunneling microscopy. Nanocrystals with a truncated pyramid shape were imaged, which result from the epitaxial growth of bcc Fe on SrTiO₃(001). By using the dimensions of the nanocrystal facets at equilibrium and an energy minimization calculation, we obtain the adhesion energy $\gamma_{\text{adh}}=(3.05\pm 0.15)\text{J/m}^2$ for bcc Fe on SrTiO₃(001)-c(4X2). © 2005 American Institute of Physics. [DOI: 10.1063/1.2008375] APPLIED PHYSICS LETTERS **87**, 063106 (2005)

Growth of Ag icosahedral nanocrystals on a SrTiO₃(001) support

Fabien Silly and Martin R. Castell^a

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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We have investigated the structure and morphology of self-assembled silver nanocrystals supported on a SrTiO₃(001)-(2X1) substrate using scanning tunneling microscopy. Ag forms nanocrystals with five-fold symmetry which have an icosahedral shape. Nanocrystals with point, edge, and face orientation (five-fold, two-fold, and three-fold symmetry, respectively) have been studied. The images of these nanocrystals allow a crystallographic identification of the supported shape of the icosahedral form.

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Encapsulated Pd Nanocrystals Supported by Nanoline-Structured SrTiO₃(001)

Fabien Silly* and Martin R. Castell

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, U.K.

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Palladium nanocrystals were grown on a nanostructured SrTiO₃(001) surface and annealed in ultrahigh vacuum

at 620 °C. This leads to the so-called strong metal-support interaction (SMSI) state, characterized by encapsulation of the metal clusters with an oxide layer. Scanning tunneling microscopy (STM) of the oxide adlayer on the Pd(111) cluster surface reveals two superstructures with different lattice parameters and crystallographic rotations. Interpretation of the STM images is most readily achieved via noncommensurate TiO_x surface layers which result in two distinct Moiré patterns.

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Growth shapes of supported Pd nanocrystals on SrTiO₃(001)

Fabien Silly, Andrew C. Powell, Marta G. Martin, and Martin R. Castell

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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Pd is deposited onto a reconstructed SrTiO₃(001) substrate in an ultrahigh vacuum environment. Elevated substrate temperature during or following deposition causes epitaxial Pd nanocrystals to form. The nanocrystal shape and size distributions are analyzed by scanning tunneling microscopy. We find that depending on substrate reconstruction and substrate temperature during deposition three shapes of nanocrystal are obtained: truncated pyramids, huts, and hexagonal shaped disks. In our previous study [F. Silly and M. R. Castell, *Phys. Rev. Lett.* **94**, 046103 (2005)] the energetics of the equilibrium nanocrystal shapes were analyzed. Here we report on the nonequilibrium growth shapes. We show that preferential growth for huts is along their (001) end facets. For hexagons growth proceeds by attachment to the side of the crystals. Truncated pyramids can grow preferentially along one of their (111) side facets resulting in an elongated shape.

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Selecting the Shape of Supported Metal Nanocrystals: Pd Huts, Hexagons, or Pyramids on SrTiO₃(001)

Fabien Silly and Martin R. Castell

Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

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Increasing interest in oxide supported nanoparticle science and technology is stimulating research into controlling nanocrystal shape. Pd forms nanocrystals on the surface of SrTiO₃(001), and depending on the crystallographic interface of the Pd with the substrate three shapes can be created: truncated pyramids, huts, and hexagonal shaped disks. Scanning tunneling microscopy reveals that the nanocrystal shapes are determined by the substrate reconstruction and the substrate temperature during deposition. A thermodynamic model is used to show that the pyramids and huts are stable structures, and that the hexagons are trapped in a metastable state.

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Bonding of Gold Nanoclusters to Oxygen Vacancies on Rutile TiO₂(110)

E. Wahlström,¹ N. Lopez,^{2,*} R. Schaub,¹ P. Thostrup,¹ A. Rønnau,¹ C. Africh,^{1,†} E. Lægsgaard,¹ J. K. Nørskov,² and F. Besenbacher^{1,‡}

¹CAMP, iNANO and Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark

²CAMP and Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark

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Through an interplay between scanning tunneling microscopy (STM) and density functional theory (DFT) calculations, we show that bridging oxygen vacancies are the active nucleation sites for Au clusters on the rutile TiO₂(110) surface. We find that a direct correlation exists between a decrease in density of vacancies and the amount of Au deposited. From the DFT calculations we find that the oxygen vacancy is indeed the strongest Au binding site. We show both experimentally and theoretically that a single oxygen vacancy can bind 3 Au atoms on average. In view of the presented results, a new growth model for the TiO₂(110) system involving vacancy-cluster complex diffusion is presented.

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