MICROSTRUCTURE AND MORPHOLOGY OF THIN METALLIC FILMS: COMPUTER SIMULATIONS AND EXPERIMENTS

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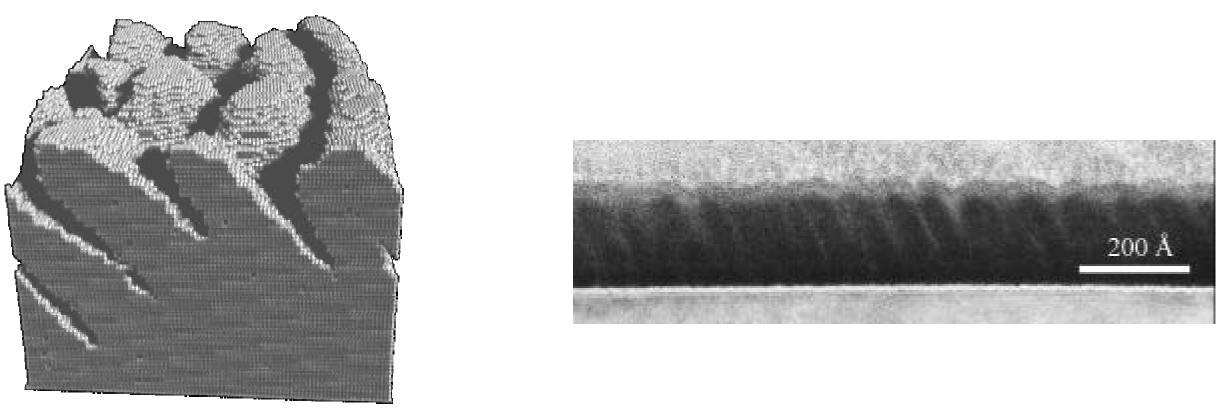
Thin metallic films have many practical applications. These applications range from interconnects in microelectronics, to protective coatings and metallic multilayers for X-Ray reflectors. The physical properties of these films depend strongly on microstructure: texture, grain size, surface and interface roughness, density etc.

Our goal is to improve the understanding of microstructure development (texture, grain and columnar growth) in thin metallic films. We thus present atomic scale simulations of such films deposited by sputtering. Our Monte Carlo model (ADEPT) includes ballistic deposition from a sputter target, surface diffusion, and allows multiple orientations corresponding to polycrystalline material. In addition, we are interested in the structure of films deposited onto non-planar (i.e. inclined) surfaces, e.g. as in deep submicron trenches and vias used in microelectronics, or as in the case of multilayer deposition onto figured substrates. For this purpose, we are using a model material implemented with aluminum parameters (e.g. diffusion coefficients, grain boundary energies, etc.), and then we scale down the Al diffusivity in order to reproduce the mechanisms involved in the growth of low mobility materials (e.g. Ti, Ta, TiN etc.).

Simulations of deposition onto inclined surfaces show that such films have lower densities and higher porosity than those deposited at normal incidence. The effect of texture on density is presented. Effects of deposition angle, grain boundaries, imperfect wetting with the substrate, Ehrlich-Schwoebel barriers (Figure 1(a)), and reduced mobility on the density and roughness of the growing layer have been investigated. The effect of the kinetic energy of the deposited atoms and of the Ar atoms (related to the Ar pressure) are included using a binary collision model. We will also present experimental results, including X-Ray Reflectance measurements, Atomic Force Microscopy and HRTEM images (Figure 1(b)) in light of these simulations.



(a) (b)

Figure 1 : Simulated morphology of a film with a large Ehrlich-Schwoebel barrier (a) and HRTEM picture of a Ta film (b), for a 60° substrate inclination.