Inline monitoring of hybrid bonding Cu recess with Vertical Traveling Scatterometry machine learning

Pádraig Timoney*[a], Stefan Schoeche[a], Nick Polomoff[a], Joseph Mittelstaedt[a], Matt Malley[a], Tyler Sherwood[a], Emad Omrani[a], Daniel Schmidt[a],
Aron Cepler[b], Paul Isbester[b], Igor Turovets[c]
[a]IBM Research, 257 Fuller Rd, Albany NY 12203
[b]Nova Measuring Instruments, 3342 Gateway Blvd, Fremont, CA 94538, USA
[c]Nova Ltd, 5 David Fikes St., Rehovot, 7632805, Israel

ABSTRACT

In recent years, advanced packaging schemes have been demonstrated to achieve greater interconnect density for advanced technology node devices. Hybrid bonding facilitates direct copper to copper interconnection, reducing performance impact of connections in traditional solder bump technologies. Such hybrid bonds require stringent surface smoothness and alignment accuracy to achieve the required bond quality level. Copper CMP is a key enabling technology to achieve the required surface smoothness of the mating surfaces. Monitoring of the surface planarity is challenging due to the struct wafer smoothness requirement (<1 nm) combined with typical pitch size of the interconnect pad array (often greater than 1 um).

Vertical traveling scatterometry (VTS) methodologies, which leverage the SI channel's unique capability, are known to enhance sensitivity for measuring surface and near-surface parameters.

In this work, vertical traveling scatterometry machine learning (VTS-ML) solutions were trained to successfully monitor copper recess from wafers with different incoming stacks. Reference data from 5 measurement dies across 15 wafers was used in the VTS-ML training. Evaluation of the VTS-ML correlation to reference was studied on 22 blind test wafers. The impact of the VTS filter position was studied in both test-on-train and blind test R^2.

Keywords: Machine Learning, scatterometry, modeless, vertical traveling scatterometry, reference metrology, hybrid bonding, copper recess, underneath layer process variation

*Corresponding author: padraig.timoney@ibm.com

1. INTRODUCTION

Heterogeneous integration increasingly relies on direct Cu–Cu hybrid bonding to improve latency, power efficiency, and security, with hybrid bonded interconnect schemes delivering thinner packaging and better electrical and thermal performance to enable next generation performance of AI systems [1]. Successful bonding requires a strong dielectric bond and a subsequent thermal anneal to form robust Cu–Cu interconnects; accordingly, post CMP Cu pad recess must be tightly controlled. The Cu recess should be small enough to ensure dielectric contact while still enabling post-bond copper closure. Inline monitoring with measurement sensitivity ~ 0.1 nm and adequate across wafer sampling is necessary to successfully monitor the CMP process for the required Cu recess. In prior work, optical critical dimension (OCD) metrology augmented with ML has been successfully used to achieve good blind-test correlation to dies not included in the model training [2,3]. These studies also demonstrated good extrapolation of the measurement for different nominal pitch and recess depth

conditions. The emphasis in this paper will be on evaluating the performance of the metrology solution on nominal process condition wafers not utilized in the training set.

2. VERTICAL TRAVELING SCATTERMETRY

Figure 1 demonstrates how Vertical Traveling Scatterometry differs from traditional scatterometry by leveraging spectral interferometry and algorithmic filtering to isolate contributions from selected upper layers while suppressing complex, variable underlayers [4,5]. This reduces modeling complexity, improves time-to-solution, and can enable model reuse across different underlayer configurations—an attractive proposition for hybrid bonding stacks with diverse incoming films.

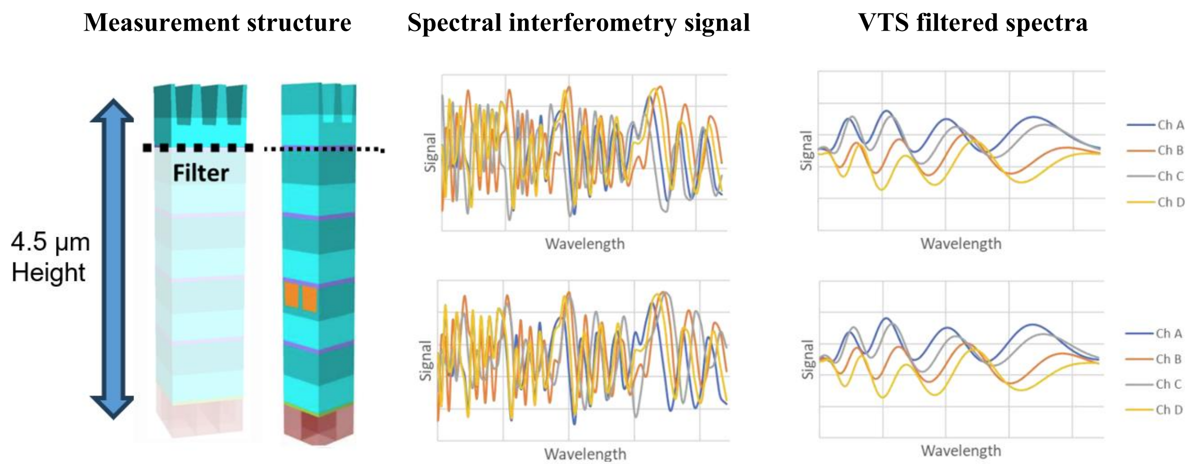

Figure 1. Interferometry spectra of complicated 4.5um tall multi-layer stack simplified to VTS filtered spectra corresponding to only the upper features of the stack [5]

Interferometry spectrum from Cu Recess wafers provides a VTS signal with peaks associated with material surface interfaces throughout the stack. Figure 2 demonstrates how interferometry spectra can be represented as VTS signals of material interfaces.

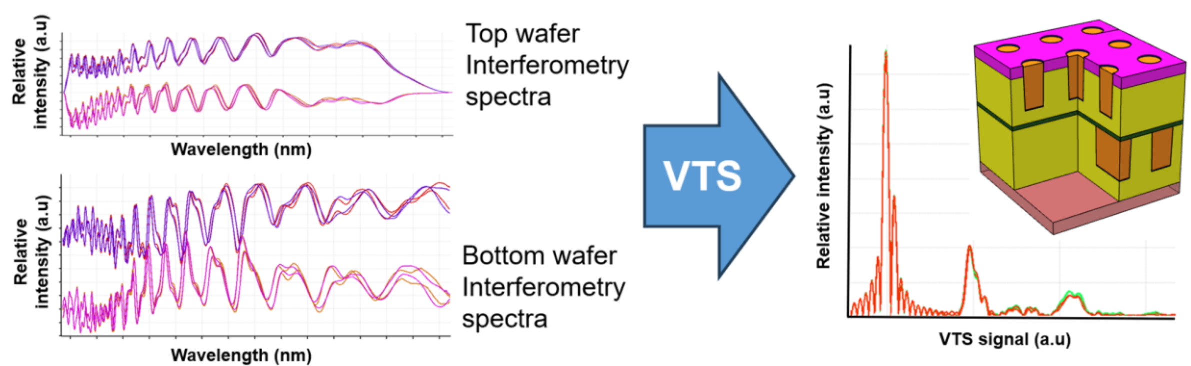

Figure 2 Interferometry spectra represented as VTS signals with numerous peaks associated with material interfaces throughout the stack.

Differences in the spectral interferometry spectra in the wavelength domain are apparent from the top and bottom wafer categories. Wafer categories 'top' and 'bottom' are introduced, where the top wafer category has a thinner underneath layer dielectric stack and some other minor structural dimension differences compared to the bottom wafer category. Regeneration of spectra resulting from isolating VTS signals provides an opportunity to evaluate spectra only associated with a specific surface or region within the structure as indicated by the different peak positions on the VTS signal axis.

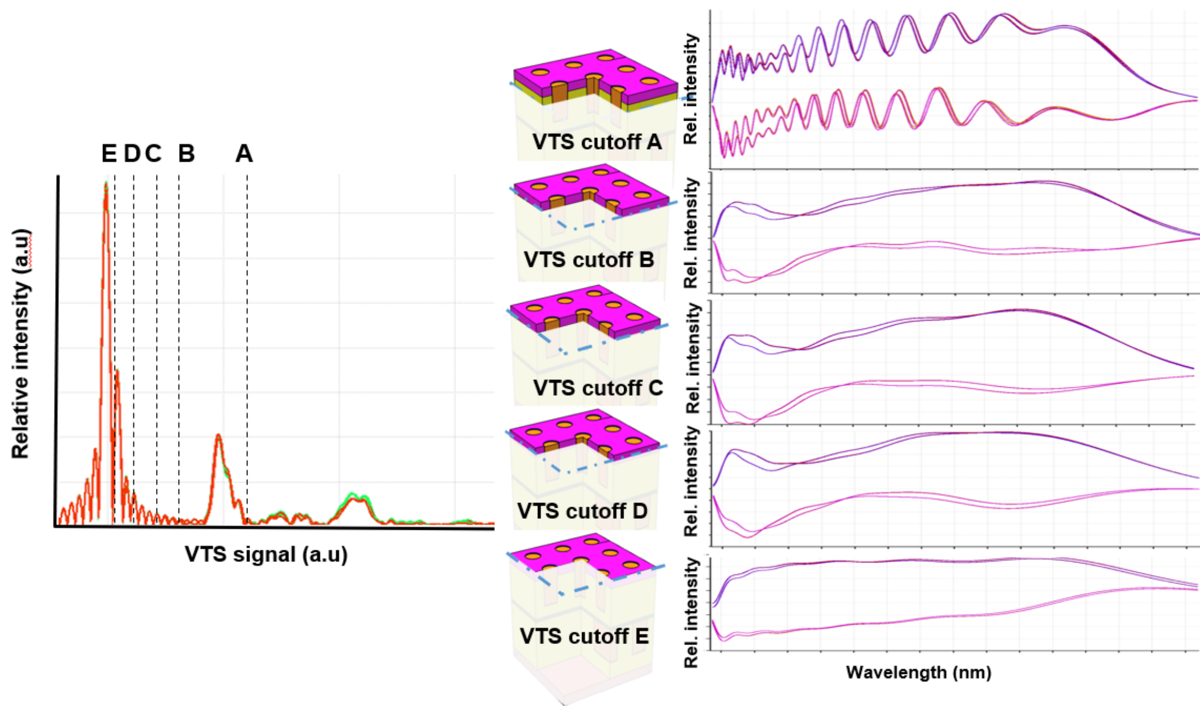

Figure 3 Different VTS peaks and regions represented in corresponding structure and resulting interferometry spectra associated with the surface structure of the corresponding stack

Figure 3 further demonstrates how different VTS peaks and regions can be assigned to vertical locations within the stack. Cutoff A represents an area from the surface to below the upper layer of the structure. The cut off positions B through E represent successively shallower signal penetration depth, thus effectively reducing the potential for underneath layer signal contributions. The VTS cut off positions are fixed on the x axis of the representative VTS spectrum and have the corresponding effect on the intensity vs wavelength spectrum shown in the right- hand portion of Figure 3. It can be initially observed from these spectra that the repetitive oscillations observed in both the pre-filtered spectral interferometry signal in Figure 2 and the VTS cutoff A filtered spectra in Figure 3 are no longer present in VTS Cutoff positions B thru E. The goal of the study is to identify the optimum compromise between minimizing the underneath layer contributions while still providing sufficient signal to successfully characterize the recess depth.

3. VTS MACHINE LEARNING

Optical machine learning solutions typically utilize a training set of known references to train corresponding spectra to identify features in the spectra which correspond to the reference [3]. VTS spectra have been

demonstrated in Figures 2 and 3 to provide ability to remove spectral contribution of surface interactions deep within the structure. This provides an opportunity to utilize VTS algorithms to focus training from machine learning to the surface features of interest to Cu bonding. Atomic Force Microscopy (AFM) was selected for high-resolution reference data at the feature scale. Since the AFM field of view is smaller than the spot size used for OCD/VTS, specific regions of interest (ROIs) were identified in the reference metrology output and statistical aggregation methods were applied across features. This approach for AFM data analysis suppresses stochastic roughness while preserving systemic recess metrics. Analysis emphasis was placed on standard deviation and sufficient replicates to ensure statistical significance. From AFM analysis a training set from 15 wafers with 5 dies per wafer and a total range of ~4nm was used. The 15 reference wafers in the training set included those corresponding to both top and bottom categories for wafer bonding. Performance was evaluated and assessed based on results from test-on-train and blind test validation utilizing a separate set of 22 wafers which were not included in the original training.

For each wafer/die, we computed ML features from the VTS filtered spectra at cut offs A–E and trained regression models to predict AFM derived Cu recess. Five condition specific models were produced (A–E). Unlike conventional OCD ML that requires detailed underlayer modeling or pre and post delta measurements, this VTS-+ML approach applies a single model applicable to both top and bottom wafer categories, benefiting metrology logistics and throughput. In an R&D environment the number of samples can be somewhat limited, and an emphasis must always be on reducing process cycles of learning. Accordingly, robustness of inline metrology solutions to accommodate incoming process differences is of particular importance.

4. RESULTS

VTS ML solution performance was assessed by evaluating the AFM correlation for each VTS cutoff solution applied to the training set (test-on-train) and 22 blind test wafers. Wafers represented those which will be the hybrid bonding top and bottom wafers and correlation results from each were combined and evaluated together for each VTS- ML solution.

Test on train results are presented in Figures 4 and 5 and provide generally acceptable results for all VTS- ML cutoff solutions with the highest correlation observed for VTS-ML cutoff A.

Reviewing Figure 3 this observed VTS-ML to AFM reference correlation result was attributed to a larger number of oscillations and features in the spectra relative to other cutoffs which provide opportunities for the ML algorithm to identify unique features consistent with reference variation and value. The R^2 degrades for VTS cutoffs D and E since not enough information is contained within the filtered spectra to capture the variability of recess depth in the training set.

Blind test results from various VTS-ML cutoff solutions presented in Figures 6 and 7 provide significantly a different AFM correlation trend than that observed for test-on-train results and for the various VTS-ML cutoff solutions. Blind test results demonstrate VTS-ML cutoff B and C provide the best correlation to AFM with cutoff A providing one of the lowest correlations to reference.

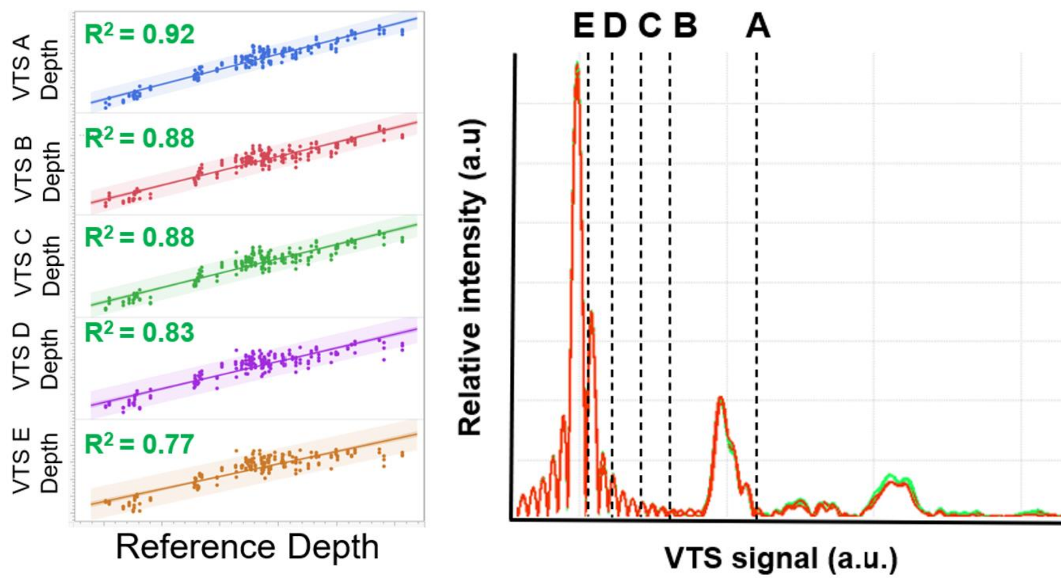

Figure 4 Test on train Cu recess correlation results for VTS-ML solutions at each cutoff. Combining results from both top and bottom wafers for bonding the VTS cutoff "A" was observed to provide highest correlation between VTS-ML Depth and AFM Reference.

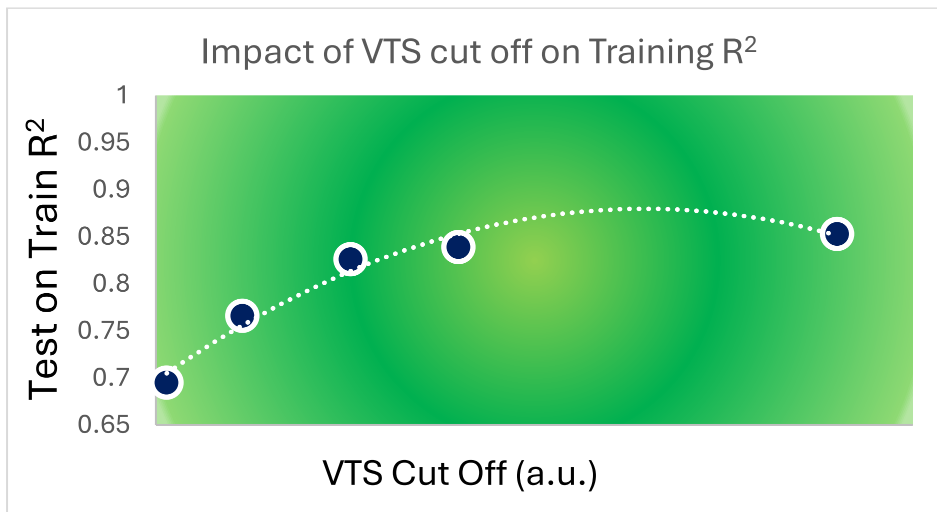

Figure 5 VTS-ML test on train Cu recess correlation results at each cutoff. VTS cutoff A was observed to provide the highest correlation between VTS-ML Depth and AFM Reference.

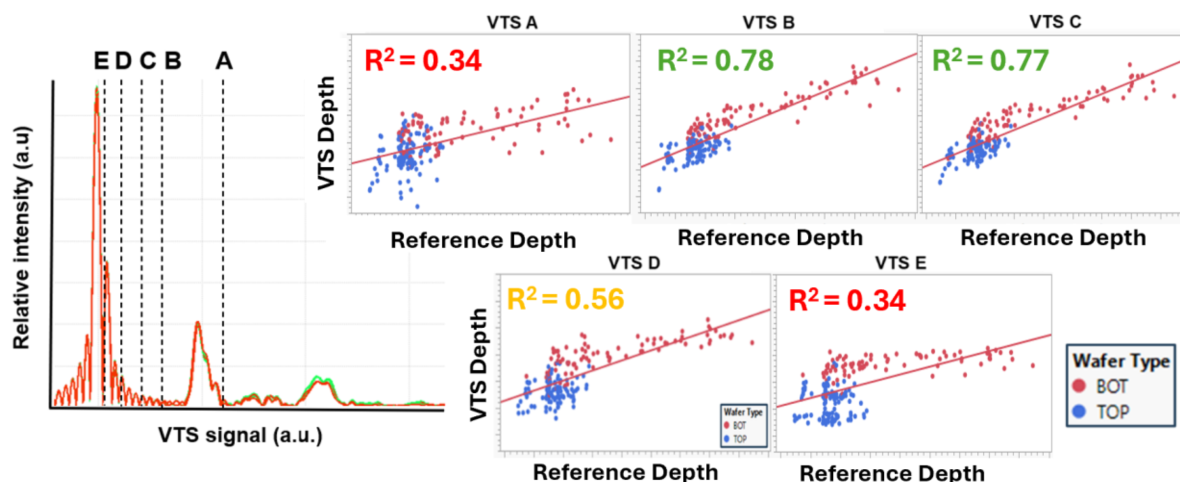

Figure 6. VTS-ML blind test Cu recess combined correlation results for both bottom and top wafers for hybrid bonding at each cutoff. VTS cutoff at B and C observed to provide the highest correlation between VTS-ML Depth and AFM Reference.

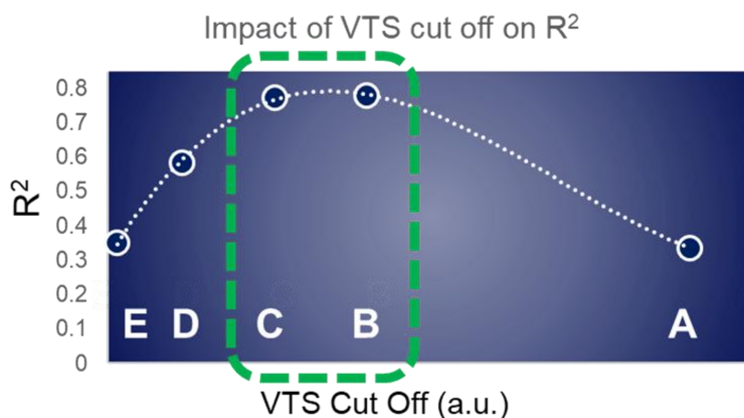

Figure 7. Compilation of VTS-ML blind test Cu recess correlation. VTS cutoffs at B and C were observed to provide the highest correlation between VTS-ML Depth and AFM Reference.

These results confirm that the test on train results for VTS-ML cutoff A did not have sufficient training samples to cater for the extent of variability modes present in the underlaying layers of the 15 wafers training samples. It is possible that with additional training, the blind test score would increase for this scenario. With VTS cutoff E primarily only encompassing interferometry signal from the surface, this result was attributed to the absence of a peak associated with the Cu Recess in the VTS training spectra. Reviewing Figure 3, the representative interferometry spectra from the VTS cutoffs B, C, and D were generally consistent. While these representative VTS spectra were generally consistent, both the test-on-train and blind test correlation results presented in Figures 4, 5, 6, and 7 demonstrate reduced performance for VTS cutoff D. It appears that the VTS-ML cutoff solution D could not fully capture the variation of the Cu Recess in the training set. This result was attributed to the proximity of the cutoff position D to the Cu Recess peak for most wafers

5. CONCLUSIONS

VTS-ML was demonstrated to provide simplified spectra, free of contributions from lower stack layers, enabling consistent Cu recess measurements with the AFM reference. Removing contributions from lower layers with VTS enabled, applying the resulting VTS-ML solution to wafers with different stacks but similar Cu recess structures, as observed with top and bottom hybrid bonding wafers.

The improved robustness and time to solution of the VTS-ML approach as compared to conventional optical modeling or machine learning approaches were apparent in the comparison of the improved correlation to reference for near-surface VTS cutoff positions as compared to deeper signal penetration cutoff positions. The result from VTS cutoff A ($R^2 = 0.35$) suggested that the VTS-ML solution appeared insufficiently trained to accommodate the variation in blind test samples, while by utilizing the same training set, VTS cutoff positions B and C ($R^2 \sim 0.8$) delivered significantly improved correlation to reference, thus clearly demonstrating the improved metrology robustness delivered by optimizing the position of the VTS cutoff position.

The study also identified two cutoff positions that delivered subsequent degradation in performance as the cut off position was moved successively from deeper to shallower signal penetration. This observation highlighted the importance of careful optimization of VTS filter cutoff position in the initial application development phase.

The outcome of this study demonstrated a methodology for leveraging limited reference metrology in an R&D environment to develop accurate and robust inline metrology using optical scatterometry enhanced by algorithmic innovation, namely vertical traveling scatterometry machine learning (VTS-ML). Future studies will be undertaken to explore other opportunities to leverage VTS-ML for improved metrology time-to-solution and robustness in R&D environment where available reference metrology sampling may be limited.

6. REFERENCES

[1] K. Sakuma, R. Yu, N. Polomoff, A. Kumar, S. Raghavan, M. Belyansky, A. Jain, R. Bonam, Y. Sulehria, H. Hsu, K. Jayanand, H. Jagannathan, D2W and W2W Hybrid bonding system with below 2.5 micron pitch for 3D chiplet AI applications Proc. IEEE IEDM 2024 2156-017X

[2] S. Chew, M. Saib, B. Zhang, A. Charley, J. Hung, A. Ger, J. De Vos, P. Leray, I. Turovets, A. Moussa, A. Miller, E. Byrne, Scatterometry Application on Cu/SiCN surface topography towards high volume manufacturing Proc. IEEE ECTC 2024 2687-9727

[3] H. Niazi, B Zhang, X. Brun, S. Krishnan, J. Chuang, Critical Dimension Scatterometry as a Scalable Solution for Hybrid Bonding Pad Recess Metrology, Proc. IEEE ECTC 2023 2377-5726

[4] J. Yoon, J. Park, M. Shin, D. Ihm, O. Bismuth, S. Ferber, J. Ofek, I. Turovets, I. Kim, Unique Spectral Interferometry Solutions for complex high aspect ratio 3D NAND structures, Proc. Of SPIE Vol. 12955, 2024.

[5] D. Schmidt, C. Durfee, M. Medikonda, M. Rizzolo, C. Silvestre, J. Frougier, A. Greene, M. Breton, A. Cepler, J. Ofek, I. Kaplan, R. Koret, I. Turovets, "Spectral interferometry for fully integrated device metrology", J. Micro/Nanopattern Mats. Metro. 22, 031203 (2023).