Incorporation of Equipment Simulation into Integrated Feature Scale Profile Evolution

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Abstract

We present three-dimensional linked reactor/feature scale simulations for integrated PVD/CVD deposition sequences applied to metal stack plug-fills. Monte-Carlo particle distributions as well as CVD equipment simulations have been incorporated into three-dimensional profile evolution.

1. Introduction

For wafer sizes ranging up to 300 mm yield and quality issues become increasingly determined by the uniformity of the processes across the wafer. This is especially important for the formation of contacts which are usually fabricated as compounds of different layers in order to fulfill the long list of requirements like low contact resistivity, metallurgical isolation, protection from aggressive reactants of subsequent process steps, sufficient adhesion, and leakage free film formation as well as void free filling.

In order to include uniformity aspects into the feature scale profile evolution, the integration of results from simulations on equipment scale is necessary for low-pressure and for high-pressure processes. These two types of processes are determined by different transport mechanisms. Therefore they require different models for the particle transport both on equipment and feature scale and different integration approaches. The presentation of the full scale integrated model for low- and high-pressure processes is the purpose of this article.

2. Low-Pressure Processes

The profile evolution of ballistic transport determined low-pressure processes such as sputter deposition, is predominantly determined by the distribution of the particles impinging on the wafer surface. Taking into account visibility conditions, the local deposition rate is given as integration of the distribution function $\mathrm{F}(\varphi, \vartheta)$

$$r = \frac{r_0}{\mathrm{N}} \int_{2\pi} \mathrm{F}(\varphi, \vartheta)\, \Omega(\varphi, \vartheta)\, d\Omega \qquad (1)$$

where r_0 is the nominal rate for a flat wafer completely visible to the particle source. N is a normalizing factor and $\Omega(\varphi, \vartheta)$ the visibility function which is either 1 for visible directions or 0 for shadowed ones.

Starting point for the reactor/feature scale integration for low-pressure processes therefore is the distribution function $\mathrm{F}(\varphi, \vartheta)$. Fig. 1 shows how the distribution of the particles arriving at different

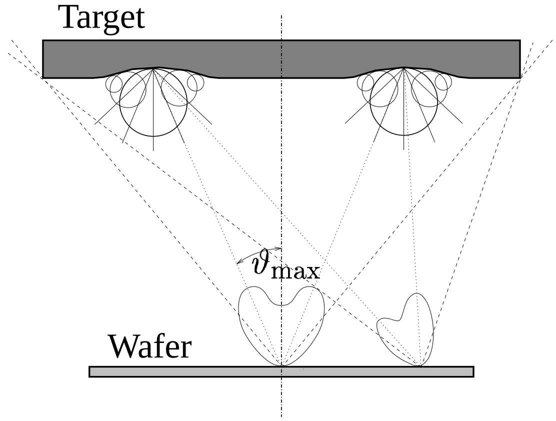

Figure 1. Relation between emission characteristics and incident particle distributions, shown by means of a sputter reactor.

positions on the wafer is determined by the angular emission characteristics of the target material and the radially varying emission intensity which can be measured by means of the target erosion profile.

2.1. Analytical Fitting Functions

The first integration step is the use of distributions resulting from Monte Carlo (MC) simulations of sputtering particle transport [1]. Fig. 2 shows how an exponential function $a\vartheta^3 e^{-b\vartheta}$ is used in order to fit the particle distributions resulting from MC simulations for different pressures.

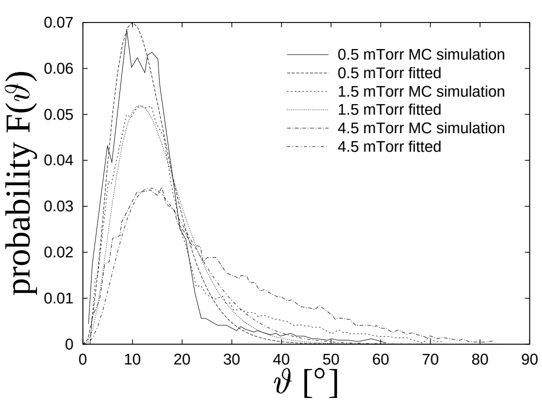

Figure 2. MC and fitted angular particle distributions for 0.5, 1.5, and 4.5 mTorr.

For a center wafer position, $F(\varphi, \vartheta)$ can be considered as radially symmetric. For

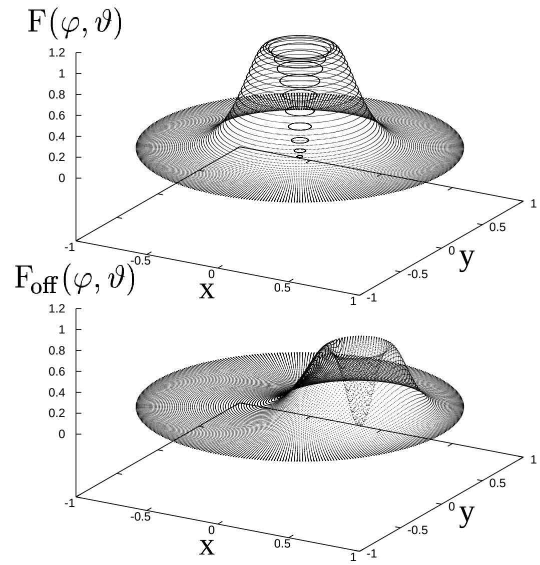

Figure 3. $F(\varphi, \vartheta)$ for a center (top) and an off-center position (bottom) on the wafer.

a peripheral position the origin of the distribution function has to be shifted and the distribution function has to be scaled in order to account for the changed intensity and particle distribution. How this is done for the given exponential function is shown in Fig. 3.

2.2. Monte Carlo Simulations

Beside analytical functions used for the approximation of particle distributions impinging on the wafer, it is also possible to include fully three-dimensional fluxes resulting from MC particle transport simulators like SIMSPUD [2]. These programs account for experimentally measured target erosion profiles and calculate particle collisions according the the prevailing process pressure and temperature for specified positions on the wafer.

Fig. 4 depicts the polar plot of particle distributions resulting from SIMSPUD simulations. The upper plot shows an almost radially symmetric distribution resulting at a center wafer position with an average azimuthal incidence direction of $\vartheta_{\rm src}$ = 1.01°.

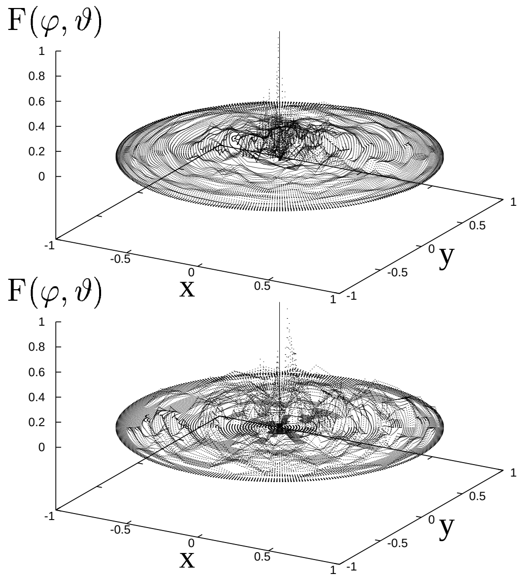

Figure 4. MC simulations for a center (top) and an off-center position (bottom).

For the peripheral position depicted below, which is shifted 72 mm off the wafer center, ϑ_{src} equals $5.12°$. This clearly reveals that the main direction of particle incidence is tilted from the vertical direction, indicated in the plot by the solid line.

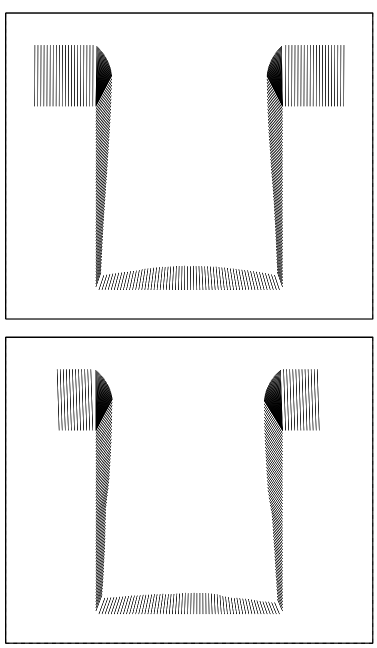

Figure 5. Cross-sections of deposition profiles using the MC distributions from Fig. 4.

The corresponding sputter deposition profiles for a cylindrical via using the distributions from Fig. 4 are given in Fig. 5. The upper figure mirrors the radially symmetric profile at the center wafer position. The profile below at the off center position not only exhibits asymmetric and irregular sidewall thicknesses but also a strongly asymmetrical profile at the bottom of the via.

3. High-Pressure Processes

High-pressure CVD processes are determined by diffusion of the reactants and by chemical gas phase and surface reactions. The equations which determine the model for the rate calculation are summarized in the sketch in Fig. 6. The complete model for the three-dimensional simulation of these continuum transport and reaction determined high-pressure CVD processes is presented in [3].

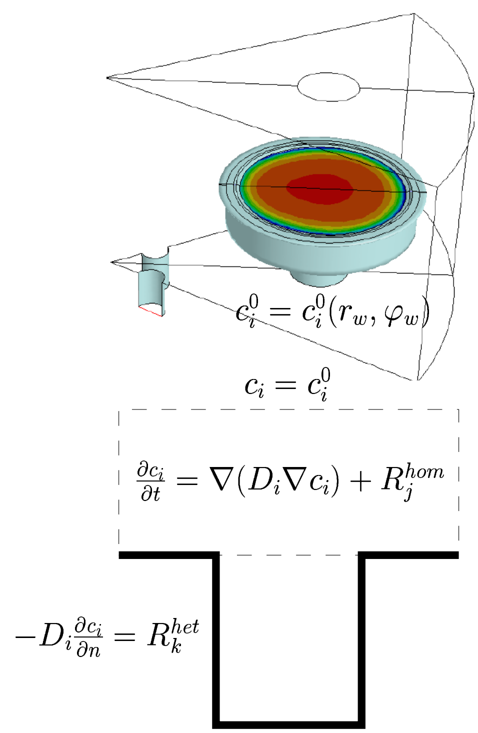

Figure 6. Linked reactor/feature scale CVD simulation.

Reactor scale simulations as feasible with programs like FLUENT[1] are linked to the feature scale profile evolution by setting the Dirichlet boundaries at the top of the feature scale simulation domain according to the concentrations resulting from the equipment level simulation. Fig. 6 shows the WF_6 concentration for a tungsten CVD process and symbolizes the link from reactor to feature scale.

4. Results

We have applied the multi scale deposition models presented above to the simulation of a metal stack gap-fill of a local interconnect (Fig. 7). As presented in [4] the four step process consists of Ti and TiN PVD films followed by TiN CVD (TDEAT/ammonia) and W bulk (reduction of WF_6 with H_2). The layers are deposited into a trench containing a spacer structure.

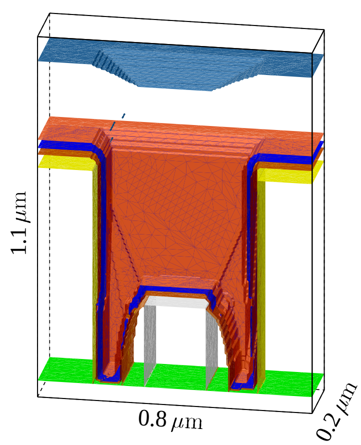

Figure 7. Ti PVD, TiN PVD, TiN CVD, W CVD metal stack.

We have simulated several positions on the wafer using the results from SIMSPUD and FLUENT simulations as boundary conditions for the profile evolution. It turned out that due to the shadowing effects for the particles traveling in line-of-sight the PVD layers exhibit the most pronounced differences whereas the conditions for the two CVD layers are sufficiently uniform across the wafer.

[1] See `http://www.fluent.com/`.

5. Conclusion

We have presented an integrated Ti PVD, TiN PVD, TiN CVD, and W CVD deposition sequence applied to a tungsten metal stack plug-fill. Both low-pressure PVD as well as high-pressure CVD parts of the profile evolution have been coupled with simulation results obtained on equipment scale. It was possible to assign the non-uniformities in the film thickness to the different steps forming the overall metal stack for the plug-fill.

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[1] A. Myers, J. Doyle, and J. Abelson, “Monte Carlo Simulations of Magnetron Sputtering Particle Transport,” *J.Vac.Sci.Technol.A*, vol. 9, no. 3, pp. 614–618, 1991.

[2] M. Sheergar, T. Smy, S. Dew, and M. Brett, “Simulation of Three-dimensional Refractory Metal Step Coverage over Contact Cuts and Vias,” *J.Vac.Sci.Technol.B*, vol. 14, no. 4, pp. 2595–2602, 1996.

[3] W. Pyka, P. Fleischmann, B. Haindl, and S. Selberherr, “Three-Dimensional Simulation of HPCVD - Linking Continuum Transport and Reaction Kinetics with Topography Simulation,” *IEEE Trans.Computer-Aided Design*, vol. 18, no. 12, pp. 1741–1749, 1999.

[4] V. Sukharev, K. Kumar, and E. McInerney, “An Integrated Simulation of Across-Wafer Uniformity in Ti/TiN/W Plug-Fill,” in *Proc. of the 15th International VLSI Multilevel Interconnection Conference*, (Santa Clara, CA), pp. 306–311, 1998.