Ballistic Transport and Reaction in Three-Dimensional Grain Structures

Max O. Bloomfield and Timothy S. Cale
Focus Center: New York—Rensselaer
RPI, CII 6015
Troy, NY 12180-3590

For deposition systems with high Knudsen numbers (Kn), *i.e.*, for structures with length scales of interest that are significantly smaller than the mean free path of gas-phase species such as in fabrication of many microelectronics and MEMS structures, transport is dominated by particle-surface collisions and is therefore "ballistic", occurring only along line-of-sight. Thus, the flux to the solid surface in high-Kn depositions can be calculated using distributions from a source volume and a set of "view factors", or transmission probabilities, calculated from the geometry of the structure and the angular distribution of the re-emitted species. These computational methods have been used for more than a decade in the investigation of structures with 2D cross-sections, such as long trenches [1] and vias [2].

With the introduction of generalized 3D interface tracking software such as PLENTE [3], it is now possible to employ the same technique for developing grain structures in vapor deposition systems (PVD and CVD). We bring several codes together to simulate the ballistic transport and chemical kinetics in a CVD system, growing from the nucleation stage and continuing through coalescence. We use FVIEW [4], which employs a ray-tracing method to calculate both the flux from a source plane above the substrate to the mesh representing the surface and the view factors from each surface element to each other surface element. FVIEW launches large numbers of rays from each surface element, tracking what each ray collides with (source plane or surface element). Surface collisions are weighted in flux calculations by the particle distribution function (PDF) of the species emitted by the target surface element. We use a Maxwellian flux from a source plane above the structure, and emission of unreacted material is considered to be diffuse.

Once the initial fluxes to the surface are calculated, EVOLVE [5] is used to determine the rate of each reaction that occurs on each surface element, considering its material. Then, the amount of unreacted flux to each element is calculated and re-emitted to the other surface elements in the system using the view factors calculated by FVIEW. Using cyclic substitution, reaction rates are determined that are consistent with all the fluxes, and the deposition rate is determined from these reaction rates [1, 2]. These deposition rates are then passed to PLENTE, which uses them to evolve the geometry of the system. After a small change in the structure, PLENTE again invokes FVIEW and EVOLVE to get new surface velocities.

As the depositing species, we consider a precursor that reacts quickly on copper but is inert on the amorphous substrate, except at nucleation sites on the surface. We assume a quick saturation of all the nucleation sites, followed by negligible nucleation. We model the deposition reaction as first order in precursor flux and material dependent. We show results from a range of reactivities for the precursor. Figure 1 show results from simulations of sticking factor 1, sticking factor 0.5, and sticking factor 10^{-3} cases. Reactive precursor flux may come directly from the source or from re-emission from elsewhere in the structure. Details about the precursor or deposition chemistry are not important for the purposes of this paper; however the overall reaction results in the irreversible deposition of copper.

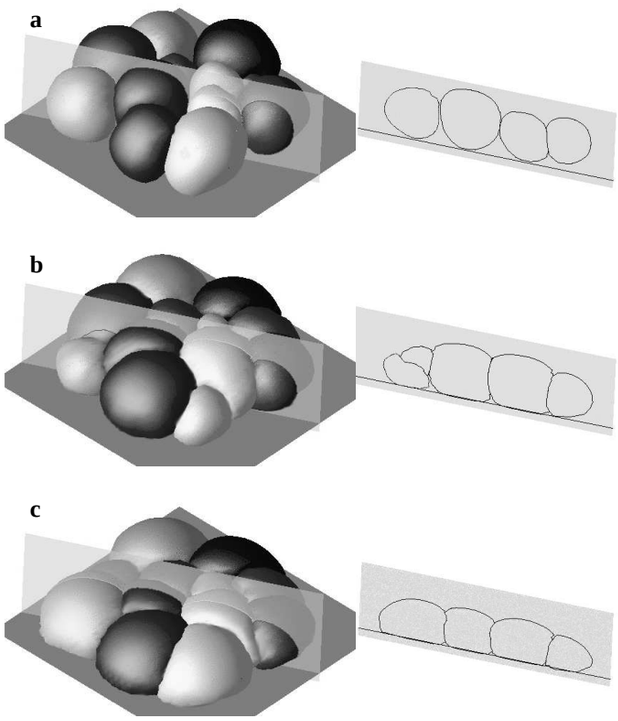

Figure 1. 3D simulated grain structure and cross sections after a short deposition of material (a) high (1), (b) moderate (0,5) and (c) low (0.001) sticking factors on copper, as noted in the text. Note the increasing density (decreasing void volume) of the film as deposition becomes more isotropic, from (a) with a prominent void structure to (c) with almost no visible voids. Note that the cross-sections do not pass through the original islands.

From analyses of these results (such as by the 2D cross-sections pictured next to each 3D picture) it is seen that the slightly and moderately reactive precursors create a denser grain structure with less void volume due to shadowing and less prominent surface seams than the highly reactive precursor. It has been observed in these and other simulations that nuclei that are positioned in the lee of larger grains become completely shadowed by their larger neighbors and are "choked off". These types of results are potentially a benefit in understanding how chemical kinetics and transport in vapor deposition systems can affect the resulting grain structure.

References

1. T. S. Cale, G. B. Raupp, *J. Vac. Sci. Technol. B*, **8**, 649–55 (1990).
2. T. S. Cale, G. B. Raupp, *J. Vac. Sci. Technol. B*, **8**, 1242–8 (1990).
3. M.O. Bloomfield, D.F. Richards, T.S. Cale, *Philisophical Mag*. **83**(31-34), 3549-68 (2003).
4. T.S. Cale, T.P. Merchant, L.J. Borucki, in *Semiconductor Process and Device Performance Modelling*, Mat. Res. Soc., v 490, 1998, p 201-212.
5. T.S. Cale, T.P. Merchant, L.J. Borucki, A.H. Labun, *Thin Solid Films* **365**(2), 152-75 (2000).