Finite Element Analysis of CVD Stripping Kinetics for *In Silico* Optimization of Semiconductor Manufacturing Parts for Sub-20 nm Technology Nodes

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Introduction

Quantum Global Technologies® (QGT: Quantum Clean® & ChemTrace®), a leader in the semiconductor parts cleaning and analytical business through their Atomically Clean Surface (ACS™) process, has developed new technologies aimed at exceeding OEM performance and meeting stringent defectivity requirements for sub-20 nanometer technologies. This is achieved by highly optimized parts cleaning and coating processes. This paper outlines recent advances in the ACS™ parts cleaning process by focusing on particle removal methods. The focus of the present work is to explain how finite element analysis is used to simulate the selective wet etching of CVD with a cleaning solution that was optimized by QuantumClean's Innovation and Technology group. Optimizing cleaning processes *in silico* for a given part surface allows QuantumClean to better predict outcomes of real surface reactions to adapt a multitude of chamber parts to the ASC™ process.

The present work considers a solid sample that is subjected to wet etch immersion clean that selectively removes layers of silicon nitride deposition from the coupon surface. The kinetic expressions associated with this chemical process for the purpose of the simulation in the present work describe the rates of adsorption and desorption of dilute species X and dilute product C onto the surface deposition B and the rate of depletion of species B through a surface reaction.

$$\text{Reactant sorption: } X + B \leftrightarrow XB$$

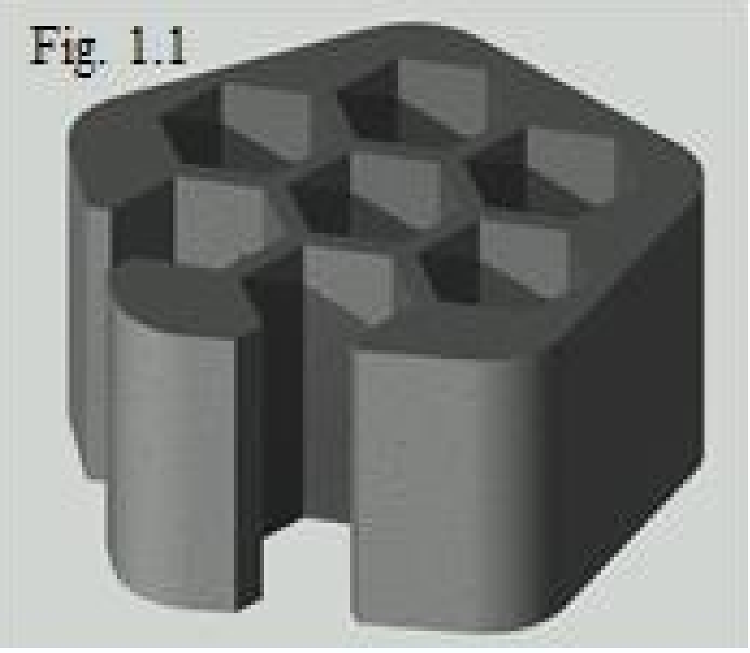
$$\text{Surface reaction: } XB \leftrightarrow CB$$

$$\text{Product sorption: } CB \leftrightarrow C + B$$

Finite element analysis allows for the facile scaling of physical phenomena such as the cleaning process of the present work. This study considers a small, metallic part with seven honeycomb-shaped ribs that is coated in silicon nitride. The part is shown in Figure 1.1 bare of any silicon nitride deposition. This part is digitally constructed arbitrarily and is not representative of any real industrial machine component. During the timespan of simulation, the part is immersed in an 800-mL cylindrical space (100 mm radius) containing upward-flowing aqueous Solution X (Figure 1.2).

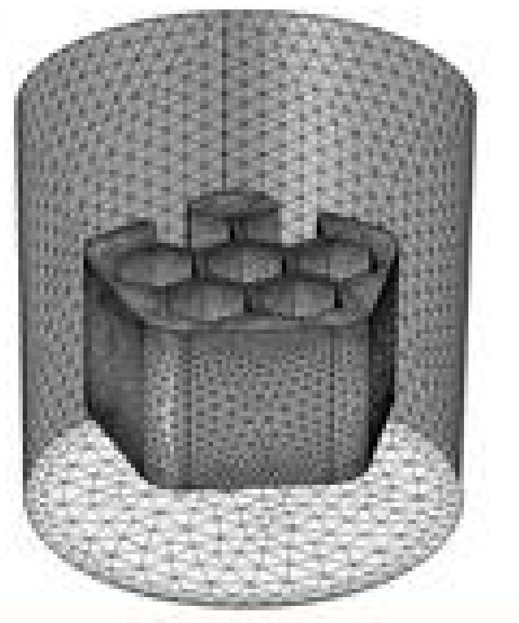
Bare Part Ray-Traced Rendering

Fig. 1.1



Simulation Space and Meshing

Fig. 1.2



This study takes advantage of the strong relationship between the thickness of thick silicon nitride layers and their observable color (Figure 2.1) to closely approximate the true color of the deposition (Figure 2.2) as it is removed throughout the simulation. Real time lapse imagery and color observation were used to estimate film removal progress without the regular use of more expensive metrology, such as refractometry or ellipsometry.

Simulation Results and Conclusions

Silicon Nitride Thickness Color Legend[1] (Fig 2.1) and Real Part (Fig. 2.2)

Fig. 2.1

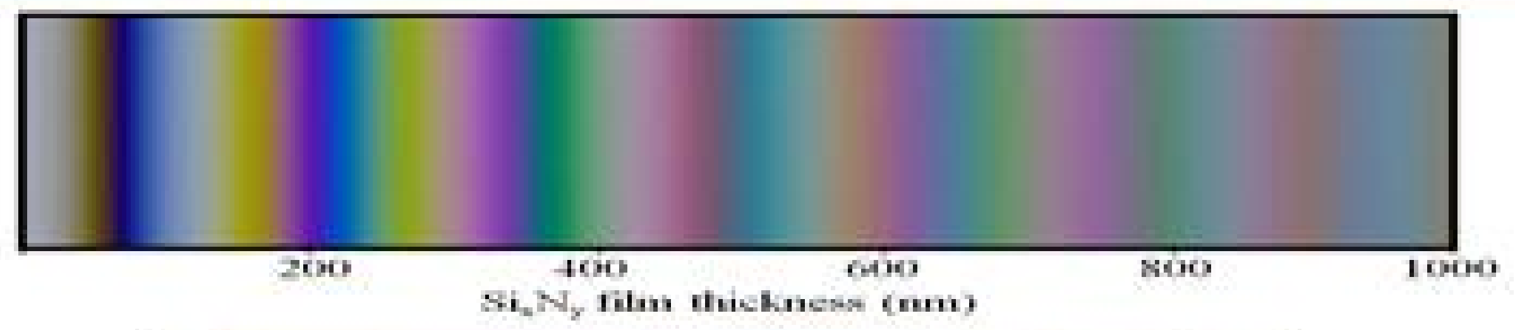
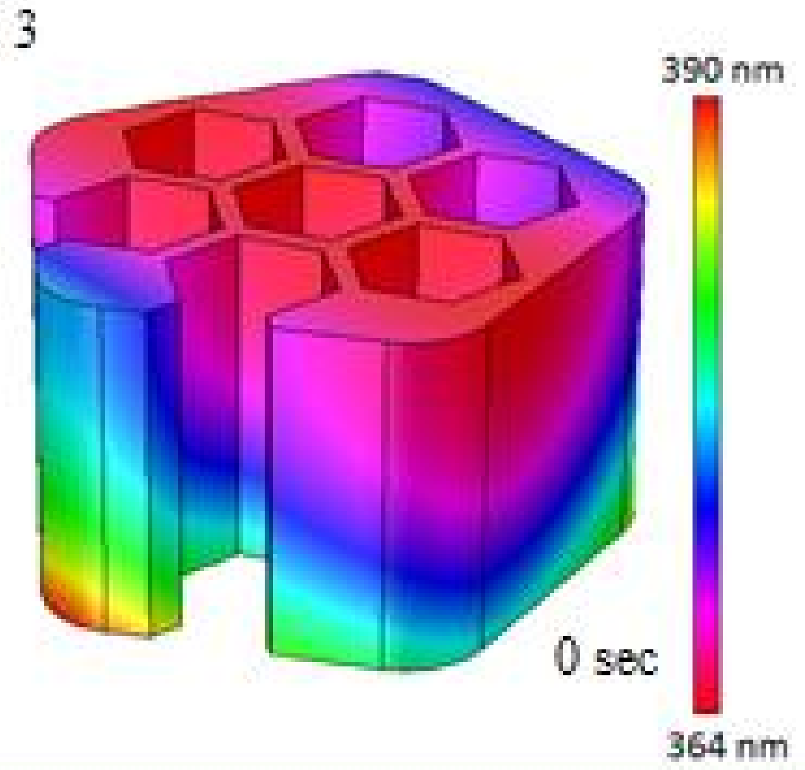


Fig. 2.2

False-Color Thickness Profile

Fig. 3



Simulation Time Lapse

Fig. 4.0

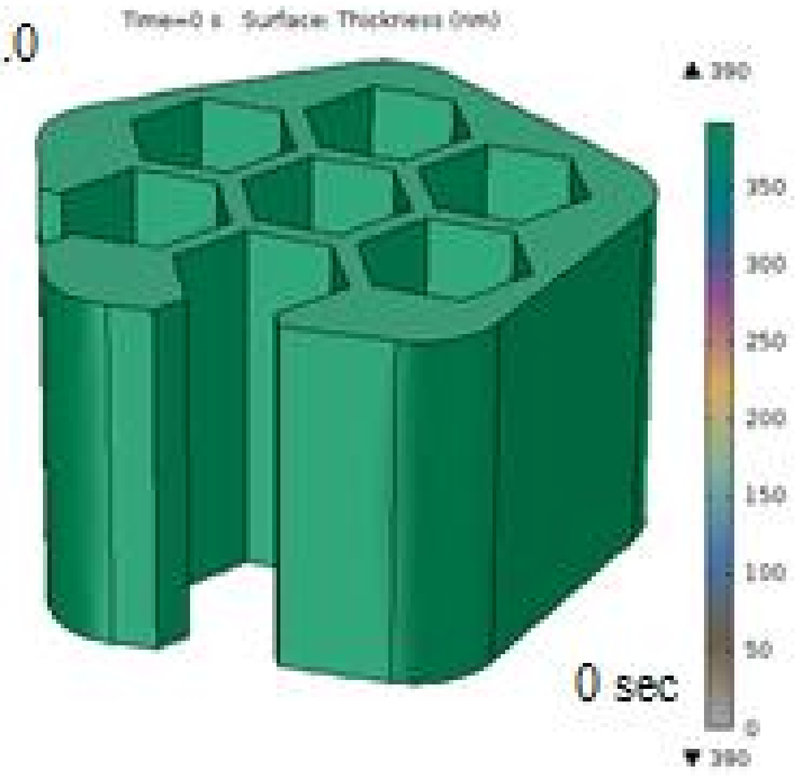


Fig. 4.1

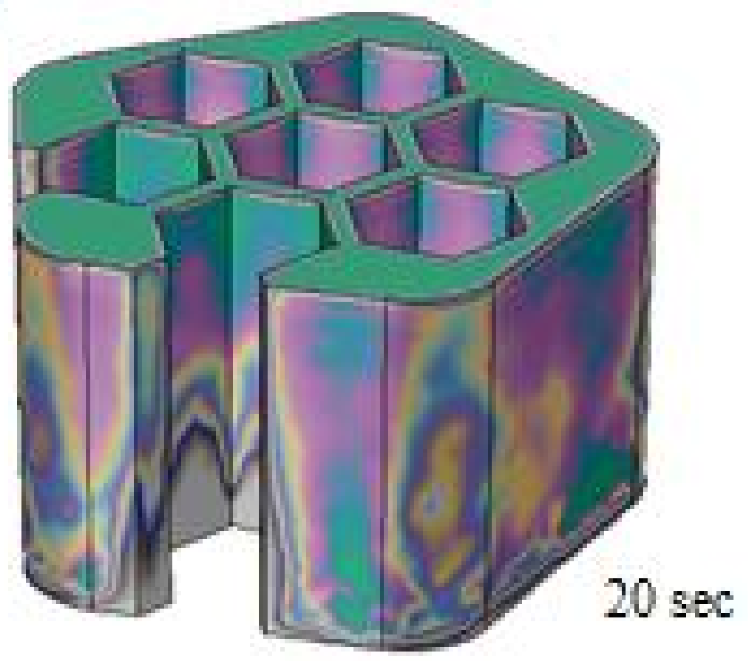


Fig. 4.2

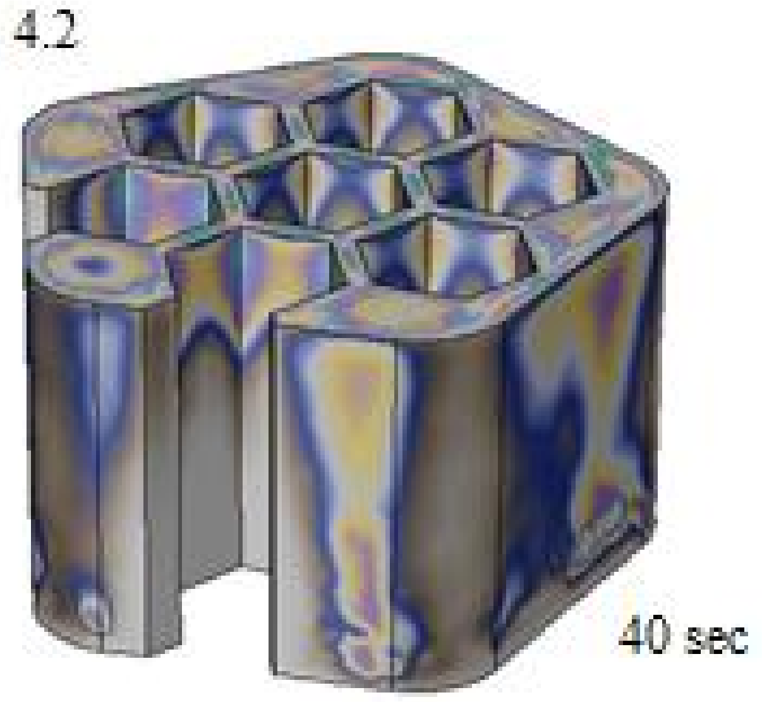
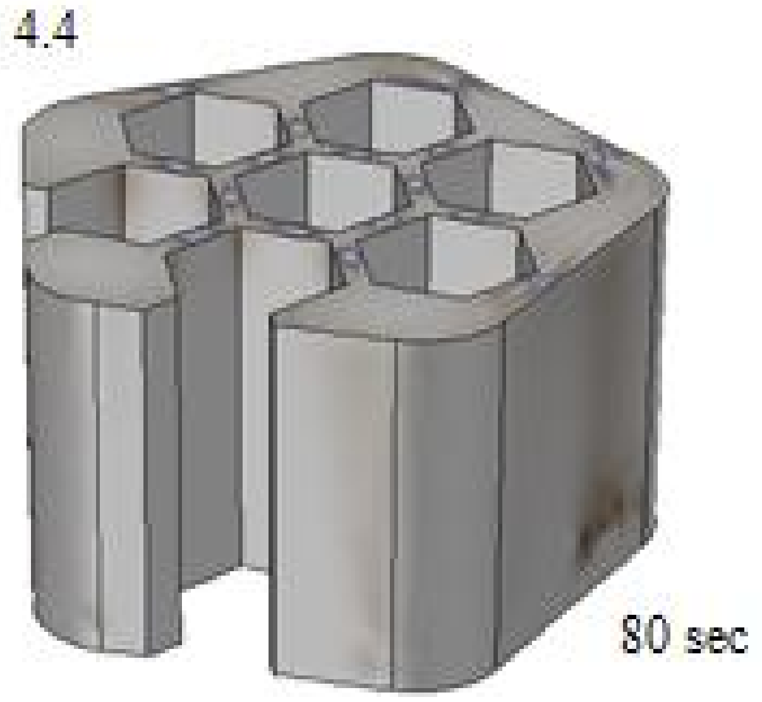


Fig. 4.3

Fig. 4.4



Cut-Line Thickness Profile Time Lapse

Fig. 5.1

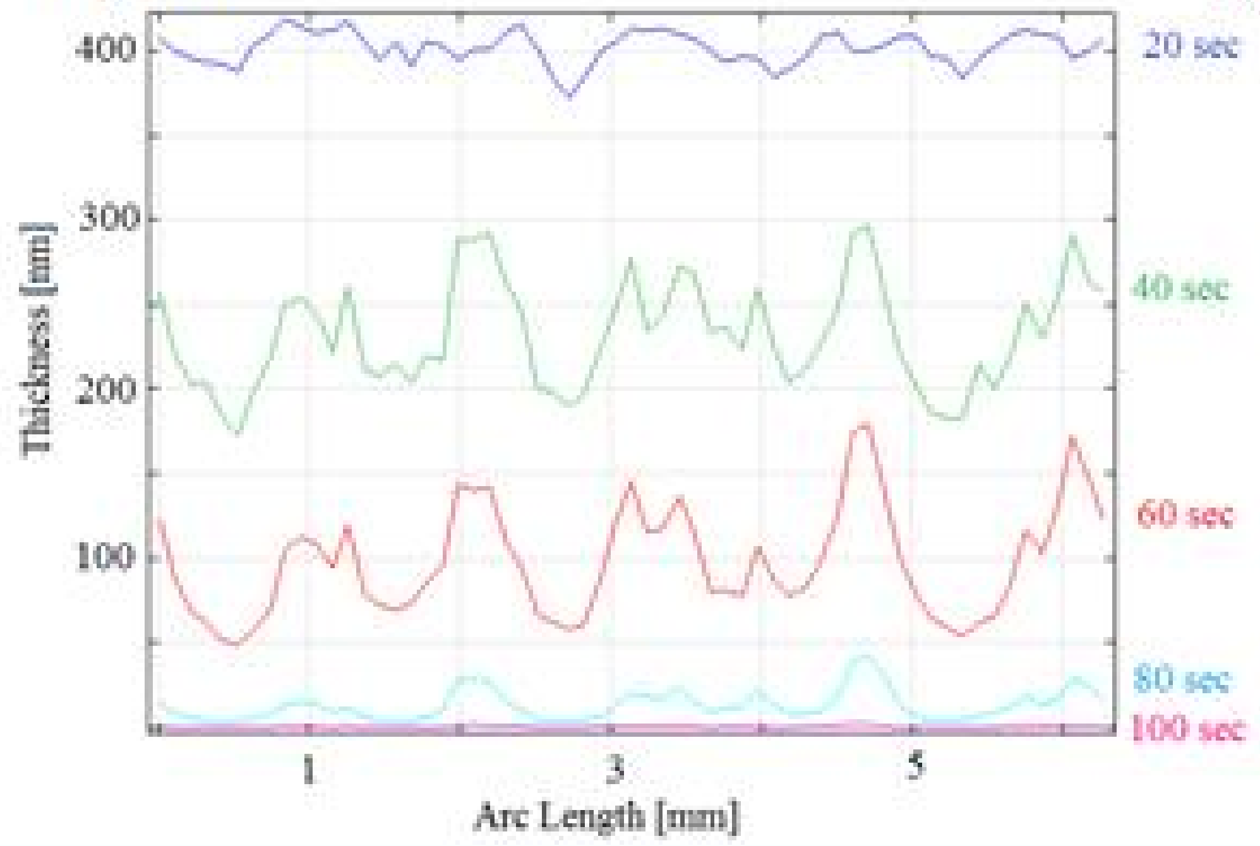
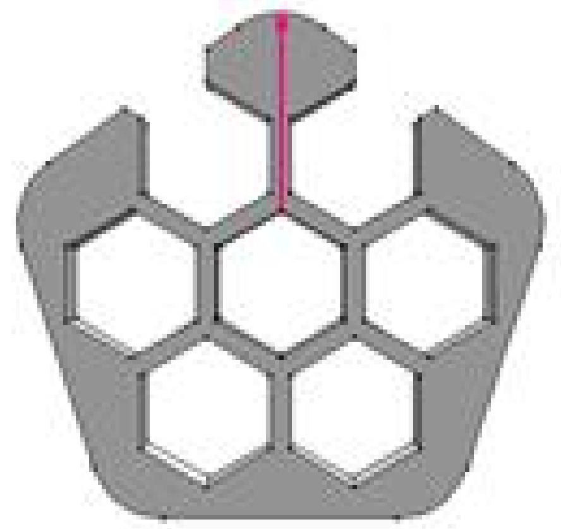


Fig. 5.2



Silicon nitride is not uniformly distributed over the part surface, but an approximate range of thickness is known, as shown in false color in Figure 3. To attempt to capture the uncertainty in the observation of the initial condition of the part surface, an arbitrary thickness (h_B) distribution function,

$$h_B(x, y, z) = a(y^2 + z^2) + b$$

is applied to the simulation volume and describes an infinite paraboloid that is used to simulate the minute degree of variance in thickness across the part surface. Figure 3 is a surface plot of silicon nitride thickness shown in false color on the part at the start of the simulation (t = 0 s). However, on the scale of the complete simulation, which encompasses the entire thickness range from 0 nm to 390 nm, variance shown in Figure 3 is indiscernible, as shown in Figure 4.0.

Figures 4.0 through 4.4 present the results of the simulation at 20-second intervals, with the color legend shown in Figure 4.0. Figure 5.1 is an overlay plot showing the thin film thickness profile along the 6.2-mm cutline shown in Figure 5.2.

This simulation was built from the observable color of the deposition on parts at different stages in the cleaning process and is effective in clearly demonstrating the kinetics of deposition removal by wet chemical etch. The model results show the impact finite element analysis can have on reducing the analytical costs of determining spatially-dependent etch selectivity on any number of parts using similar kinetics models.

References

[1] Henrie, J., S., K., S.M., S., & A., H. (2004). Electronic color charts for dielectric films on. Optical Society of America, 12 (7), 1464-1469.

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