QUANTUM OSCILLATIONS IN THE WORK FUNCTION OF ATOMICALLY-UNIFORM FILMS: THEORY AND EXPERIMENT FOR AG/FE(100)

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As the size of a solid specimen is reduced to the nanoscale, its physical properties may be modified by the quantization of its valence electronic states. Observations of these "quantum size effects" (QSE's) dates back at least to 1966 when Orgin et al. reported variations in the conductivity of thin Bi films with thickness[v]. Subsequent jellium calculations by Schulte revealed oscillations in the work function with film thickness[vi]. More than 20 years later Zhang et al. showed how the QSE could influence the physical stability of a growing film and so determine its morphology[vii]. Against a backdrop of increasing interest in nanofabrication, this 'electronic growth model' revived interest in the QSE and triggered a large number of publications and discussions about the effect of quantized valence states on various material properties in the nanoscale regime.

In the work presented here, the work function of atomically uniform Ag films grown on Fe(100) is measured as a function of film thickness. Oscillations are observed as a result of quantum confinement of the valence electrons. A first-principles calculation reproduces the observed variations except for very thin films (one and two monolayers), and the differences can be attributed, in part, to strain effects caused by the lattice mismatch between Ag and Fe. These results illustrate the close interaction between interface effects and surface properties. The agreement between the experimental results and those given by density functional theory is excellent, which lends confidence in the ability of modern theory to give a good understanding of quantum size effects in thin solid films.

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