

# Proactive Particle Control in Ultrapure Water (UPW) in Silicon Wafer Cleaning Process, IRDS, 2021

## Introduction

The evolution of the semiconductor device design from planer to FinFET has enabled the ability to continue advancement of technology node to a device pitch of 24nm by 2022, which translates to a spacer width of 6nm. The spacer width then defines the killer particle size of 3.0nm of the Fin module. In addition, The FIN height will have reached 60nm translating to a FIN aspect ratio of 10:1 leading to potential device reliability issues related to FIN collapse. This will move device design strategy by 2025 to require Lateral Gate All Around (LGAA) transistor design using nano wires and nano sheets to elevate structural problems related to FIN transistor design. Finally, by 2031, device design will move to 3D stacked device design adding more complexity such as P over N, memory on Logic, and Logic on Logic. This continuation of enabling device shrinking with the addition of device complexity is driving the need to further enable the ability to detect and remove the critical particles that are the major source of defects that prevent device yields to improve. This problem has been a challenge for a decade and is now more complicated as the capability of measuring critical particle size on the wafer surface has also been reached. The consequence we are now faced with is to rely on measuring particles much larger than the critical particle size with the expectation that we can predict the behavior of the critical particles that we cannot measure. We are also finding other factors that are concerning and problematic:

1. The most advanced UPW particle filtration technology cannot control particle removal at the current killer particle size.
2. There are indications that high purity materials shed a considerable number of particles at or above the current killer particle size.
3. There is a concern that high molecular weight polymers may form particles on the wafer surface during the wafer drying process that are at or larger than the current killer particle size.

This white paper describes the PROACTIVE approach of UPW IRDS team to deal with the technological gap and associated risks described above.

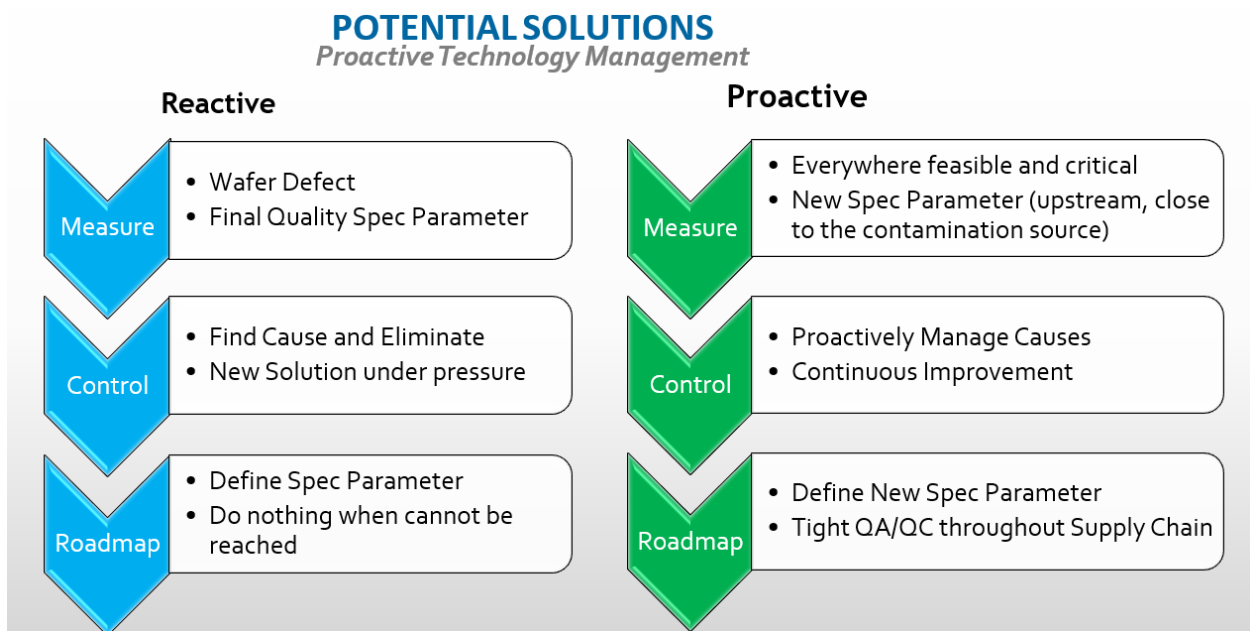
## Part 1: Proactive Approach for Particles Control

Traditionally, particle control is dealt with in a reactive manner. It assumes that the particles should be detected first and then their causes identified and resolved. This approach has been used throughout the history of semiconductor manufacturing at all levels. However; since we no longer can detect killer particles, compounded by the increasing occurrence and risk associated by the killer particles it has become necessary to find ways to control particles with the means available. This idea requires proactive approach to particles control, leveraging best available metrology and standardized processes. The following steps are required to enable proactive particle control:

1. Define particle level targets on the wafer and other critical surfaces based on the device sensitivity to particles as defined by device and process experts.

2. Using highly controlled deposition experiments determine the particle deposition rate on the wafer compared to the known particle count in the UPW.
3. Based on the above, define the target level of the particles in UPW.
4. Using highly controlled experimentation, determine the retention efficiency of particles by filtration at the killer size using the best available final filtration technology available.
5. Develop a projection for the level of particles upstream to the final filters which will result in an acceptable level of killer particles level in the UPW supply to the process tool as defined by the wafer deposition rate study.

Figure #1 below illustrates the benefits of using the proactive approach compared to the reactive approach:



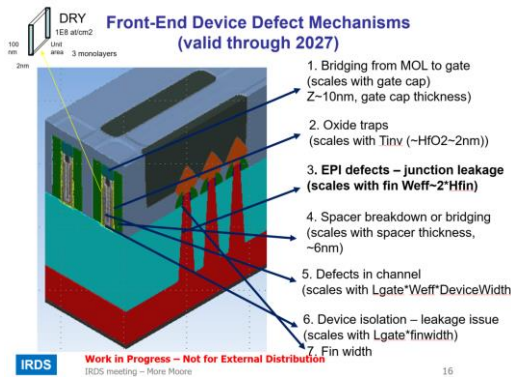
**Figure 1. Proactive vs. Reactive Approach for Contamination Control**

It is expected that the implementation of this process will drive the following proactive development:

- Tighter filtration and more effective use of existing SEMI standards (i.e., SEMI C79) for evaluation of the UPW filters performance.
- Better quality of the materials used in UPW delivery and more effective use of the particle related SEMI standards (i.e., SEMI F104).
- Focus of UPW system design and operation ensuring low particle load into the feed to the final filters. This implies design rules that would lead to less hydraulic instability and lower friction forces. SEMI F61 can be used for reference.

## Methodology

**Target particle size.** The following image illustrates key points of discussion between UPW and the device experts (More Moore IFT, International Focus Team) that helps to deconstruct the sensitivity of the device to particle related defects and define the killer particle size as defined in IRDS table YE03.



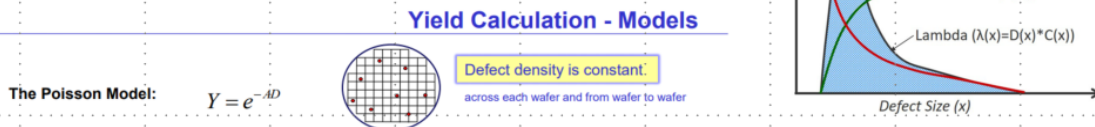
**Figure 2. Understanding Particle Killer Effect Based on the device Structure**

**Target particle density.** In addition to the killer particle size, it is important to determine the target level of the defect density distribution of each layer in order to meet the required product yield as defined by IRDS More Moore. This targeted defect density distribution is estimated using typical key parameters such as k (process risk) and q (fab constant).

Below is the Yield calculation model referenced from published method as agreed between Yield Enhancement Team and More Moore chapters of IRDS:

## Yield distribution

- ▶  $D0 = \text{Integral of } D(x) = k/x^q \text{ from } x = Xc \text{ to } \text{Inf.} = k/2/Xc^2$  where  $Xc$  : minimum critical size, for  $x < Xc$ ,  $D(x) = 0$
- ▶  $K, q = \text{Fab constants, } q \sim 3$ .



The Yield distribution calculation uses the Poisson distribution model which is a highly effective tool in a discrete process such as device defect analysis. Using this model, the critical area for each layer can be determined with respect to defect size, defect density, and feature dimensions. The following table provides the calculated defect density for the smallest size affecting the layer (killer particle size) for the minimum target of 80% yield. Yield <80% is considered cost ineffective.

**Table 1. 2020 target of maximum allowed defect density (Dx/wafer) for the killer particle size or larger**

2020	Width (nm)	Defect Size (nm)	Pitch (nm)	Critical Area (cm <sup>2</sup> ) in 80mm <sup>2</sup>	Dx/wafer	Dxi	1/(A*Dxi)^n	1/(A*D0i)^n	Defect Mechanism	Process Type for predominant defect mechanism
Gate	20	10.0	48	0.267	5.7	0.0405	0.992	0.978	Patterning, Gate stack	Dry etch, Wet Etch (GAA), Wet Clean
Fin	7	3.5	28	0.080	133.5	0.3306	0.981	0.978	Gate stack, EPI	Dry etch, Dry Clean (SiCoNi) or Wet Cleans
VC	16	8.0	48	0.017	11.2	0.0633	0.998	0.978	Clean	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
MetalC	16	8.0	48	0.213	11.2	0.0633	0.971	0.978	Patterning, Metal	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Via0	15	7.5	42	0.017	13.6	0.0720	0.999	0.978	Clean	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Metal0	15	7.5	30	0.320	13.6	0.0720	0.919	0.978	Patterning, Metal	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Viax	18	9.0	51	0.010	7.9	0.0500	0.999	0.978	Clean	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Metalx	18	9.0	36	0.320	7.9	0.0500	0.932	0.978	Patterning, Metal	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Viay	40	20.0	113	0.005	0.7	0.0101	1.000	0.978	Clean	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean
Metaly	40	20.0	80	0.320	0.7	0.0101	0.993	0.978	Patterning, Metal	Dry etch, Wet Clean, Wet Fill (Electroplating), Wet Clean

A similar table was produced for the following two generations of technology based on their respective critical dimensions of the device as published in the More Moore table.

**Table 2. Summary of the Dx/wafer for the three generations of technology**

2020	2022	2025	2020	2022	2025
Defect Size (nm)	Defect Size (nm)	Defect Size (nm)	Dx/wafer	Dx/wafer	Dx/wafer
10.0	9.0	7.0	5.7	5.0	6.6
3.5	3.0	3.5	133.5	136.1	52.8
8.0	9.0	9.0	11.2	5.0	3.1
8.0	9.0	9.0	11.2	5.0	3.1
7.5	6.0	5.0	13.6	17.0	18.1
7.5	6.0	5.0	13.6	17.0	18.1
9.0	8.0	6.0	7.9	7.2	10.5
9.0	8.0	6.0	7.9	7.2	10.5
20.0	20.0	20.0	0.7	0.5	0.3
20.0	20.0	20.0	0.7	0.5	0.3

Where Dx is the defectivity value for Gate and Fin layers obtained from the Table 1 for 2020 and similar tables for the subsequent two generations of technologies.

Based on the calculations critical defects depend on both size and the source of the contamination. While some contaminants are coming from UPW and chemicals in the wet processing, others are related to dry processing and may originate from air or gasses/precursors. For example, for the UPW roadmap, the smallest killer size is 3.5nm of conductive particles at limit of 136 particles per 300mm wafer in year 2022, whereas the gate would be limited by any particles of the size of 9 nm or greater at a limit of 5 particles per 300mm wafer.

**Particle deposition rate.** The UPW IRDS Team has conducted several particles deposition studies and estimated the ratio of particles in UPW that would result in target density of particles on the critical surface. It is expected that the leading mechanism of the particle deposition is drying, meaning that particles present in the water film on the wafer surface will attach to the wafer as the result of wafer drying process.

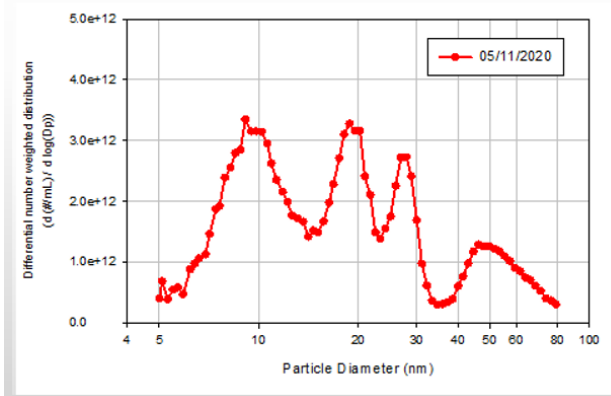
The following diagram illustrates the details of the latest particle deposition test conducted with help from CT Associates and Unisers laboratories. In this test, particle mixture was prepared out of silica particles

standard solutions of a known sizes of the silica particles. The particle size distribution vs. concentration was characterized using LNS as illustrated in the figure below.

## UPW IRDS – Particle Deposition Test

- Spin Coater was provided to CTA by Entegris
- Intel and Pall covered some of the cost

Sample preparation @ CT Associates



- Particle size from 5nm to 70nm
- Liquid concentrations for spin-drying:
  - Wafer-1: 1Eg/ml
  - Wafer-2: 1E7/ml
  - Wafer-3: 2E6/ml

## Wafer-scanning @ UNISERS

Shipped to Zurich

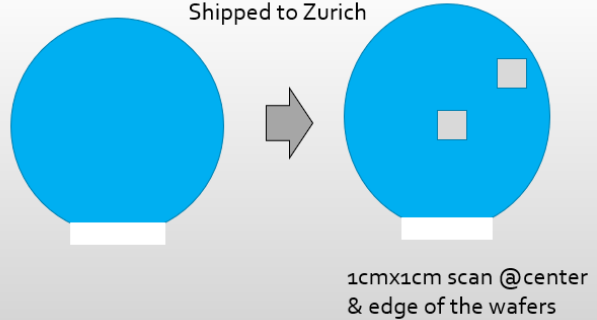


Figure 3. Particle Deposition Test Procedure

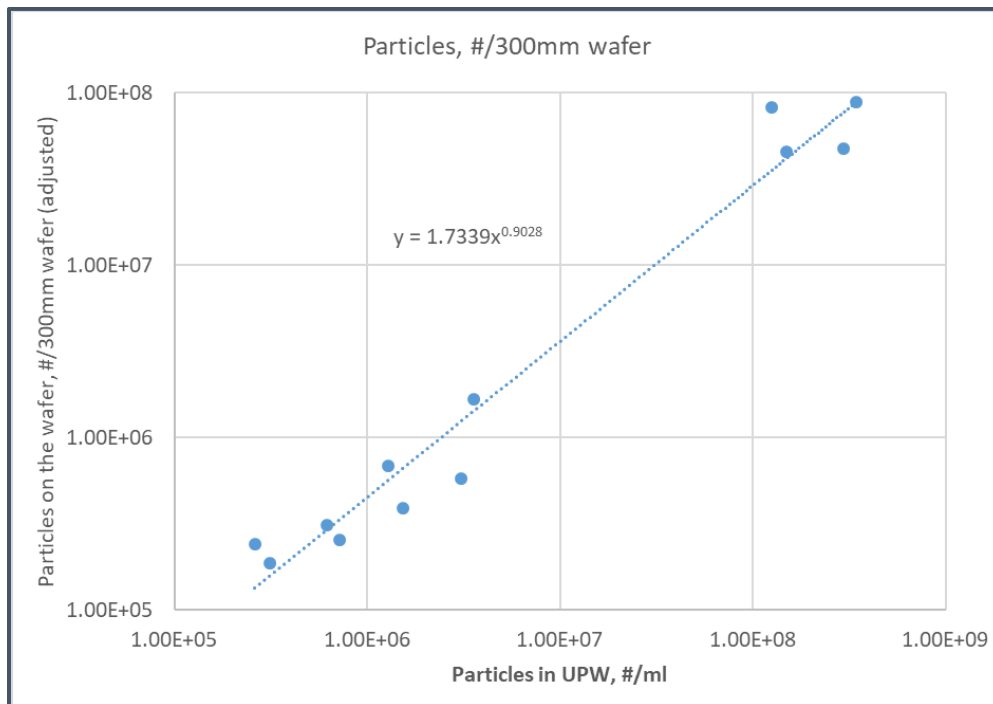


Figure 4. Particle Deposition Test Results

The data in Figure 4 provided basis for the following correlation:

**Table 2. UPW Roadmap Particle Development**

2020	2022	2025	2020	2022	2025	2020	2022	2025	2020	2022	2025
Defect Size (nm)	Defect Size (nm)	Defect Size (nm)	Dx/wafer	Dx/wafer	Dx/wafer	Cx, #/ml UPW	Cx, #/ml UPW	Cx, #/ml UPW	IRDS value, Cx' #/ml	IRDS value, Cx' #/ml	IRDS value, Cx' #/ml
10.0	9.0	7.0	5.7	5.0	6.6	3.8	3.3	4.4	1	1	1
3.5	3.0	3.5	133.5	136.1	52.8	122.9	125.6	43.9	100	100	10

Note: UPW target (Cx'), particles per milliliter in UPW, was determined by rounding down projected maximum level of particles in UPW (Cx).

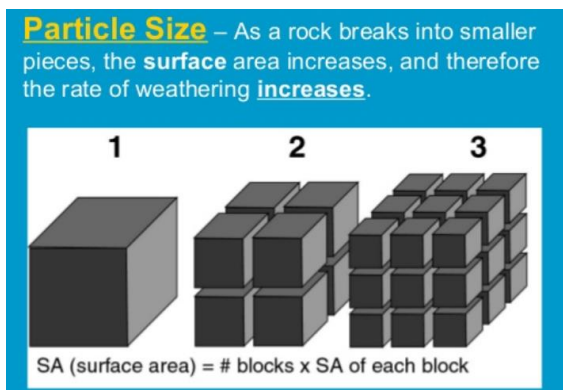
**Filtration efficiency.** In recent years, there has been a lot of effort by leading filter companies to develop tighter filters and evaluate their performance. Although the information is insufficient to accurately define performance, there is reasonable ability to estimate particle retention capabilities based on the existing published information.

**“Proactive” particle target.** To drive proactive operation on a DI water/UPW system, the measurable particle level in the feed to the final filters is projected using power law approximation. This approximation is done in two steps:

Step 1 uses the target level of killer particles (both the size and the concentration) and calculates the concentration of the killer particle (size per YE03 table) in the feed to the final filters (current assumption is 8X removal by both final filters and the POU filters, based on suggestion of the filter vendors).

Step 2 uses that calculated value of Step 1 and calculates the concentration of the 50nm particles, using power law value of 3.

The image below illustrates the reasoning behind commonly observed correlation with power law between 2 and 3 (most often near 3), meaning that decrease of the particles size in half results in 8x number of the corresponding smaller particles. This correlation is valid for unfiltered water where particle size distribution is unaffected.



**Figure 5. Physical meaning of power law dependency**

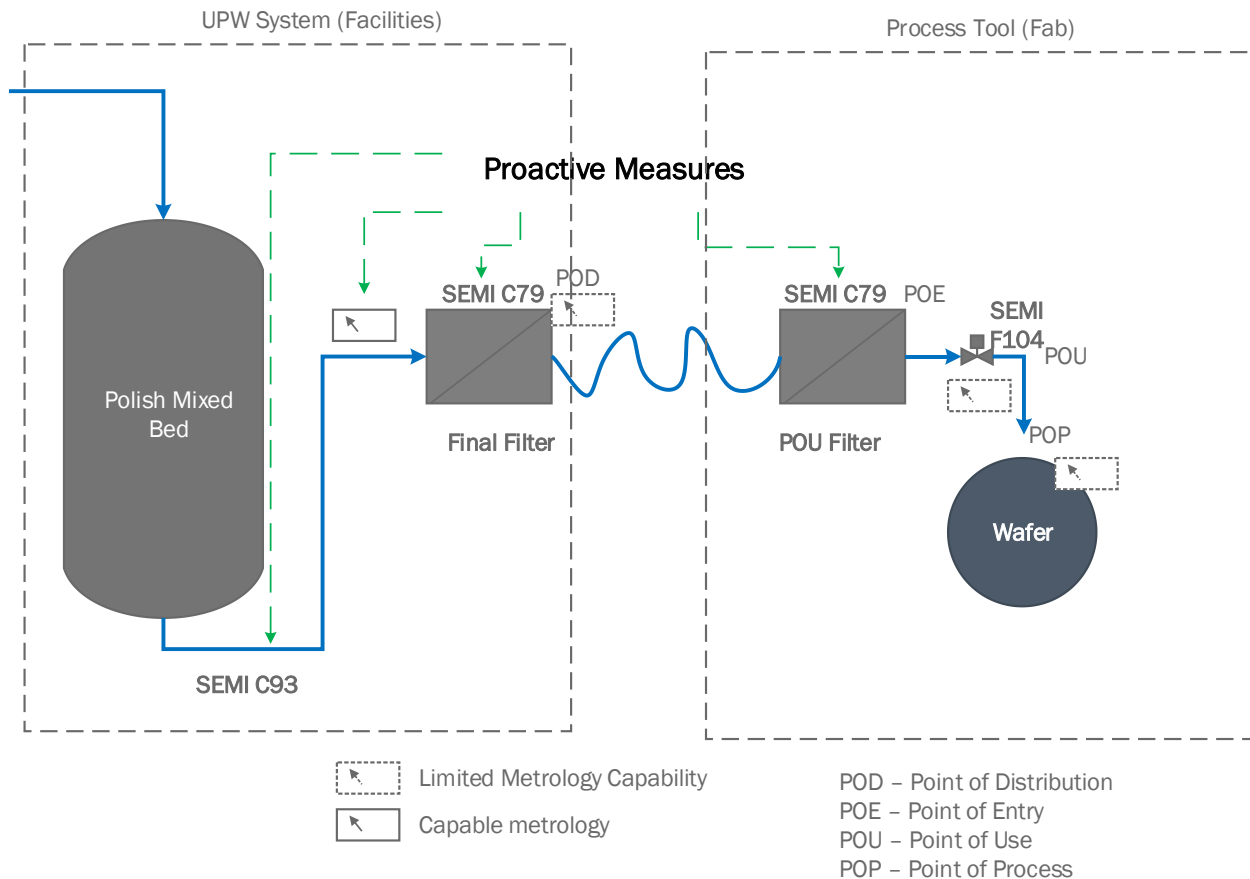
As the result, the proactive roadmap target is calculated from the target UPW killer particle concentration divided by filter retention factor and projected into larger measurable size of the particles, using power law coefficient of 3.

The following example demonstrates the specific calculations used to set the proactive particle target.

### UPW IRDS “Proactive” Particle Targets

**Note: the following section describes methodology for proactive managing of particle risks based on IRDS data. UPW IRDS forum is currently focused on the particle deposition model to be able to better correlate the defect density with particle concentration in UPW. This may lead to different particle target concentrations in UPW, subject for future roadmap update.**

The following schematic diagram represents UPW Particle control system.



The diagram above includes Polish ion exchange (IX) column that while treating traces of ions is also capable of highly effective particles removal. At the same time, the IX resin was found to be able to produce extremely high number of the particles larger than the killer size. SEMI C93 standard was developed to help to control the cleanliness of the IX resin.

Final filtration step follows Polish IX and is the last treatment step in the UPW system. The most advanced filters have been first introduced more than 2 decades ago and have not changed ever since, despite

substantial geometrical scaling in more than 10 generations of technologies in this period. As the result, currently used final filters are expected to reduce the level of particles in the feed only approximately by 50% (based on experts' opinion and published data). There is also possibility that POU (point of use) filters can be added next to critical tools. This possibility is considered in the proactive target development. The particle retention rate estimated for the POU filters is 75%.

Note: above filter retention values are used for illustration purpose only. It is recommended to test filters using SEMI C79 standard and develop a system specific calculation based on the actual filter retention.

Given the fact that most (if not all) advanced semiconductor manufacturing facilities have ability to monitor particles of the size of 50nm, the following calculation was developed for the proactive particle control at this size.

Key assumptions:

**IRDS target**

- see table 2

**Key assumptions:**

POU filter retention - 75%

FF retention - 50%

Power law - 3

**Table 3. Power law calculation to determine Proactive roadmap value**

year	D', nm	Cx', #/ml	Incl Filter			UPW Roadmap, #/ml	Zero Count, #/ml
			#/ml	Dp, nm	Cp, #/ml		
2020	3.5	100.0	800	50	0.274		0.05
2020				30	1.270		0.05
2020	10.0	1.0	8	50	0.064	0.05	0.05
2020				30	0.296	1.00	0.05
2022	3.0	100.0	800	50	0.173		0.05
2022				30	0.800		0.05
2022	9.0	1.0	8	50	0.047	0.05	0.05
2022				30	0.216	0.70	0.05
2025	3.5	10.0	80	50	0.027		0.05
2025				30	0.127	0.05	0.05
2025	7.0	1.0	8	50	0.064		0.05
2025				30	0.296		0.05

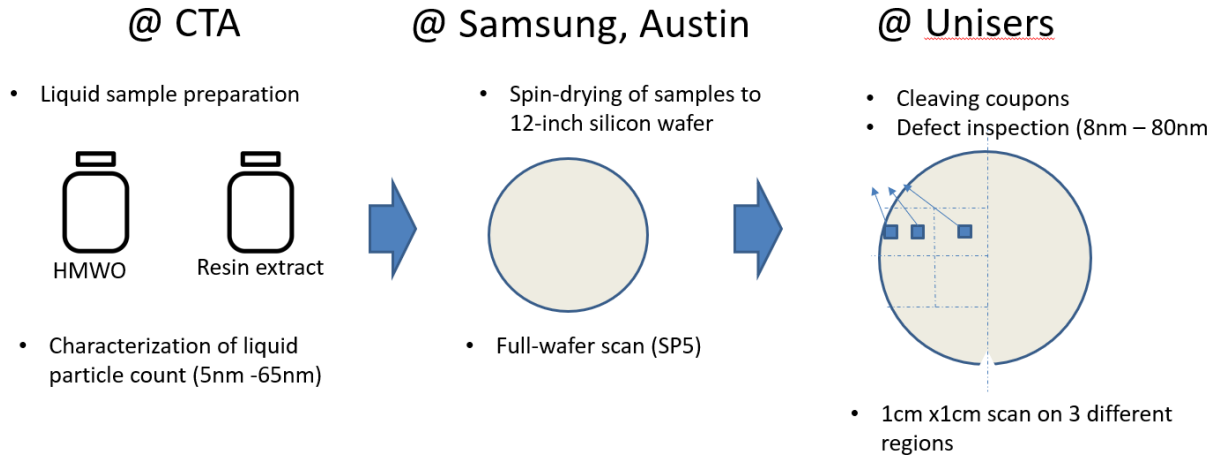
Note: this methodology is valid if zero count represents actual capability of the used particle metrology

C<sub>p</sub> is the calculated target proactive particle concentration in the feed to the final filters.



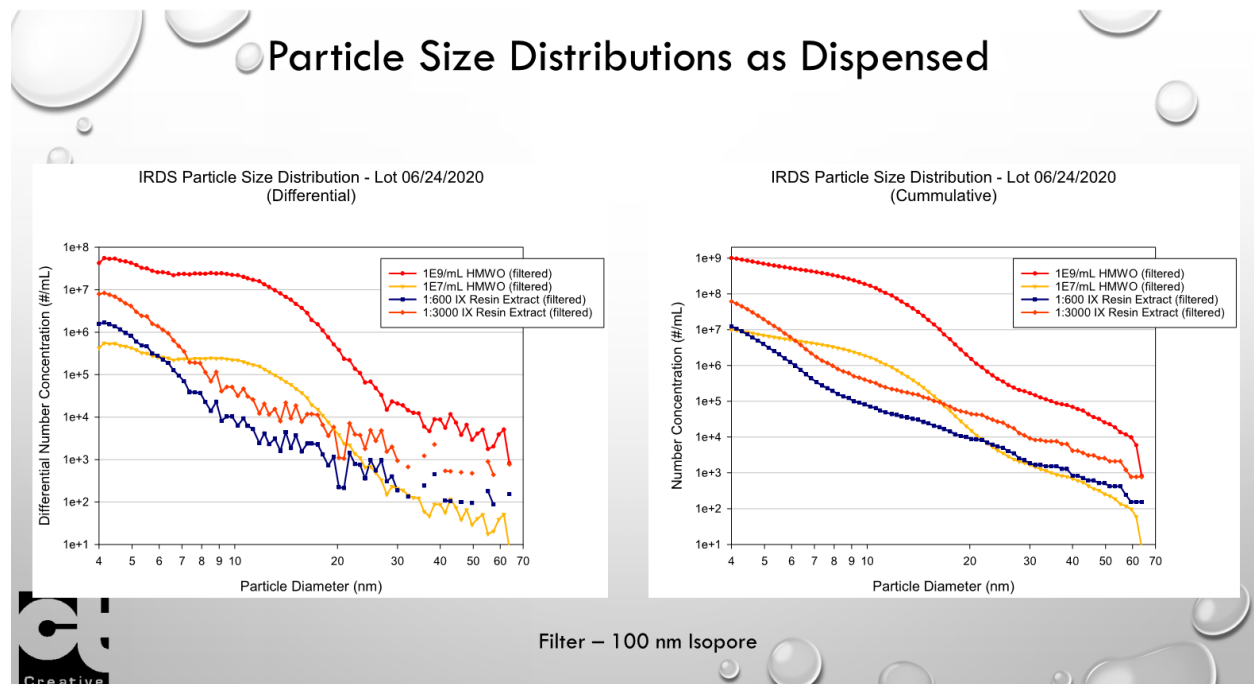


Recently, the UPW IRDS team organized an experimental study to confirm and quantify the risk of particle precursors in UPW. One goal of the study was to propose a target level of the particle precursors for the UPW roadmap. The experiment was conducted with support from CT Associates, Samsung, and Unisers. The following diagram (see Figure 7) illustrates the test process.



**Figure 7. Particle Precursor Deposition Test Workflow**

Particle precursors' solution used in the test were first characterized by the particle size distribution.



**Figure 8. Particle precursor characterization**

The 300mm blank un-patterned silicon oxide wafers were pre-cleaned using SC1 followed by DI Water rinse using single wafer processing tool prior to dispensing the solution on the wafer. The solution was

then hand poured about a third of the way in from the edged of the wafer using a pipet while being rotated at various speeds indicated in the table. The wafer was then rotated at a higher speed as indicated in the table under nitrogen gas stream to dry the wafer surface. Particles were then counted on the dried wafer using a KLA Tencor SP5 surface scan tool (particles size detection of 19nm). Wafer processing conditions and results of the particles formation are indicated in Figure 9.

Wafer Preparation Details						19NM Defect Scan Results			
Run Order	Slot ID	Spin-Coated Solution	Process Recipe Cleaning Steps	Process Recipe Spin-Coating Step	Process Recipe Spin-Drying Step	Defect Map Before Coating	Defect Map After Coating, Only Added Defects Shown, Blue = PCs with Images	Defect Size Distribution for the Scan Map after HMW/O Coating	Post-Scan Details
1	24	DI Water Only	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream				373 Added, 25 Imaged, 3 PCs found
2	22	Resin Extract 1:600 Dilution in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream				873 Added, 30 Imaged, 12 PCs found
3	17	Resin Extract 1:3000 Dilution in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream				480 Added, 31 Imaged, 11 PCs found
4	16	1MDa HMW/O 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream				3890 Added, 35 Imaged, 9 PCs found
5	9	1MDa HMW/O 1E7/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream				89934 Added, 29 Imaged, 15 PCs found
6	4	None (BLANK)	SC1 Rinse and DI Water Rinse	No Liquid Dispense while spinning at 80rpm (BLANK)	Spin at 1500rpm under a Nitrogen Gas Stream				60 Added, 23 Imaged, 3 PCs found
7	3	1MDa HMW/O 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 10rpm	Spin at 150rpm under a Nitrogen Gas Stream				2506 Added, 35 Imaged, 31 PCs found
8	2	1MDa HMW/O 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Slowly Pour 120 mL solution while spinning at 1800rpm under a Nitrogen Gas Stream	Spin at 1800rpm under a Nitrogen Gas Stream				960 Imaged, 33 Imaged, 9 PCs found
9	1	1MDa HMW/O 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 200rpm	Spin at 1500rpm under a Nitrogen Gas Stream				652 Added, 32 Imaged, 21 PCs found

Figure 9. Particle Precursor Deposition Test

The same wafers were shipped to Unisers for subsequent analysis of the particles with particle detection of 8nm.

The results of the Unisers analysis are shown in Table 4.

Both SAS (Samsung Austin Semiconductor) SP5 and Unisers data confirmed similar particle distribution and added particle counts per bin size of the dissolved HMW/O compounds. The defect level on the wafer was also consistent with the level of particle equivalents as characterized by CTA.

**Table 4. Unisers results of the particle precursor deposition (focusing on 8-19nm particles)**

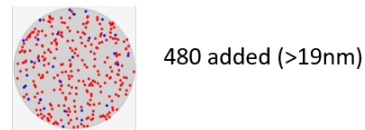
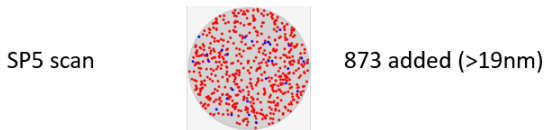
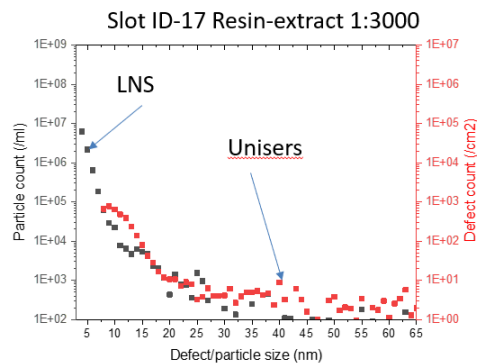
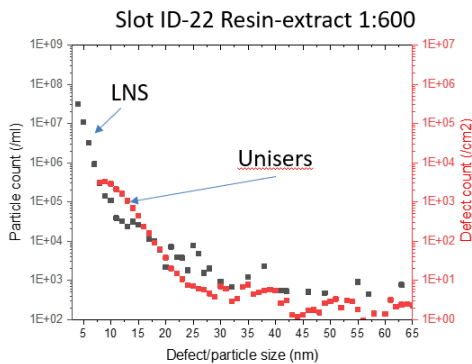
Run Order	Slot ID	Spin-Coated Solution	Process Recipe Cleaning Steps	Process Recipe Spin-Coating Step	Process Recipe Spin-Drying Step	Unisers defect count (8nm-19nm) / cm <sup>2</sup>	SP5 defect count (>19nm) / wafer
1	24	DI Water Only	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream	473	373
2	22	Resin Extract 1:600 Dilution in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream	15,759	873
3	17	Resin Extract 1:3000 Dilution in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream	3,495	480
4	16	1MDa HMWO 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream	9,693	3,890
5	9	1MDa HMWO 1E7/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 80rpm	Spin at 1500rpm under a Nitrogen Gas Stream	181,180	89,934
6	4	None (BLANK)	SC1 Rinse and DI Water Rinse	No Liquid Dispense while spinning at 80rpm (BLANK)	Spin at 1500rpm under a Nitrogen Gas Stream	662	60
7	3	1MDa HMWO 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 10rpm	Spin at 150rpm under a Nitrogen Gas Stream	546,893	2,506
8	2	1MDa HMWO 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Slowly Pour 120 mL solution while spinning at 1800rpm under a Nitrogen Gas Stream	Spin at 1800rpm under a Nitrogen Gas Stream	341,703	960
9	1	1MDa HMWO 1E9/mL in DI Water	SC1 Rinse and DI Water Rinse	Pour 120 mL solution while spinning at 200rpm	Spin at 1500rpm under a Nitrogen Gas Stream	327,343	652

For the UPW roadmap development, Resin extract data were used for reference

### Defect/particle size distribution (Resin Extract)

LNS: 8nm-19nm particle count (/ml): 7.55 E5  
 Unisers: 8nm-19nm defect count (/cm<sup>2</sup>): 1.58 E4

LNS: 8nm-19nm particle count (/ml): 1.51 E5  
 Unisers: 8nm-19nm defect count (/cm<sup>2</sup>): 3.49 E3



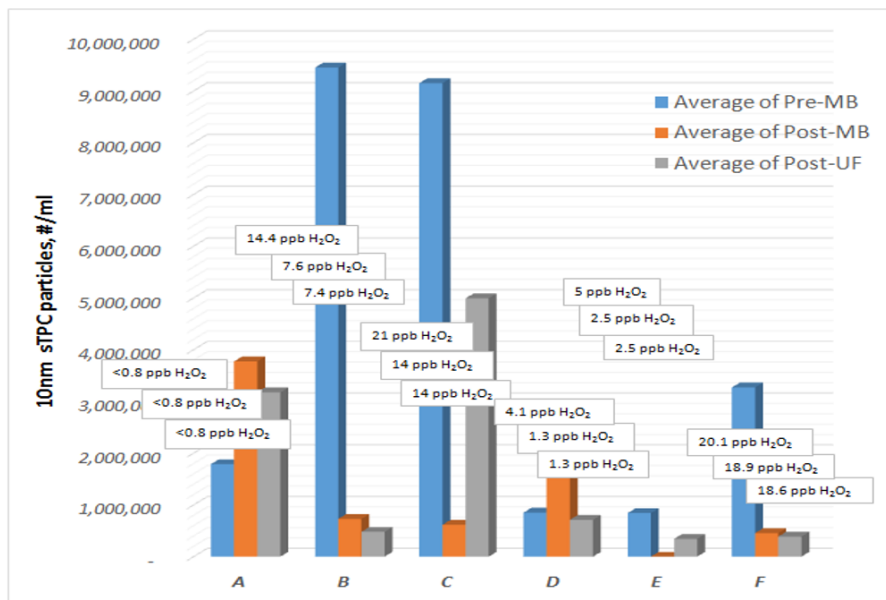
**Figure 10. Particle precursor deposition results for the UPW IX resin extract (presented at UPM2020, November 2020)**

The results of Figure 10 indicate that 7.55E+5 particle equivalent in milliliter of UPW produced 1.58 E+4 particles per cm<sup>2</sup> of the wafer or 1.1E+7 particles per wafer, or one particle equivalent per ml produces 14.8 particles on the wafer. Using the data of the second wafer where resin extract solution was diluted to 1.51E+5 #/ml, the result is similar to the 1<sup>st</sup>: one particle equivalent per ml produces 16.6 particles per wafer (average of 15.7 #/wafer).

Given the target for the particle density on the wafer (example 5 defects per wafer for 2022), this means that the particle precursors in UPW should be limited to 5/15.7 = **0.32 particle equivalent per milliliter**. This result suggests that the risk can potentially be significant. This is based on the data published by UPW ITRS (now UPW IRDS), suggesting that such particles concentration in the high-volume manufacturing facilities that participated in that study can be as high as **~1E+6/ml in UPW**.

Note: the results are based on the limited number of the data points and should be viewed as having limited accuracy.

### sTPC 10nm particles in UPW Polish vs. H<sub>2</sub>O<sub>2</sub> levels



ULTRAPURE WATER Conference, Portland, OR, 2017

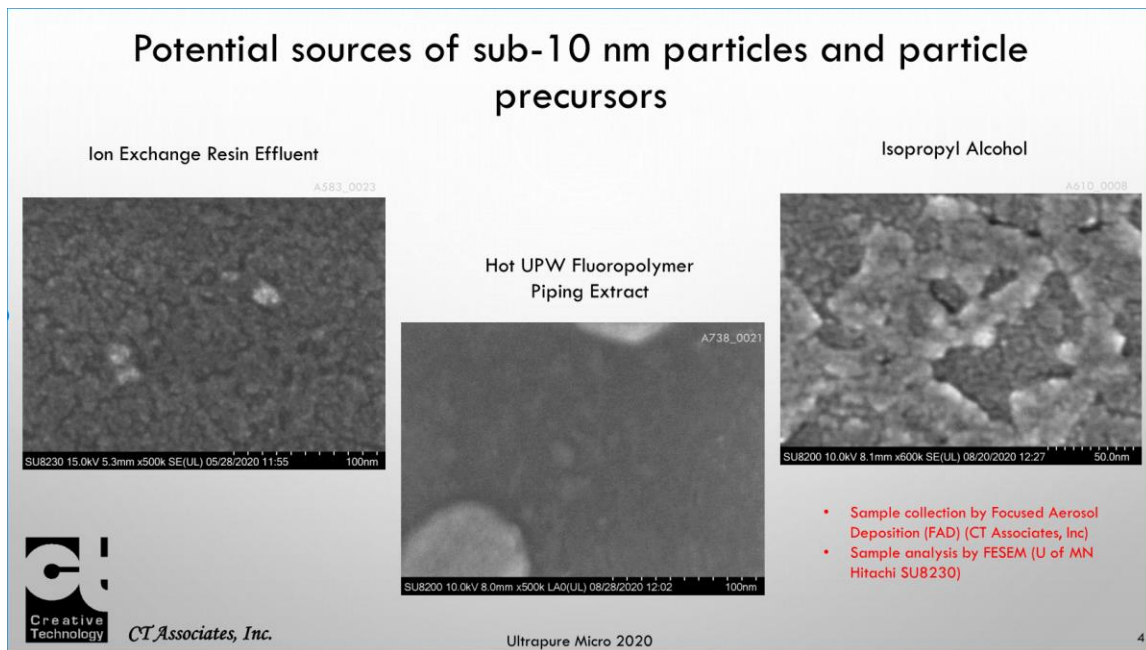
**Figure 11 Particle (likely Precursor) Level in UPW as measured by sTPC** (same technology used in definition of the particle precursor). Scanning Threshold Particle Counter, a particle measurement device currently being offered by Kanomax FMT.

### Discussions

When considering the definition for the roadmap parameters, it is important to do this in the context of the following factors:

- Actual manufacturing process includes steps protecting yield from contamination – this means that actual risk to yield can be lower than perceived. However, it is common to use test wafers and run them under conditions similar to those used in the experimental work above. Thus, these experimentally observed defect levels can potentially lead to impacts to production.

- New devices have increasing sensitivity to contamination due to smaller features and higher complexity
- A past sTPC benchmarking study indicated different performance of HVM (high volume manufacturing) UPW systems on final particle quality. This means that sTPC metrology does distinguish quality differences.
  - o SEMI C93 data suggest significant difference in quality of different resins, potentially explaining the difference.
- There are anecdotal reports of wafer issues during IX resin replacements
- Variability of filtration performance is well known (SEMI C79 data)
- Evidence of residue on the wafer due to precursor deposition was recently reported



## Summary

The experimental work conducted by the UPW IRDS Team suggests substantial risk of particle deposition caused by particle pre-cursors; however, it is unclear how this may impact semiconductor device yield directly. The recommendation to the material providers is to expedite the improvement of the cleanliness of the ion exchange resin and other materials used in UPW to reduce the elution of high molecular weight organics from these materials.