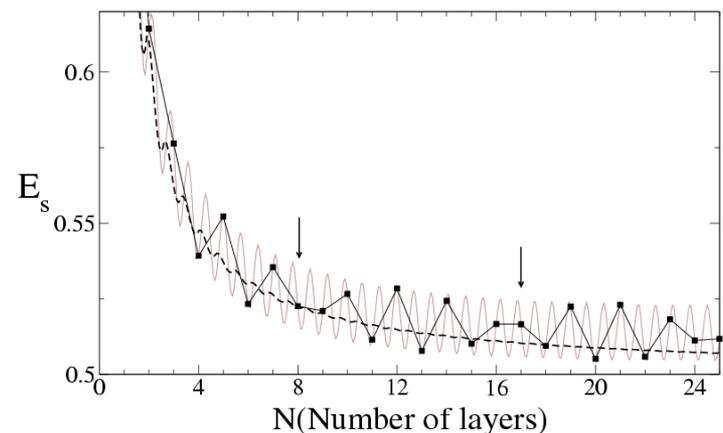
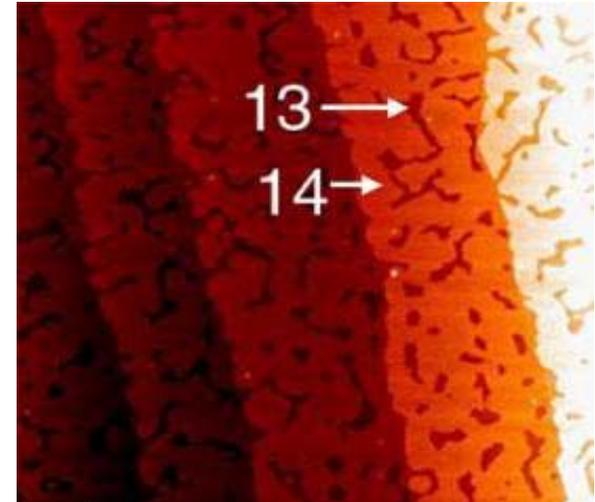


Electrical Transport in Thin Film Nanostructures

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Understanding electrical transport through nanostructures requires perfect control of their structure and morphology, which can sometimes be achieved via *self assembly*. Quantum size effects (QSE) in metallic nanostructures appear to be a strong driving force toward self assembly. For instance, ultrathin Pb films on Si and Ge can be grown in a quasi *bilayer-by-bilayer* fashion due to the QSE. This self-assembly mechanism produces films that are atomically flat over *macroscopic* distances.

Although quantum confinement leads to the quantization of kinetic energy, this effect alone cannot explain the robust quasi bilayer-by-bilayer growth seen in experiment. Instead, we find that this growth pattern can only be explained by the Coulomb potential resulting from an interface-induced Friedel oscillation or charge density wave.



M. Ozer et al., submitted for publication.

There is an increasing body of experimental evidence suggesting that the morphology of ultrathin Pb (lead) films is determined by quantum mechanical principles, provided that the growth conditions are precisely tuned. Already in 1989, Hinch and coworkers claimed that atomic Pb layers grow in a bilayer-by-bilayer fashion on a copper crystal at relatively low temperature. Normally one would have expected a layer-by-layer growth mode. Hinch and coworkers attributed this unusual growth mode to the quantum size effect. Many researchers later refuted their claim but now we have provided conclusive evidence for robust bilayer growth up to 25 monolayers of Pb, using scanning tunneling microscopy.

The QSE implies that the thickness of the film is comparable to the wavelength of the electrons. Pb has the peculiar property that the wavelength of the highest occupied electron level (i.e., the most energetic electron) matches the atom-layer spacing in the film almost perfectly; that is, every bilayer of Pb approximately accommodates one-and-a-half “Fermi wavelengths”. Although this matching argument had been used successfully to explain the electrical properties of thin Pb films, it does not easily explain why the film grows two atom layers at a time. Nonetheless, our observations strongly indicate that this simple matching argument has profound consequences for the thermodynamic stability of the films. We observe that Pb films on Si (silicon) evolve in a bilayer-by-bilayer fashion, starting at 5 monolayers. Atomically smooth films have been grown with layer thicknesses of 5, 7, 9, 11, 13, 14, 16, 18, 20, 22, and 25 monolayers. Evidently, bilayer growth is occasionally interrupted by the growth of a single-atom layer. Bilayer growth resumes after completion of this single atom layer. This even-odd crossover is a beating phenomenon typical of a wave-like interference patterns, and is to be expected from the above matching argument. In this case, the beating effect involves the periodicity of the crystal lattice and the Fermi wave length. The figure shows a microscopy image of a Pb layer near the first even-odd crossover point (13-14 ML). Large atomically-flat terraces are 14 monolayers thick. Because we slightly underdosed the amount of Pb, one can see holes that are one layer deep. This morphology is a dramatic manifestation of quantum growth. It furthermore shows that the Pb terraces can be as wide as the underlying Si terraces. This level of smoothness is astonishing for metal growth on semiconductors.

To fully understand this bilayer growth, we have calculated the total energy of the film, using a simple text book model. Interestingly, quantum confinement alone is not enough to explain bilayer growth. We need to explicitly introduce a potential reminiscent of the charge density oscillations near a surface or interface (Friedel oscillations). The graph shows how the total energy of the film oscillates as a function of thickness, nicely reproducing the bilayer oscillations. The model calculation even catches the even-odd crossover phenomenon (indicated by arrows). This simple picture is confirmed by much more rigorous calculations based on Density Functional Theory (DFT).

This work has produced films of amazing quality and also provided fundamental understanding into their formation mechanism. The interplay between structural stability and quantum mechanics could be significant for other nanoscale objects (especially when they are metallic), and possibly lead to a new paradigm in nanofabrication that fully exploits the quantum mechanics of the growth object.

The theoretical model calculations and DFT calculations were done in collaboration with Drs. Biao Wu and Zhenyu Zhang at Oak Ridge National Laboratory. This work is currently under consideration for publication.

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Education:

One graduate (Murat Ozer) and one undergraduate student (Jason Smith) contributed to the experimental work. Murat Ozer started his dissertation research in the Fall of 2002. Jason Smith graduated at the University of Tennessee in the spring of 2003 and has started his graduate career also at The University of Tennessee. Both students have become skilled operators of the new Molecular Beam Epitaxy system in the PI's laboratory. The theory was done in collaboration with postdoctoral scholars Biao Wu and Jia Yu at ORNL, and with Zhenyu Zhang at UTK/ORNL (staff).

Societal Impact:

Nanoscience represents one of the most promising avenues for future innovations in e.g. physical sciences, medicine, and information technology. A key requirement for making functional nano devices is the ability to acquire perfect control of their structure and morphology. A viable way to accomplish this is to exploit quantum mechanical laws while tuning and assembling nanostructures. This work represents an important case-study, showing how quantum mechanics can be understood and used to engineer thin film nanostructures of desired morphology.