



White Paper

Equipment & Process Co-Optimization (EPCO), Artificial Intelligence & Machine Learning Challenges for Semiconductor Manufacturing

Updated July 2021

Background

CopyExactly! Methodology

The CopyExactly! (CE!) philosophy and methodology was famously developed by Intel in the late 1990's for matching development site processes to manufacturing. The general premise is that you use exactly the same process equipment with exactly the same process recipes. By controlling the variables associated with the equipment and process recipes, you can achieve the same production yield results—as you have seen in development—in a shorter period of time.

(CE!) has morphed into CopySmartly!, the difference being matching performance across different equipment. Whether your new process 'corridor' is in the same FAB or on another continent, (CE!) and CopySmartly! represent the gold standard in fast, low-risk, deterministic process bring-up.

The Problem

Increasing Process Complexity

Despite the advancements pioneered by CopyExactly!, today's high-volume, advanced logic processes—including Fin-FET and gate-all-around transistors, and high aspect ratio etch techniques used in 3D-NAND memories—require a new approach to the established basic CopySmartly! methodology.

As process nodes have shrunk, new variables affecting process yield and challenging the established process methodologies have emerged. Even on the exact same equipment, small variations can cause deviations from the process mean, for example, in the many single wafer processing chambers attached to a processing mainframe. Localized virtual vacuum leaks, subtle reaction gas partial pressure variations, wafer surface saturation due to changes in pumping performance, surface reactivity due to changing wafer temperature, chamber clean end points, and chamber seasoning profile can all affect the objectives of the CopySmartly! methodology.

Additional emergent challenges include inter-layer adhesion, 300mm wafer mechanical stresses, new atomic level deposition and etch chemistries, exotic low resistance contact and fill metals, stringent cross contamination protocols, and maximizing throughput by managing the trigger conditions for preventative

maintenance cycles—all of these require greater insight to how the process and equipment are interacting.

The Solution

Equipment and Process Co-Optimization (EPCO)

The Advanced processes now require Equipment and Process Co-Optimization (EPCO), which demand higher accuracy metrology tools and add a new layer of in-situ molecular complexity to the (CE!) methodology protocols.

The idea of using EPCO for semiconductor manufacturing is one that is being looked at beyond CopySmartly! In a recent paper by McKinsey & Co.¹, long term semiconductor process manufacturing optimization potential, using big data, artificial intelligence (AI) and machine learning (ML), represented an estimated \$38B cost saving opportunity from a combination of reduced maintenance costs, improved yields, and increased throughput. Further, McKinsey stated their strongest opportunity for realizing these benefits was adjustment of tool parameters, specifically using live tool sensor data from current and previous steps to enable AI/ML algorithms to optimize the usually non-linear relationship between process operations.

Key to successful AI/ML deployment is actionable real-time data that allows for appropriate models to be created and tested with data correlation between real world and ML model inputs and outputs. The digital transformation brought about by in-situ, real-time molecular diagnostics and its cloud-connected data sets are a key technology enabling CopySmartly!, as well as AI/ML for semiconductor process control optimizations.

If It Isn't Broken...Should You Fix It?

One of the barriers to adoption of AI/ML in semiconductor fabrication lies in the risk averse mindset of "It's qualified, don't touch it". The question of invalidating existing expensive and protracted process qualifications by dynamically changing process tool settings is a legitimate one and needs to be rationally considered.

The gold standard for requalification is the 3F-test—which examines whether the proposed change have an effect on Fit, Form or Function (3F) of the process or

1: <https://www.mckinsey.com/industries/semiconductors/our-insights/scaling-ai-in-the-sector-that-enables-it-lessons-for-semiconductor-device-makers#>

end product. More specifically, is the effect of the change outside of normal operating variances seen from expected and historical statistical process control (SPC) variations? Given that the AI/ML dynamic process tooling changes are designed to tighten process variation mean and standard deviation, they should lie comfortably within the constraints of the 3F-test criteria and no requalification should be needed.

However, this can be further mitigated by clearly having limit-stop safeguards in place, a best practice approach when the AI/ML algorithms are designed and deployed.

Minor low-level process ‘tweaks’ are necessary and common in all fabs and a routine part of process continuous improvement, the only difference here is the EPCO autonomous deployment and control over the equipment and process.

Key to a successful EPCO deployment is the availability of appropriate in-situ metrology solutions to enable real-time observability, quantification, and control. Measurements taken after processing is completed i.e., in-line measurements, are sequential in nature, costing throughput and cycle time, and lack the immediacy to affect meaningful real time process change and optimization. One of the fundamental changes needed to optimize FAB management is the switch from in-line to in-situ metrology solutions.

You Can’t Fix (or Optimize) What You Don’t Measure

In-situ molecular metrology has historically been particularly challenging. Optical techniques, while useful for wafer surface thickness measurements and identification of spot defects, lack quantification and sensitivity to enable real-time EPCO. Residual gas analysis (RGA) metrology is useful for leak detection, but lacks the robustness and run-to-run consistency needed for reliable EPCO process profiling.

The semiconductor process includes radiation, charged particles, corrosive and reactive gases, and small to large particulates.

Such a harsh environment quickly and irreversibly alters the performance of sensitive in-situ process metrology equipment. To meet the needs of real-time molecular data collection, it is critically important that the molecular sensor be robust, and that the data source is highly dependable.

The Atonarp Aston™ molecular sensor (Table 1.) is unique in deploying a self-contained ionization mechanism called MicroPlasma, which, unlike regular RGA electron ionizing sources, is not affected by corrosive process gas. Aston’s MicroPlasma ionization source enables a scheduled maintenance period that is up to 100x longer than regular RGAs. Other common molecular sensor technology, like optical emission spectroscopy (OES), require plasma emissions to identify byproducts and reactant molecules of interest. Further OES solutions do not work with increasingly common processes that may have pulsed plasmas, dim plasmas, or no-plasma present near the wafer. Additionally, OES requires clear line-of-sight to the process plasma and condensate build-up on the chamber’s optical metrology window is another source of poor measurement data or frequent preventative maintenance-based tool down time. Atonarp Aston’s ReGen™ mode allows the sensor to self-clean in situations where vapor and particulate condensates may be present.

Table 1. Key Aston Specifications

Parameter	Typical	Units
Mass resolution	0.8	u
Mass number stability	0.1	u
Sensitivity (FC/SEM)	5x10 ⁻⁶ /5x10 ⁻⁴	A/Torr
Minimum detectable partial pressure (FC/SEM)	10 ⁻⁹ /10 ⁻¹¹	Torr
Limit of Detection	10	ppb
Maximum operating pressure	1 x 10 ⁻³	Torr
Dwell time per u	40	ms
Scan update rate per u	37	ms
Emission current	0.4	mA
Emission current accuracy	0.05	%
Start-up time	5	mins
Ion Current Stability	< ±1	%
Concentration Accuracy	< 1	%
Concentration Stability	±0.5	%
Power consumption	350	W
Weight	13.7	Kg
Size	400 x 297 x 341	mm

[Refer to Aston datasheet for full list of specifications](#)

To ensure maximum effectiveness and efficiency, data must be prioritized that enables multiple use cases since this will have a much greater impact on EPCO, CopySmartly!, AI/ML, than a single tool or initiative. For

example, in the machine learning paper by Timoney et al.² variations in FinFet critical dimension (CD) after reactive ion etch (RIE) is seen based on processing chamber used. The paper outlines that some chambers were observed to have wide wafer to wafer variability of FinFET CD and applying machine learning to the same chambers provided significant improvement in the CD linearity. Critically, chamber variations were not identified by the in-line optical critical dimension metrology but were clearly identified when reference metrology was correlated to machine learning predictions. Impact of training set size was evaluated, and it was found that reducing the number of lots in the training set did not significantly degrade the correlation.

Further, the paper identifies that incorporating additional metrology techniques will enable more comprehensive and accurate outputs for thorough process monitoring or control and this is becoming particularly significant as process technologies advance to 7nm process node and below.

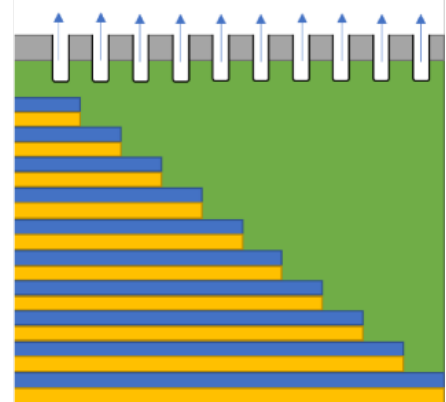
Atonarp Aston is suitable for:

- Chamber clean end point detection (EPD)
- Chamber leak testing
- Chamber seasoning and matching prior to release to manufacturing
- Process profiling
- Process EPD
- Atomic level etch (ALE) and atomic level deposition (ALD) monitoring with or without plasma
- Chemical vapor deposition (CVD)
- EUV lithography (dry resist)
- High aspect ratio (HAR) etch
- Small open area (OA%) etch and contamination detection
- Gas purity and residual gas analysis

End Point Detection without Plasma

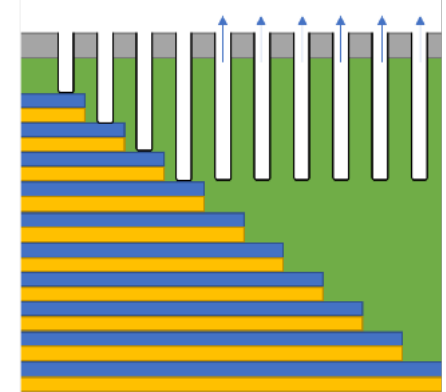
While optical emission spectroscopy (OES) has been widely adopted for etch EPD, the trend for low open area (OA) and HAR designs make it ineffective for many etch tasks. OES techniques require plasma 'on' and light emitting species. More sensitive techniques to achieve prompt and deterministic EPD are required as dim and remote plasmas are increasingly used in 3D devices and atomic level etch (ALE) processes. Further, pulsed plasma is often used to manage the etch profile

Small Open Area gives
low signal to noise ratio



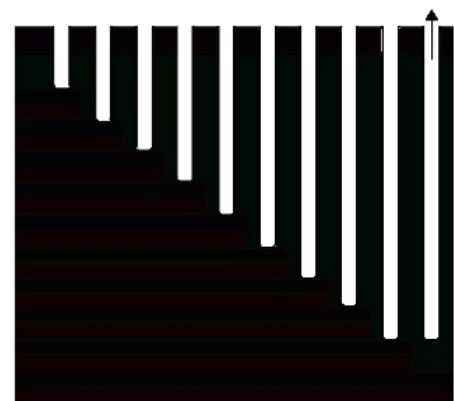
T₁

Byproduct abundance reduces
with each stair step



T₂

Pulsed plasma required
for HAR anisotropic etch



T₃

Figure 2. OES end point detection ineffective for 3D memory structures

2: Padraig Timoney, Taher Kagalwala, Edward Reis, Houssam Lazkani, Jonathan Hurley, Haibo Liu, Charles Kang, Paul Isbester, Naren Yellai, Michael Shifrin, Yoav Etzioni, "Implementation of machine learning for high-volume manufacturing metrology challenges," Proc. SPIE 10585, Metrology, Inspection, and Process Control for Microlithography XXXII, 105850X (21 March 2018); doi: 10.1117/12.2300167

in HAR and low OA processes making OES an impractical solution for EPD. In 3D structures, multi-layer film and multiple contact depths hinder the ability to get a sharp step change in optical emission signal for endpoint as each row of contacts reaches the bottom (figure 2).

New uses for molecular sensors are being identified in the semiconductor process environment on a continuous basis, as the versatility of the technology becomes increasingly understood and deployed by process and equipment engineers alike.

How Fresh Is Your Data?

In There are basically three main types of data in the semiconductor process control FAB environment:

1. In-Situ data taken real time on the process tool
2. In-line data to measure results (usually immediately) after a processing step
3. Parametric or post-Fab data (used for wafer line yield and wafer ship acceptance criteria)

Additionally, these three main data can be further categorized into three sub-types (examples of the type of data collected shown in **bold**):

- Target data i.e., this is what the tool was targeting as part of the recipe e.g., target temperature: **327°C**, target SiF₄ molar concentration: **0.100 mol/l**
- Measured data i.e., is this is what was actually measured at a given point in time e.g., measured temperature **325.9°C**, , actual CF₄ molar concentration: **0.097 mol/l**
- Informational data i.e., wafer lot number: **8F2342G**, equipment serial number & chamber: **32FF4567-4**, and process flow and step: **22nm eFlash - gate etch (1207)**

For CopySmartly! and AI/ML, data should be prioritized. The quality and richness of the data is highly leveraged vis-a-vis its impact on risk reduction or cost savings. Measured in-situ, real-time data at the molecular level gives true insight as to how the process is set-up and proceeding—actionable data available in cycle. Reactants, by-products and partial products can be identified and quantified, allowing for dynamic process control to ensure tight mean and standard deviation control across run-to-run, chamber-to-chamber, tool-to-tool, and even site-to-site for a given process

module. Managing overall complex semiconductor process control and line-yield starts with having tight control on individual process steps and ensuring low variability and tight statistical process control (SPC).

EPCO Examples: Plasma Impedance and Process End Point Detection (EPD)

As process times become shorter with fine, processing structures, the plasma RF stability requirements are becoming more stringent. Etch rate excursions, even for short periods of time, can have significant detrimental effects on electrical performance. Managing the critical plasma impedance matching behavior from can be greatly influenced by different chamber’s physical differences and chamber specific process gas flow management, both of which result in changes in gas composition. When a chemical mixture of gases—used for etching, deposition, or cleaning—is injected into the plasma chamber, the resulting ions present a fluctuation (low) in impedance to the impedance matching network that is supplying the RF power to the plasma chamber. The impedance matching network needs to quickly—within 100 ms or less—respond to the impedance change and return the system to predicable, stable plasma impedance.

End point detection EPD is used in many semiconductor processes and is challenging to get right. A common use of EPD is in etch, and in particular the critical etch steps for transistor contacts, critical dimension vias (M1 to M2), 3D-NAND HAR staircase etch, and MRAM stack etch.

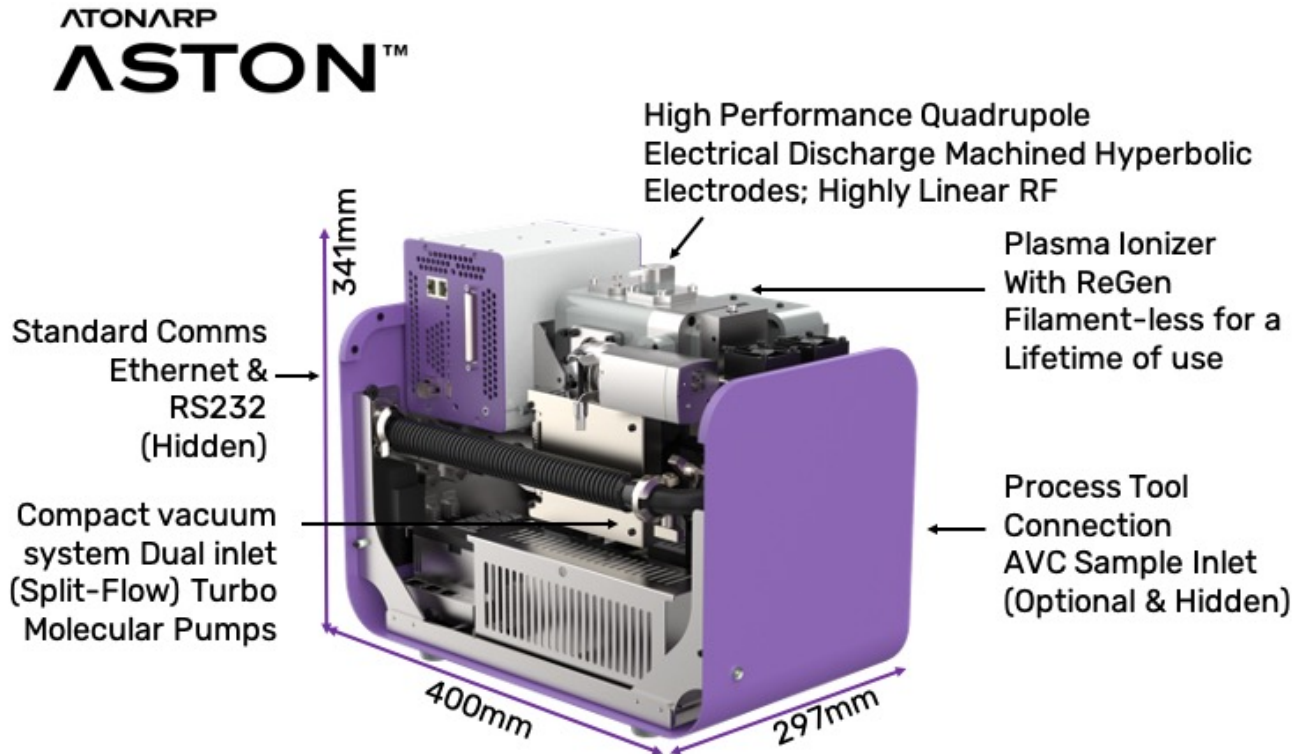
In these etch processes, under-etch is a yield killer (contact opens or high resistance) and over-etch can lead to metal fill and planarization challenges causing knock-on processing, electrical, and yield issues later in the process. Further complicating etch are issues like wafer material thickness uniformity across a 300mm diameter wafer and even wafer curving (called ‘potato chipping’ as the wafer mechanically deforms with increasing and non-uniform material thickness). To address these issues, many processes are designed to have selective etch materials deposited as a blocking layer against slight to moderate over-etch and generally these etch processes are time-based. Alternatively, optimizing the etch process by specifically 1) monitoring the quantity of etch byproducts and 2) looking for a clear end point and flattening of the etch rate curve, will provide optimum throughput and a consistent etch profile, reducing risk

in subsequent processing steps and providing more consistent electrical performance.

In-Situ Molecular Sensors for EPCO

Robust real-time in-situ molecular sensor solutions are now required to offer true insight into how a process is setup and proceeding, and to offer data that is actionable and impactful for operational performance and bottom line improvement. Reactants, by-products, and partial products can be identified and quantified,

allowing for dynamic process control to ensure tight mean and standard deviation control for a given process module across run-to-run, chamber-to-chamber, tool-to-tool, and even site-to-site. Managing overall complex semiconductor process control and line-yield starts with having tight control on individual process steps and ensuring low variability and tight statistical process control (SPC). Aston from Atonarp (figure 3) was designed from the ground up to meet the needs of in-situ molecular analysis to enable EPCO.



Atonarp is advancing medical diagnostics, life sciences research, and industrial process control through next-generation digital molecular profiling. In-situ molecular profiling in advanced manufacturing means higher throughput, improved efficiency, and reduced waste. Real-time, quantitative diagnostic tests can improve outcomes and patient satisfaction at lower cost.