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The Growth of Nanostructures and Composite Films on Solids: Simulation and Phenomelogical Theory

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13. ABSTRACT (Maximum 200 words)

We have studied how the morphology of films grown by epitaxy changes after deposition, if we change the temperature. We have determined by simulations how isolated islands on a solid surface move or shrink by evaporation. We developed new methods to study how an ensemble of islands evolves when heated or when strain is imposed on the surface. This work provides an understanding of basic phenomena taking place during epitaxy.

14. SUBJECT TERMS

nano-structures, composite films, phenomenological theory.

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Final Report, Grant F 49620-98-1-0366 "The Growth of Nanostructures and Composite Films on Solids: Simulations and Phenomenological Theory"

The resources provided by this grant were used for theoretical research in several areas. We performed simulations of a number of phenomena taking place in the early stages of film growth by epitaxy. We have provided a complete description of how the islands formed on the surface during deposition, move[3], evaporate[9], and change shape[4]. We developed a method to simulate coarsening of these islands on a very long time and space scale[5,7]. We proposed and documented by simulations[8,10] that nucleation and growth can be controlled by imposing a periodic strain on the substrate, which will lead to the formation of a periodic array of islands of equal size. To achieve this kind of control has been one of the main goals of nano-science. It has been observed that islands grown on a surface prefer a specific size. We have shown[1] that this may happen because the island size fits a natural length of the electronic wave-function.

In the second part of the grant's duration, we switched to studying various catalytic systems. We have shown that surface strain modifies very substantially the adsorption isotherm[11] and this may explain why ultrasound passing through a catalyst changes its activity. Our current work examines the electronic properties of the γ-alumina[13] (which is the support of choice in most catalysts). This is the first calculation on this very demanding system. We have also determined how Pd atoms migrate on γ-alumina surface[14]. The adsorption of a metal on the surface of another metal, can modify its properties and we looked[16] at how the capacity of adsorbing CO is modified when Fe, Cu, or Ni islands are adsorbed on Ag. We were prompted to do this by very elegant single-molecule experiments by Wilson Ho, whose conclusions are confirmed by our calculations. Finally, we developed a new method for deriving potential expressions from *ab initio* energy calculations[2], proposed a new numerical method for performing quantum dynamics[15], developed an algorithm for solving Maxwell equations and used it to examine how the electromagnetic field under an STM tip is enhanced[12], and wrote a review article of our work on rate theory in quantum systems.

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