QUANTUM SIZE EFFECTS IN NANOSTRUCTURES: METAL THIN FILMS AND SEMICONDUCTOR NANOWIRES*

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Many physical properties of nanostructures are affected by the quantum confinement of electrons. In this talk I will discuss two examples: metal thin films and semiconductor nanowires. An intriguing and unexpected feature has recently been discovered during epitaxial growth of metal thin films on semiconductors. Instead of forming three-dimensional (3D) islands of various size as commonly observed for nonreactive interfaces, the metal atoms can arrange themselves into plateaus or islands of selective heights with flat tops and steep edges under certain growth conditions. This unusual behavior has been observed in quite a few systems including Ag/GaAs, Ag/Si(111), and Pb/Si(111). The implication could be significant, since the formation of these uniform, self-organized atomic structures points to a potentially interesting pathway to prepare functional nanostructures. It is believed that this extra stability of metal films with specific thickness has an electronic origin, and can be explained by the so-called quantum size effects due to electron confinement. These quantum well (QW) states also give rise to an oscillatory work function as the thickness varies, and thus affect the details of the surface adsorption processes. In addition, the QW states are directly connected to the oscillation in the exchange coupling between two magnetic materials across a nonmagnetic spacer layer of various thicknesses. I will present our recent density-functional calculations to study the electronic structure and film stability in Ag/Fe(100), Pb/Si(111), and various freestanding films [1]. The role played by the substrate and the crystal band structure will be discussed.

Another interesting class of nanostructures is semiconductor nanowires that have potential applications in many fields such as optoelectronics, photovoltaic cells, and especially device miniaturization. I will discuss the structural, electronic, and optical properties of hydrogen-passivated silicon nanowires along [110] and [111] directions with diameter up to 4.2 nm. The size and orientation dependence of the band gap is investigated. Quantum confinement becomes significant for $d < 2.2$ nm, where the dielectric function exhibits strong anisotropy and new low-energy absorption peaks start to appear in the imaginary part of the dielectric function for polarization along the wire axis [2].

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[2] X. Zhao, C. M. Wei, L. Yang, and M. Y. Chou, Phys. Rev. Lett. 92, 236805 (2004).