MOLECULAR DYNAMICS SIMULATION OF ION EFFECTS ON THE GROWTH OF THIN FILMS

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Molecular Dynamics simulations are becoming increasingly helpful in understanding the atomic-scale processes that are instrumental in thin film formation and ion-beam modification. An overview will be given of the results of current work on Mo and Cu films deposited on Mo substrates. Ion effects will be discussed from the viewpoints of ion-beam assisted deposition (IBAD), post-deposition ion etching, and post-deposition ion-beam probing. The work concentrates on the complexities that one encounters in thin-film manufacuring, rather than on the simple mechanisms. After all, grain boundaries, textured surface patterns, and crystallographic mismatch at interfaces are just a few of the conditions that distinguish real-life applications from textbook thin films. We will examine the results of MD simulations - employing Embedded Atom Methods – in a variety of cases and discuss some of the limitations and future prospects. A few examples are:

(1) Strong surface patterns develop when a Mo film is grown on a Mo(110) substrate, while they are absent for Mo on Mo(100). The causes of this difference in nanofaceting and the resulting difference in defect topology are discussed.

(2) Depositing a Mo film on a substrate containing two (100)/(910) grain boundaries of different orientation leads to complicated film morphologies in the grain boundary regions. Dislocations, mosaic spread, and regions of fcc Mo are observed. Stress development after annealing and ion-bombardment is also discussed.

(3) Cu films deposited on Mo substrate form a model system for the latest metallization technologies in IC manufacturing. The influence of the fcc/bcc interface mismatch on the Cu film properties is analyzed for thermally evaporated and IBAD films.

(4) Primary and side effects of ion beam etching of amorphous Mo films as a technique for obtaining films with desirable optical properties are evaluated.