Using Principal Component Analysis for Photomask CD signature investigations

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ABSTRACT

Reticle critical dimension (CD) errors must be minimized in order for photomask manufacturers to meet tight CD uniformity (CDU) requirements. Determining the source of reticle CD errors and reducing or eliminating their CDU contributions are some of the most relevant tasks facing process engineers. The AMTC has applied principal component analysis (PCA) to reticle resist CD measurements in order to examine variations in the data. PCA provided the major components of resist CD variation which were rescaled into reticle CD signatures. The dominant component of CD signature variation is very similar in shape and magnitude between two different chemically amplified resist (CAR) processes, most likely indicating the variation source is a common process or tool. CD variational signatures from PCA were used as a basis for launching investigations into potential reticle CD error sources. PCA was further applied to resist CD measurements from alternate process tools to assist efforts in judging the effectiveness of resist CD signature matching.

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Keywords: critical dimension (CD) errors, CD uniformity (CDU), principal component analysis (PCA), chemically amplified resist (CAR), stability

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1. INTRODUCTION

Reticle critical dimension uniformity (CDU) continues to be one of the most challenging specifications for photomask manufacturers. Each new wafer technology node has reticle CDU specifications tighter than its predecessor, requiring the elimination or at least the minimization of systematic reticle CD errors, such as center to edge, side to side effects, and localized CD deviations, often referred to as hot/cold spots. For some CARs, the optimization of resist bake and/or develop processes have proven effective in lowering reticle CDU.[1,2,3,4] Other methods such as feedback correction strategies have also been employed when the source of reticle CD error is unknown.[5] Despite these improvement techniques sub 45nm wafer technology nodes demand mask manufacturers fulfill 2nm 3σ CDU specifications,[6] which will require novel approaches for photomasks manufacturers to elucidate the source of CD errors as well as eliminate or minimize their impacts. To this end, the AMTC examined resist CDU signatures using PCA, a statistical technique for revealing patterns in large data sets.[7,8,9] While PCA examines only variations in a data set the resulting components of this variation can be converted into reticle CD signature variations giving process engineers evidence of potential CD error sources. PCA enabled the identification of systematic resist CD signature variations on two different CAR systems which were not evident by other examination methods. The shape and magnitude of the dominant CD signature variations were very similar between two different CAR processes suggesting a common process or tool as the potential error source. PCA was similarly applied to determine the effectiveness of resist CD signature matching using alternate processes tools such as resist develop and post exposure bake (PEB). This report presents AMTC's application of PCA to photomask resist CD signatures.

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2. EXPERIMENTAL

The AMTC processes test reticles at regular intervals in order to gauge line performance and stability. Commercially available 193nm phase shift blanks with widely used positive and negative CARs (pCAR, nCAR) are written with 50kV e-beam (PG) lithography and processed identically to customer reticles, except without the use of feedback compensation strategies. Each test reticle has the identical dense feature layout (560nm pitch) distributed uniformly over ~130mm^2 and 169 measurement points are collected with a CD SEM after the resist develop and final etch processes (*i.e.*, resist and final CD). Resist CD measurements are fitted with a thin plate spline smoothing (TPS) routine in order to obtain a resist CD signature.[10] The TPS fits from resist CD measurements of ~60 test reticles per CAR were examined with PCA.

3. RESULTS

3.1 Resist CDU data for each CAR

For each CAR process there are multiple tools available at each unit process step however, only test reticles processed with the identical coat, PEB and resist develop tools within each data set were selected for this initial PCA examination. This choice was necessary because PCA will later be utilized to compare resist CD signatures between alternate and primary process tools. However, multiple PG and metrology tools were used within each CAR data set and those were not excluded in this analysis. Figure 1 shows histograms of resist CDU for each CAR process with the number of test reticles in each data set.

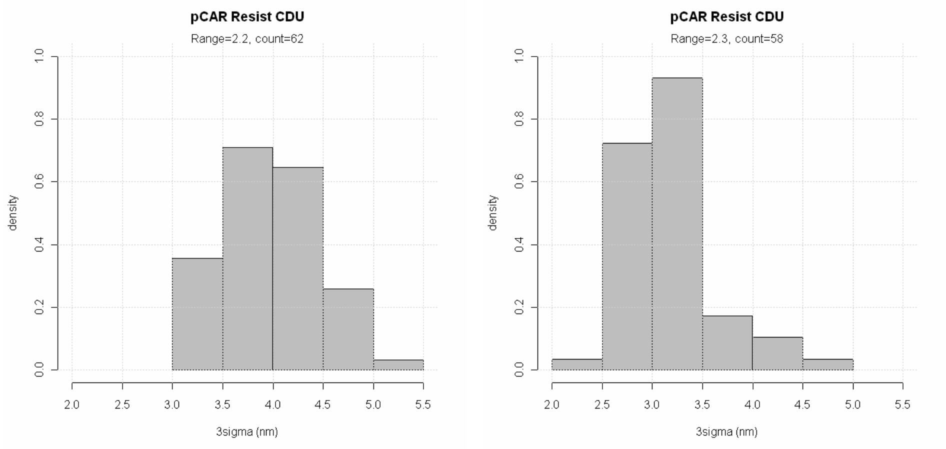

Figure 1. Resist CDU of pCAR and nCAR test reticles.

The average CDU level differs by ~1nm between these two CAR processes and the CDU variation around the respective centers is 25-35%. Despite strict statistical process control (SPC) of relevant process parameters such as resist thickness, exposure dose, temperatures and flow rates, pCAR CDU performance exhibits a 25% variation around a mean of 4nm whereas nCAR varies ~35% around a 3.2nm mean. Understanding the root cause of this variation is vital for the identification of process contributions to the overall CDU and its variations.

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Figure 2 depicts average resist CD signatures for both CAR processes obtained using point by point averages of TPS fits for all test reticles and then normalizing by the mean of each data set.

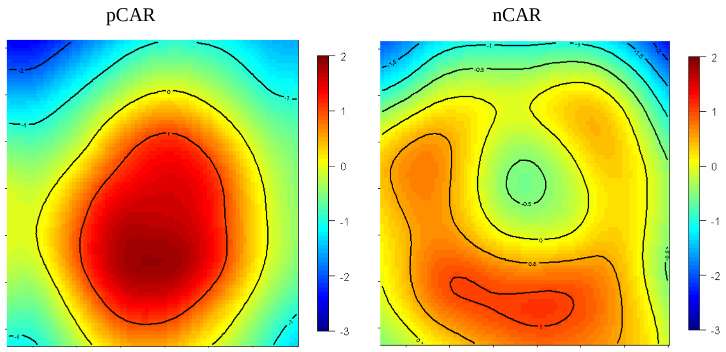

Figure 2. Normalized average resist CDU signatures for pCAR and nCAR processes

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The characteristic pCAR resist CD signature is a center (hot) to edge (cold), radial shape, while that for nCAR is a top (cold) to bottom (hot) orientation. However, variations from this average CDU signature were routinely observed within each CAR process. Consider Figure 3 which depicts resist CD signatures for three pCAR test reticles, processed several months apart, yet with identical PG and metrology tools.

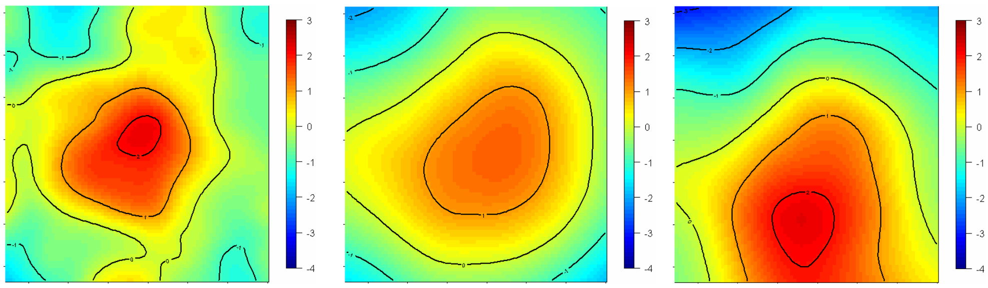

Figure 3. Typical pCAR resist CD signatures.

All pCAR test reticles have radial resist CD signatures yet to varying degrees. This variation was often observed and seemed random, making CD error source determinations problematic. Similar fluctuations in nCAR resist CD signatures were also observed as displayed in Figure 4.

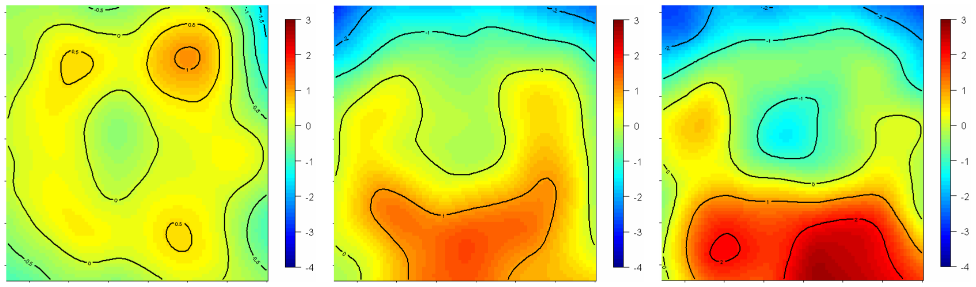

Figure 4. Typical nCAR resist CD signatures.

As with pCAR the identical PG and metrology tools were used for these three nCAR test reticles and process time differed by several months. The left diagram of Figure 4 has essentially no top to bottom CD signature while it is very pronounced in the right diagram, resulting in a poorer CDU. Similar to pCAR, variations in nCAR top to bottom resist CD signatures were routinely observed yet without a known CD error source.

Since the CD measurements were obtained in resist for each CAR, etch and subsequent processes could be eliminated as potential error sources. Efforts thus focused on front end processes such as blank preparation, resist coat & bake, PG, PEB, resist develop, and resist metrology (scatterometry and CD SEM). When preliminary investigations into baking temperatures, temperature uniformities and developer flow rates provided no clear indication of the resist CD error source, the AMTC turned to PCA in order to examine the variation in these two resist CDU data sets.

3.2 PCA on pCAR and nCAR resist CDU

The PCA technique for revealing patterns in large data sets is detailed elsewhere.[7,8,9] As the focus of this study is the resist CD signature variation and not the variations in resist CD off targets, resist CD measurements for each test reticle were normalized by the average in order to obtain a mean of zero for the entire data set.[9] R (version 2.11.1) was utilized to compute the essential principle component elements: the correlation matrix (function *cor*), eigenmodes (values & vectors using function *eigen*), normalized percentages for each variation mode, and scores for each CAR data set.[11] This PCA computation returned a set of eigenmodes for each CAR data set equal to the number of variables (169 in this case, the number of resist CD measurements on each test reticle) yet only the first few eigenmodes will be considered here because they account for the majority of data set variations. Figure 5 shows a Pareto chart of the first 10 eigenmodes for each CAR data set along with the associated eigenvalues and normalized cumulative percentages of each eigenmode.

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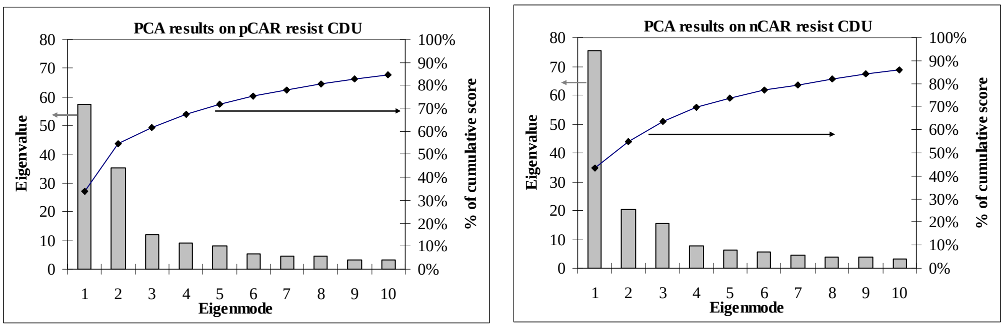

Figure 5. First 10 eigenmodes with eigenvalues and cumulative percentages for pCAR and nCAR resist CD data sets.

The eigenvalue represents the weight of its corresponding eigenmode within the data set. The resist CD signature variation is not random in each CAR data set because some eigenvalues are much larger than others. This clearly indicates a deterministic mechanism as the source of resist CD variation. A flat distribution of eigenvalues, for example, would indicate a dominance of stochastic variations.

It is clear from Figure 5 the weight of nCAR eigenmode 1 is more than for pCAR, while the inverse is true for eigenmode 2. However for both data sets, the first and second eigenmodes account for >50% of the resist CD signature variation. Eigenmodes 3-10 collectively account for ~30% of the data set variation and will not be examined in detail in this report. While 30% resist CD variation is not trivial, the AMTC elected to focus on the most important, principal components of each data set, and selected those eigenmodes responsible for the highest impact on CD variation (*i.e.*, the ones with the highest eigenvalues). We further assumed the first 2 eigenmodes would be the easiest CD error sources to isolate and reduce or eliminate. Lastly, eigenmodes 5-10 in each data set have similar eigenvalues which could indicate random variations as described above.

For every eigenmode and its associated eigenvectors, a score (s) can be calculated by summing the products of the variables and eigenvectors for that eigenmode, as depicted below:[7]

$$s = \sum_{i=1}^{169} \left(v_i * \mu_i \right) \tag{1}$$

Where ν_i represents the normalized TPS fit value from resist CD measurements and μ_i the mode eigenvectors. Principal component scores project the data onto the eigenvectors and assists efforts to describe the different variation modes. [9] Scores for eigenmodes 1 and 2 versus resist CDU (3σ) are displayed graphically in Figures 6 and 7 for every test reticle each CAR data set.

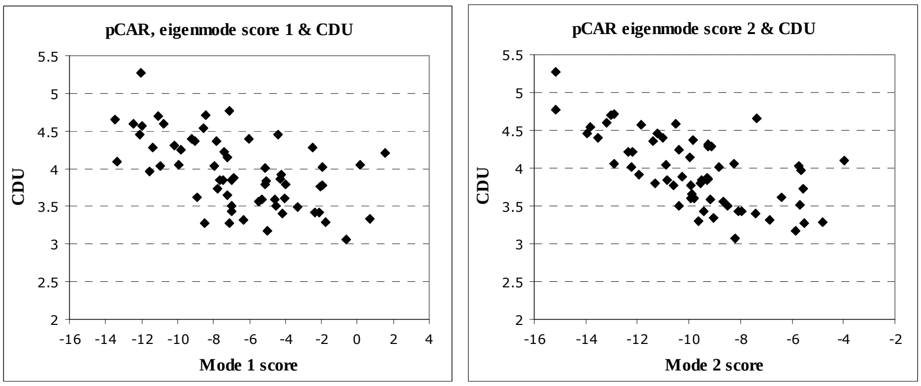

Figure 6. pCAR resist CDU versus mode 1 & 2 scores.

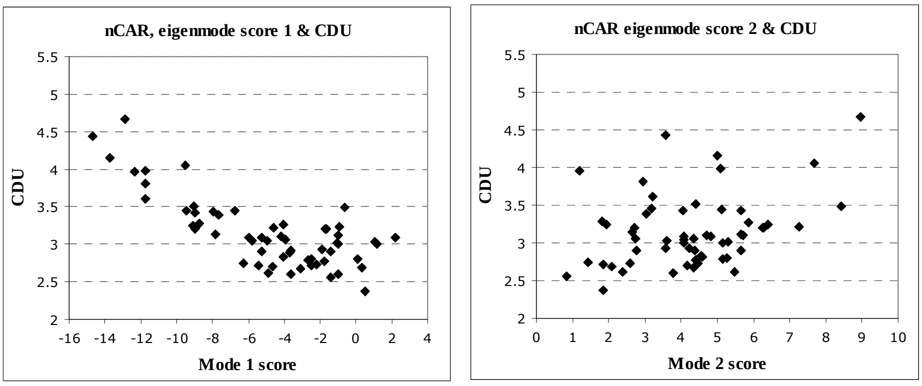

Figure 7. nCAR resist CDU versus mode 1 & 2 scores.

Using the functions *lm* and *anova* in R[11] to examine CDU as a function of mode 1 and 2 scores simultaneously, results in statistically significant models for both CAR processes as detailed in Table 1.

Table 1. Multivariate model information for pCAR and nCAR data sets.

Data Set	**R^2**	**Mode 1 p-value**	**Mode 2 p-value**
pCAR	0.7834	6×10^{-13}	2×10^{-16}
nCAR	0.7568	3×10^{-16}	9×10^{-08}

These CDU models are shown graphically in Figure 8 for both CAR processes.

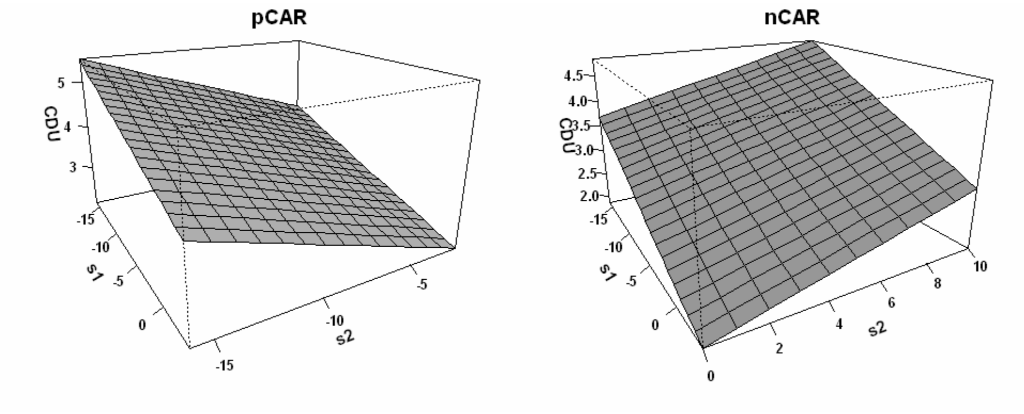

Figure 8. pCAR and nCAR CDU models as functions of mode 1 & 2 scores.

The two planes in Figure 8 are graphical representations of the modeled relationships between CDU and only the first two variational mode scores yet these relationships are only valid within the range of the score data. For pCAR, larger mode 2 scores impact CDU much more than mode 1, while modes 1 and 2 have opposing yet similar impacts on nCAR CDU (with mode 1 contributing slightly more than mode 2 to nCAR CDU). Such trend information is useful if process parameters can be found that relate to these scores for each CAR process. If obtained, we could then limit these contributions to resist CD variation by an appropriate control of the CAR process parameter.

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Figures 6-8 also illustrate the limitations of the classical method of examining only 3σ to characterize resist CDU quality. Resist 3σ is a condensation of a complex process of variables that contribute collectively to CDU and is inadequate to completely describe the uniformity. Similarly, visual examinations of resist CD signatures also fail to provide valuable trend information. Applying PCA however to a large population of reticles, each with 169 measurement points, yields much more information that potentially leads to resist CDU improvements.

3.3 PCA's relation to CDU signatures

Transforming PCA variation modes into reticle CD variational signatures requires rescaling the modes with the following expression:[12]

$$\mu_i^* = \mu_i * \sqrt{\lambda} \qquad (2)$$

Where μ_i^* represents the rescaled mode eigenvector, μ_i the original eigenvector for each variable *i*, and λ is the corresponding mode eigenvalue. Performing this operation followed by plotting the rescaled mode eigenvectors using the resist CD measurement coordinates provides a reticle CD signature variation for each mode. Figure 9 shows rescaled mode 1 and 2 eigenvectors for both CAR processes.

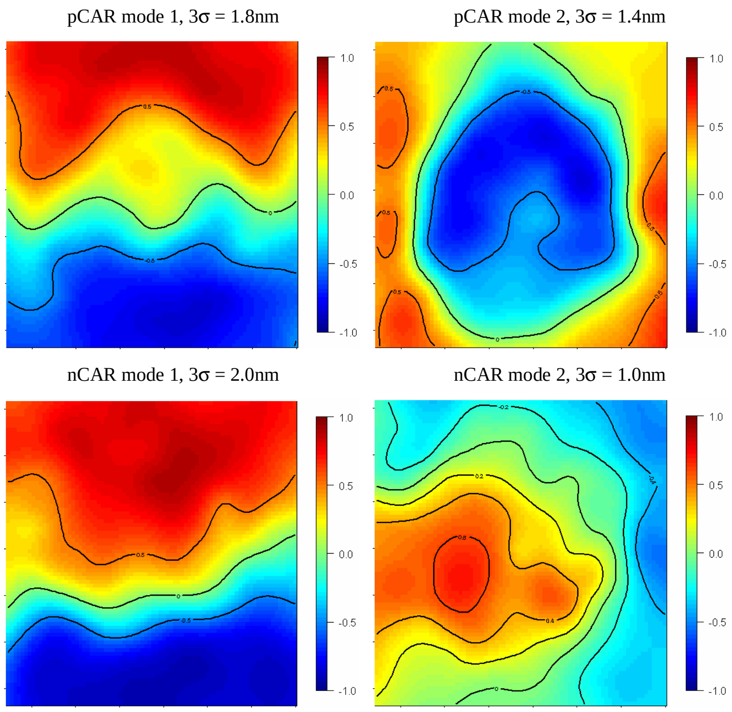

Figure 9. CD variational signatures obtained from modes 1 and 2 for nCAR

Both CAR processes show a very similar top to bottom resist CD variation for mode 1, both in shape and magnitude. The sign in both mode 1 CD signatures (top hot, bottom cold) is opposite from the average nCAR signature (top cold, bottom hot) due to negative mode 1 score results for both CAR data sets (the signs of eigenvectors can be changed without altering the variations they describe [9]). Such a strong similartiy for both CAR processes is surprising since each CAR is unique in chemical composition, additives, and properties, as well as having completely different resist baking temperatures and develop processes. Furthermore, different PEB tools are utilized for these two different CAR processes which should introduce dissimilar variations from different hardware. Similar, dominant CD variation modes, indicates the mode 1 source is likely a common unit process or tool to both CAR processes.

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Mode 2 variations on the other hand are very different between these two CAR processes, with pCAR displaying a center cold, radial type variation, while that for nCAR is also radial but center hot with an obvious side to side CD impact (left hot, right cold). The mode 2 sign for pCAR (center cold radial) conflicts with the average pCAR signature (center hot radial) again due to negative mode 2 score results for pCAR. This difference in mode 2 CD variations could mean the mechanism responsible is something unique to each CAR process.

Although mode 1 for pCAR is the dominant CD variation, it is not visible in the average resist CD signature (Figure 2), while the dominant nCAR mode 1 variation is similar to the average nCAR resist CD signature. Conversely mode 2 for pCAR is very similar to the average resist CD signature while nCAR's mode 2 is unlike its average signature. The correlation between CDU (3σ) and the two dominant modes of variation depicted in Figure 8 can be understood from the shapes of modes in Figure 9. For pCAR adding or subtracting mode 2 to the average resist CD signature will alter the resist CD signature and CDU, as predicted by Figure 8. The same is true for the relation of mode 1 to nCAR CDU (3σ), also shown in Figure 8, as its CDU impact is slightly larger than mode 2 .We thus stand to gain the greatest improvement in CDU and CDU stability by working to

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eliminate mode 2 variations from pCAR and mode 1 variations from nCAR. Eliminating or simply reducing these modes from each CAR process should remove 1-2nm 3σ from the resist CD variation.

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With this information the AMTC began investigations in an attempt to isolate the error source(s) responsible for these CD signature variations. Initial efforts focused on processes where multiple tools were used such as PG and metrology, in an attempt to uncover potential tool mismatches. To date, no strong correlations were observed between these tools yet this investigation continues and results will be presented in a follow up report.

From the PCA examination of potential tool mismatches, the AMTC found another useful application of this technique: determining if alternate process tools provide a suitable match in resist CD signatures to the primary tools.

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3.4 PCA's utility in process matching determinations

PCA was similarly applied to determine the effectiveness of resist CD signature matching using alternate PEB and resist develop tools. Another, smaller set of the same test reticles described in Section 3.1 were processed on alternate tools and compared using PCA scores to the set of reticles that all utilized the primary process tools. Eigenmode results from this PCA application are very similar to those reported above, both in eigenvalues and cumulative percentages of each mode, indicating no new resist CD variations were introduced by these alternate process tools. As previously, only scores from the first two eigenmodes are compared against resist CDU and Figure 10 shows this comparison for pCAR where several reticles were processed on alternate PEB and resist develop tools.

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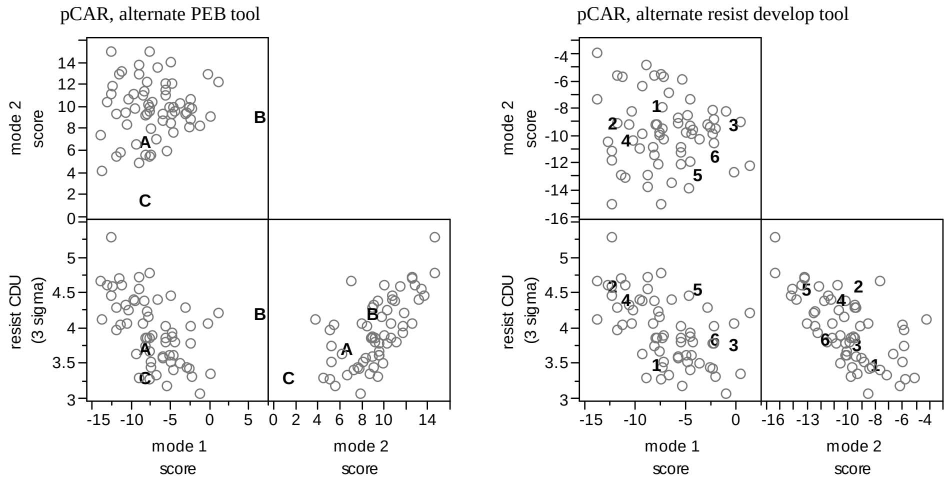

Figure 10. pCAR modes 1 & 2 scores versus CDU; Left: 3 reticles (labeled A, B, and C) processed on an alternate PEB tool; Right: 6 reticles (labeled 1-6) processed on an alternate resist develop tool.

In the case of an alternate pCAR resist develop tool, all reticles display scores and CDU very similar to those of the primary tool, indicating a sufficient match in resist CDU for these two variation modes. For the alternate pCAR PEB tool, reticle "A" is similar to the primary PEB tool while reticles "B" and "C" have outlier scores in modes 1 and 2, respectively. Reticle "A" is thus considered to match resist CDU from the primary PEB tool as well as reticle "B" since mode 1 CD variations were shown previously to have little CDU impact for pCAR and also because reticle "B" has a CDU 3σ value near the average for the entire data set. The low mode 2 score for reticle "C" warrants further study since this was the dominant CD variation mode for pCAR and because Figure 6 showed low mode 2 scores correlate with higher resist CDU. However reticle "C" has quite a good CDU 3σ value and it is thus accepted as part of the mode 2 CD variation with the alternate PEB tool.

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A close examination of Figure 10 reveals the same trend observed in Figures 6 and 8: CDU correlates to pCAR mode 2 scores. In this case however, mode 2 scores have the opposite sign of those in Figure 6 because the sign of the mode 2 eigenvectors has changed. PCA sign choices are not unique, causing scores in this case to have the opposite sign as those in Figure 6.

Figure 11 shows a similar score and CDU comparison for nCAR test reticles where alternate PEB and resist develop tool were used for several test reticles.

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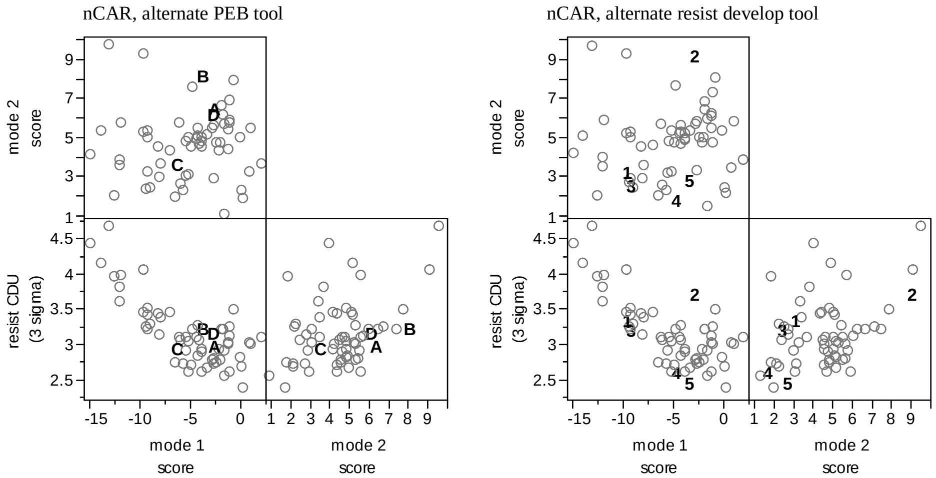

Figure 11. nCAR scores for modes 1-3; Left: 3 reticles (labeled A, B, and C) processed on an alternate PEB tool; Right: 5 reticles (labeled 1-5) processed on an alternate resist develop tool.

In the nCAR case, all reticles processed on the alternate PEB and resist develop tools have scores and CDU similar to those on the primary tool, indicating a suitable resist CD match.

Obvious in these PCA comparisons are score and CDU outliers for test reticles processed on the primary tools however, it was AMTC's intent to avoid, if possible, the introduction of additional resist CD variation from alternate process tools. It shall be pointed out this PCA score and CDU comparison was used to judge resist CD uniformity matching which is just one of many criteria (*e.g.*, mean CD, linearity, defectivity) examined to determine alternate tool capabilities. The AMTC found PCA to be a more rigorous CD uniformity check than simply examining 3σ values or visually comparing resist CD signatures. In the 4 examinations above, PCA shows there are no new dominant modes of resist CD variation introduced by the alternate process tools, which is an important result when viewed in terms of overall line CDU and CDU stability.

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4. CONCLUSIONS

PCA was applied to different sets of CAR, 50kV exposed, photomask resist CD measurements in order to determine the data set variations. At least one mode of variation in each CAR data set related to the classical, 3σ value for reticle CD uniformity. Modes of variation from each CAR data set were converted into resist CD signature variations and the dominant mode was very similar in shape and magnitude between two different CAR systems, most likely induced by a common process or tool. This result was not observed via other methods of CD signature investigation. These CD variational signatures derived from PCA were used as a basis for launching investigations into potential reticle CD error sources. PCA was further applied to resist CD signatures derived from alternate PEB and resist develop tools, which assisted efforts in judging the effectiveness of resist CD signature matching from alternate process tools and also demonstrated no new dominant CD variation modes were introduced by alternate process tools.

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ACKNOWLEDGEMENT

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