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Table-top extreme ultraviolet Grazing-Reflection
Ptychography with Full-Pose Self-Calibration

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054 Abstract

055 Table-top extreme ultraviolet (EUV) reflection ptychography has gained increas-
056 ing interest in semiconductor metrology due to its nanometer-scale resolution,
057 nondestructive character, and laboratory-scale cost-effectiveness. However, its
058 widespread adoption remains constrained by alignment challenges inherent to
059 grazing-reflection geometry, which have prevented reflective configurations from
060 achieving image quality comparable to those of transmission-mode systems.
061 In this study, we introduce a table-top EUV grazing-reflection ptychography
062 system that enables full-pose self-calibration through holistic system modeling
063 and highly efficient optimization. The developed system is validated using a
064 customized wafer sample and real chip sample. Experimental results indicate
065 that the system successfully corrects image distortions, improves resolution, and
066 enhances surface metrology quality. Furthermore, we discuss algorithmic and
067 physical issues including the feature-domain phase-retrieval for ptychography
068 and coupling effect among pose parameters. The proposed approach not only
069 accelerates the transition of EUV reflection ptychography toward real-world use
070 but also opens avenues for methodological advances to a wider range of imaging
071 applications.
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073 **Keywords:** Extreme ultraviolet, reflection imaging, ptychography, self-calibration
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1 Introduction

As semiconductor manufacturing progresses toward nanometer-scale features, there is an escalating demand for advanced metrology that can address critical dimensions and overlay errors [1]. Short-wavelength techniques such as extreme ultraviolet (EUV) imaging offer distinct advantages [2, 3], including nanometer resolution, deep penetration, and nondestructive inspection, making them suitable for semiconductor metrology. Furthermore, the development of tabletop EUV sources based on high harmonic generation provides high brightness and coherence, effectively facilitating laboratory-scale imaging [4–6].

However, progress in EUV-based metrology has been hindered in recent years by several fundamental challenges. A primary obstacle is the scarcity of high-quality, high numerical aperture (NA) optics suitable for this spectral band. Within the EUV regime (approximately 10–100 nm), all materials strongly absorb radiation, necessitating the use of mirrors instead of lenses. The fabrication of these EUV mirrors demands specially designed multilayer coatings and exceptional surface smoothness, with height variations significantly smaller than the wavelength. These rigid requirements render EUV mirrors extremely difficult and costly to manufacture [7–9].

Ptychography has opened new avenues for lensless imaging [10–12]. Unlike conventional approaches that rely on complex optical systems, ptychography does not require any optical elements between the sample and detector; instead, it reconstructs the sample image directly from diffraction patterns. By leveraging redundant information from spatially overlapped scanning, ptychography recovers the illumination probe and image nonisolated specimens [13–16]. The NA in this technique is determined by the diffraction distance and detector size, and therefore, it approaches the theoretical limit [17]. Thus far, ptychography in transmission geometry has proven to be an effective tool for high-resolution imaging in the EUV waveband, and several studies demonstrated its utilization in the analysis of lithographic components [11, 18, 19] and biological samples [20, 21], and in the multiwavelength characterization of EUV optics [22, 23]. However, the application of EUV ptychography in reflection configurations remains limited.

In practice, EUV reflection ptychography can be implemented across three distinct ranges of reflection angles: small angles ($<10^\circ$) [24–26], which are commonly used for photomask inspection in lithography; moderate angles ($<60^\circ$) [27, 28], typically employed to explore the fundamental principles of reflective diffraction imaging and seldom applied in practical inspection tasks; and large reflection angles ($\sim 70^\circ$) [29–32], which corresponds to grazing-reflection geometry. Within this grazing reflection range, most materials are reflective, and the phase response shows significant angular sensitivity, making it suitable for tasks such as defect analysis and compositional analysis in semiconductor inspection. Further, reflective diffraction imaging at other wavelengths uses grazing reflection systems [31, 33].

However, such a grazing-reflection configuration poses significant challenges to system alignment and calibration for ptychography. Moreover, the limited power of tabletop EUV sources results in weak reflected and diffracted signals. Consequently, the effect of system misalignment is exacerbated by a low signal-to-noise ratio (SNR), which significantly degrades imaging quality. This issue becomes pronounced for larger

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139 numerical apertures, wherein the high-frequency signal content is sparse. Transmission
 140 ptychography involves calibrating the diffraction distance and scan positions, which is
 141 a subject thoroughly addressed in many studies [34–37]. However, calibration methods
 142 for reflection ptychography remain relatively underdeveloped.

143 Although some efforts have been made to correct system misalignment [38–40],
 144 they are constrained by the oversimplified assumption that all parameters are correct,
 145 except for one or two corrections. Maintaining this assumption requires using highly
 146 precise hardware alignment solutions, which undoubtedly increase system cost and
 147 complexity and hinder its general applicability in practical scenarios. Further, this
 148 assumption remains unrealistic even with highly sophisticated hardware alignments
 149 because of inevitable discrepancies between idealized models and real physical systems.
 150 Consequently, improvements in image quality remain limited. Thus far, there is no
 151 comprehensive and holistic solution that can perform the integrated calibration of full-
 152 pose parameters in reflection ptychography systems, and the need for such a solution
 153 is genuine and urgent.

154 In this study, we report a grazing-reflection ptychography system operating on a
 155 17.9 nm table-top EUV source that features full-pose self-calibration capability. The
 156 full-pose calibration is based on an advanced optimization framework that includes
 157 comprehensive system modeling, feature domain phase retrieval, and automatic dif-
 158 ferentiation. The system is used to image a customized sample and a real chip, and
 159 the proposed self-calibration algorithm demonstrates an unprecedented improvement
 160 in image quality. Our method addresses a fundamental challenge in reflection pty-
 161 chography and significantly advances its practical application. This study has inspired
 162 progress in diffraction-based imaging techniques across broader regimes, including
 163 visible light, X-ray, and electron microscopy.

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165 2 Results

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167 2.1 Principle

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169 In transmission ptychography, the camera is placed parallel to the sample to capture
 170 diffraction signals in reciprocal space after the illumination probe interacts with the
 171 specimen. These signals are distributed in the Ewald sphere. Under paraxial approx-
 172 imation with a low numerical aperture, the pixel array on the detection plane can
 173 sample the reciprocal space diffraction signal uniformly. In the EUV reflection pty-
 174 chography system (Fig. 1a), the detector is positioned perpendicular to the outgoing
 175 light but tilted relative to the sample. This configuration leads to the nonuniform sam-
 176 pling of the reciprocal space signal on the Ewald sphere. Diffraction patterns appear
 177 significantly distorted compared to those under normal-incidence illumination. In con-
 178 ventional approaches, the degraded imaging performance in reflection ptychography
 179 is largely attributed to the insufficient correction of this distortion.

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181 To address this issue, we describe the mapping relationship \mathbf{T} between the diffrac-
 182 tion pattern distributed on the Ewald sphere and tilted detector plane as a function
 183 of the pose parameters of the reflection system, including diffraction distance d , three-
 184 dimensional illumination angle $\boldsymbol{\theta} = [\theta_x, \theta_y, \theta_z]^\top$, and three-dimensional detection
 rotation angle $\boldsymbol{\gamma} = [\gamma_x, \gamma_y, \gamma_z]^\top$. A detailed derivation of the mapping operator \mathbf{T} is

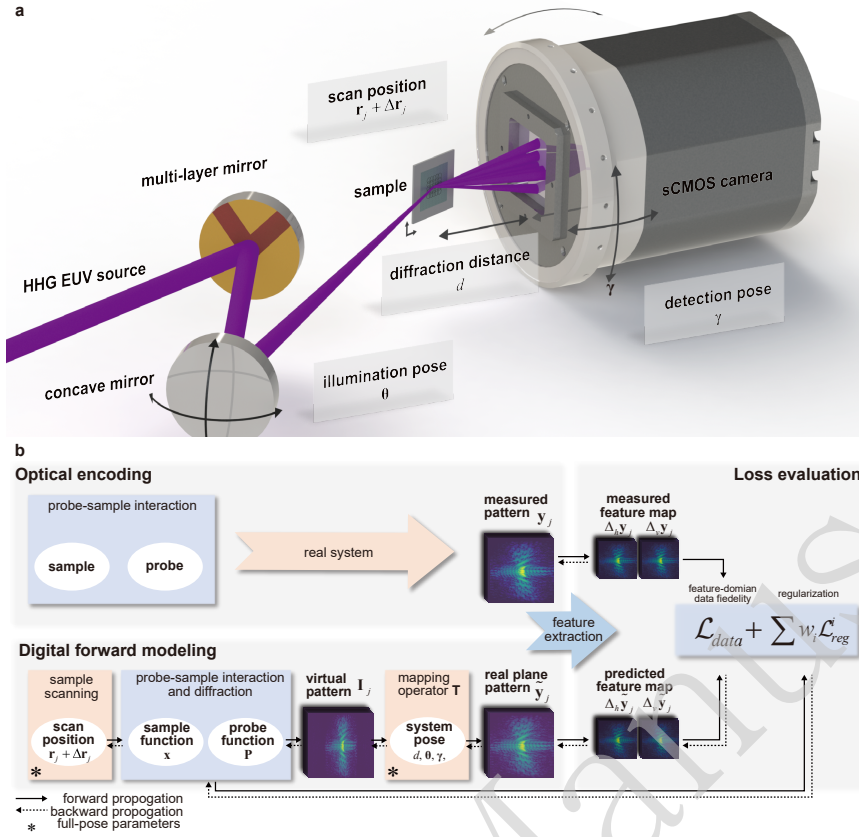


Fig. 1 Principle of full-pose self-calibration for table-top EUV reflection ptychography. **a** Schematic of table-top EUV reflection ptychography system with grazing illumination. Misalignment attributed to scan position, diffraction distance, illumination pose, and detection pose. **b** Flow work of proposed method. The optical encoding block represents a physical experimental setup, whereas the digital forward modeling block simulates how system parameters are combined to generate predicted diffraction patterns. Following loss evaluation using a feature-domain (FD) loss function along with regularization terms, the gradients of each variable are computed via auto-differentiation and back-propagated. Finally, variables are updated using an optimizer.

provided in the Materials and Methods section. As depicted by the digital forward modeling block in Fig.1b, we further integrate this relationship into the forward model of ptychography.

$$\mathbf{y}_j = \mathbf{T} \left\{ \mathbf{I}_j = |\mathbf{A} [\mathbf{P} \odot \mathbf{Q}_j(\mathbf{x}, \mathbf{r}_j + \Delta \mathbf{r}_j)]|^2, d, \boldsymbol{\theta}, \boldsymbol{\gamma} \right\}, j = 1, 2, \dots, N \quad (1)$$

where \mathbf{y}_j , \mathbf{I}_j , \mathbf{A} , \mathbf{P} , \mathbf{x} , \mathbf{Q}_j , \mathbf{r}_j , and $\Delta \mathbf{r}_j = [\Delta x_j, \Delta y_j]^\top$ represent the j th diffraction pattern in total N frames, virtual pattern on the Ewald sphere, propagation operator, probe function, sample function, translation operator, two-dimensional estimated scan position, and position error, respectively. The scan position error is integrated

231 using the Fourier shift theorem [?]. After modeling the full-pose integrated forward
 232 propagation, we use the feature domain (FD) loss [42, 43] for data fidelity assessment
 233 between the measurement \mathbf{y}_j and prediction $\tilde{\mathbf{y}}$.

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$$\mathcal{L}_{data} = \sum_{j=1}^N \left\| \nabla \sqrt{\mathbf{y}_j} - \nabla \sqrt{\tilde{\mathbf{y}}_j} \right\|_{Huber} \quad (2)$$

239 where $\nabla = [\nabla_x, \nabla_y]^\top$ represents the first-order differentiation operator. Further,
 240 $\|\cdot\|_{Huber}$ represents the Huber norm [44], which is a hybrid loss function combining L_1
 241 and L_2 components to balance robustness against outliers with optimization efficiency.
 242 Compared to the element-wise loss functions such as the mean squared error (MSE)
 243 used in traditional phase retrieval, the FD loss is less sensitive to model degeneration.

244 Prior knowledge can be incorporated through regularization terms to enhance
 245 reconstruction stability, including support and denoising constraints. The complete
 246 loss function is expressed as $\mathcal{L}_{full} = \mathcal{L}_{data} + \sum_i w_i \mathcal{L}_{reg}^i$, where w_i represents the
 247 weighting coefficient of the i th regularization term. The complete workflow of the pro-
 248 posed method is shown in Fig. 1b. The optical encoding block represents the physical
 249 measurement process in the actual system, whereas the digital forward modeling block
 250 implements computational mapping from variables to the predictions. The loss func-
 251 tion evaluates and backpropagates through a computational graph for accumulating
 252 the gradients of each variable using automatic differentiation. Materials and Meth-
 253 ods present more details about the implementation of the experimental algorithm,
 254 including the sampling conditions, regularization, and optimizer settings.

255 We conducted a series of investigations into method performance and system
 256 behavior after completing the forward modeling and inverse problem design. The
 257 following investigations provide profound algorithmic and physical insights into reflec-
 258 tion ptychography, which offers essential guidance for robust algorithm designs and
 259 optimized experimental configurations:

260 **I.** We validate the effectiveness of the FD loss function used in ptychography.
 261 Simulations are performed under different illumination doses and source coherence
 262 conditions. The detailed implementation is provided in Section S1. As shown in Figs.
 263 S1 and S2, the FD-Huber loss successfully recovered images under moderate noise
 264 levels and coherence degradation, outperforming both MSE and FD- L_1 loss. This
 265 conclusion is corroborated by experimental results shown in Fig. S3.

266 **II.** In Section S2, we explore the sensitivity of image reconstruction to different pose
 267 parameters under varying reflection angle settings with simulation results presented
 268 in Fig. S4. We find that misalignment in all parameters can degrade reconstruction
 269 quality. The sensitivity to misalignments in θ_x , θ_y , and $\Delta \mathbf{r}_j$ increases significantly
 270 as the geometry approaches grazing reflection. This sensitivity analysis explains why
 271 grazing-reflection ptychography yields poorer image reconstruction quality compared
 272 to normal-incidence or small-angle illumination and underscores the necessity of full-
 273 pose self-calibration.

274 **III.** We identify coupling relationships among the parameters, which are dis-
 275 cussed in detail in Section S3. Parameter coupling indicates that the error of one
 276 parameter can be compensated by adjusting other parameters. This effect is most

pronounced between the pose parameters and scan positions. Consequently, we introduce a segmented updating optimization strategy to decouple parameters during self-calibration.

IV. We discuss the illumination-dose dependence of full-pose self-calibration. The simulation results in Section S4 indicate that full-pose self-calibration is effective when the illumination dose reaches or exceeds 10^7 photons.

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323 2.2 Self-calibrated reflection ptychography on 17.9 nm EUV
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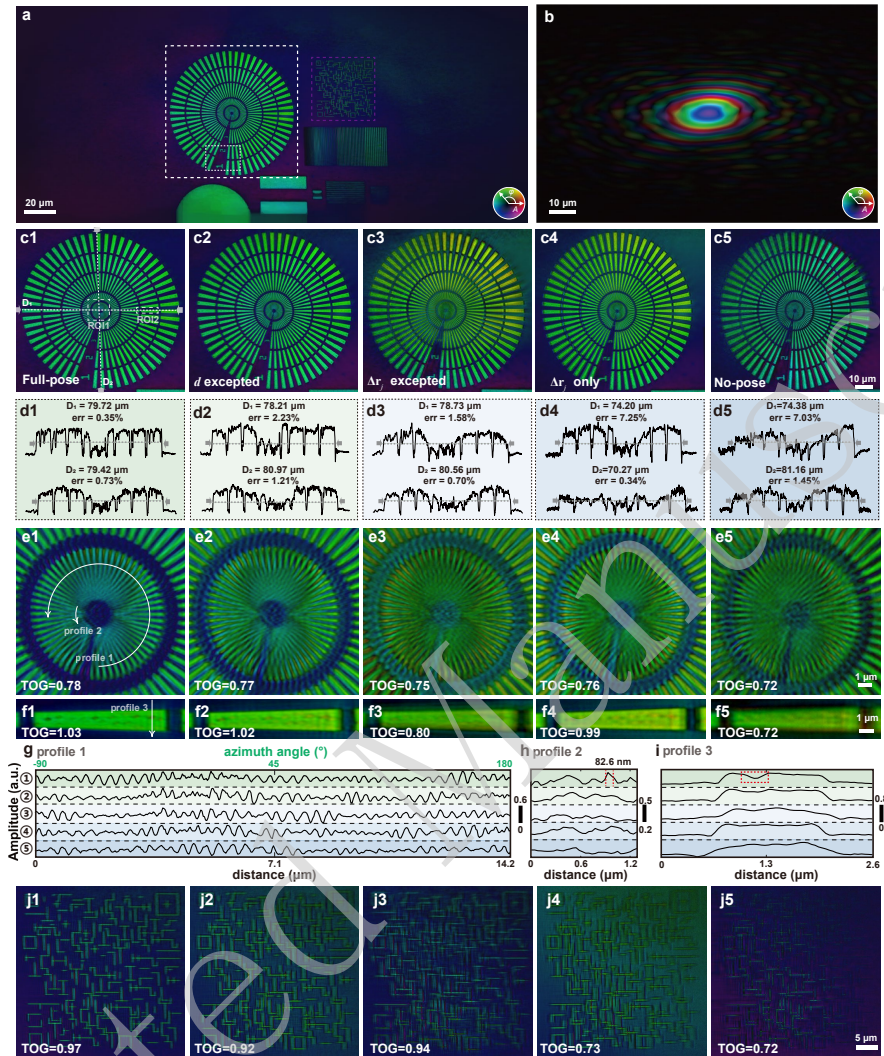


Table 1 Calibrated pose parameter values on the customized wafer sample with different strategies.

	d (mm)	θ ($^\circ$)	γ ($^\circ$)
No pose/ $\Delta\mathbf{r}_j$ only	50.00	[0.00, 70.00, 0.00]	[0.00, 0.00, 0.00]
Full pose	48.42	[-0.80, 71.72, 0.35]	[9.13, 2.23, 0.01]
Partial pose: d excepted	50.00	[-0.42, 70.94, 0.15]	[4.13, 2.18, 0.01]
Partial pose: $\Delta\mathbf{r}_j$ excepted	49.44	[-8.30, 71.37, 0.18]	[4.42, 0.39, 0.01]

Our reflection ptychography system uses a table-top 17.9 nm EUV source based on high-order harmonic generation (HHG). Detailed information is provided in Section S7. The focused 17.9 nm beam illuminates the sample at a grazing angle, and a scientific complementary metal-oxide-semiconductor (sCMOS) camera (Dhyana XF95, 2048×2048, 11 μm pixel size) was placed perpendicular to the reflected beam. Incidence angles relative to the normal and sample-camera distances of the sample surface were 70° and 50 mm in the design, respectively. Sample scanning was driven by a two-dimensional slip-stick piezo stage (LS35x.Lab, MultiFields Technology).

In this experiment, we employed a Fermat spiral-scanning strategy with 400 positions [45] and scanning overlap ratio of $\sim 82\%$. At each position, four patterns were recorded with increasing exposure times to enable high dynamic range image fusion. Data recording at each position took approximately 1 s, whereas stage movement and stabilization required approximately 1.2 s. Full data acquisition was completed within approximately 15 min.

The pseudocolor imaging results of a customized wafer sample (silicon substrate with a gold pattern; scanning electron microscope (SEM) image provided in Fig. S9) and corresponding probe functions are presented in Figs. 2 (a) and 2b)). The probe inherently carries a linear phase gradient along the horizontal direction because of the highly tilted illumination. However, in our forward model (mapping operator \mathbf{T}), this linear phase term is equivalently represented as a translation of the wavevector coordinates of the Ewald sphere. Consequently, the reconstructed probe wavefront does not explicitly contain this phase component. The pixel size of the reconstructed image is 43.5 nm \times 70.0 nm at a numerical aperture (NA) of 0.19 \times 0.095. Table 1 lists posture parameter values under their default settings ($d = 50$ mm, $\theta_y = 70$, and rest = 0) and after calibration using different strategies. Figs. 2c1–c5 show the overall outline of the Siemens star pattern reconstructed with full-pose, partial-pose, and no-pose calibrations. The outer diameter of the Siemens star pattern is 80 μm , and the pattern includes five groups of radial gratings from the outside with a minimum line width of 30 nm.

The outer diameters are measured in the horizontal (D1) and vertical (D2) directions for images reconstructed using different strategies (Figs. 2d1–d5). The reconstructed patterns exhibit severe compression in the horizontal direction when the scan position error ($\Delta\mathbf{r}_j$) is calibrated without pose parameters or when no calibration is performed. This perspective distortion stems from inaccurate θ_y estimations, leading to incorrect sampling intervals in the reciprocal space. In contrast, calibrating

415 pose parameters while neglecting $\Delta \mathbf{r}_j$ partially alleviates the distortion. The full-
416 pose strategy yields the smallest errors, with both D1 and D2 deviations below 1%,
417 outperforming other strategies including the one in which d is fixed.

418 Figs. 2e1–e5 display the central region (ROI1) of the Siemens star pattern. Images
419 reconstructed without full-pose parameters show artifacts and reduce contrast near
420 the center (Figs. 2e2–e5). The corresponding amplitude profiles (No. 1 in Figs. 2g)
421 and (h) confirm this observation. Figs. S9b and d in Section S6 provide a direct
422 visual comparison of Siemens star patterns under an SEM and full-pose EUV pattern,
423 which shows high consistency between two modalities. For quantitative comparison,
424 we calculate the Tamura coefficient of the gradient (TOG), which is a metric that
425 characterizes the clarity of the complex-field image within each ROI [46]. TOG values
426 align with the visual assessment, which confirms that full-pose reconstruction yield
427 the sharpest results. However, grating features are not fully resolved even in full-pose
428 reconstruction, and the horizontal gratings appear clearer than the vertical gratings.
429 This discrepancy can be attributed to the anisotropic nature of the NA of the system.
430 Profile No. 1 in Fig. 2 h indicates that the full width at half-maximum (FWHM) of
431 the measured minimum grating is 82.6 nm, which is approximately equal to 1.9 pixel
432 sizes. Images of ROI2, which contain a larger line pattern with punctate defects, are
433 shown in Figs. 2f1–f5. As demonstrated by the profiles in Fig. 2 (i), only the full-pose
434 strategy successfully resolved the defects.

435 Figs. 2j1–j5 show enlarged views of the maze pattern, and a direct comparison with
436 the SEM image is shown in Figs. S9 c and e. With full-pose self-calibration, the EUV
437 image clearly resolved both the horizontal and vertical lines while presenting a flat
438 background, thereby indicating high consistency with the SEM image. In contrast, all
439 other strategies were severely contaminated by artifacts.

440 In EUV reflection ptychography, material-specific surface characterization is
441 enabled by rich information in the complex-field imaging mode. The amplitude of the
442 complex value corresponds to the reflectance at each pixel, whereas its phase angle
443 reflects the phase change induced by the interface phase shift governed by Fresnel
444 relations and surface topography of the sample. The quality of sample characteriza-
445 tion depends on both the image reconstruction quality and precision of the system
446 parameters.

447 We used the phase of the reconstructed results to segment the gold patterns and
448 silicon substrate and calculate the height using the specific method provided in Section
449 S5. Figs. 3a and 3b show the surface topography of the regions of number “1” and “2”
450 under the full-pose and no-pose conditions, respectively. These regions correspond to
451 the yellow dashed areas in Fig. 2a. The height map in Fig. 3a exhibits sharp well-
452 defined edges, indicating clear segmentation between the silicon substrate and gold
453 pattern. In contrast, Fig. 3b shows significant glitch artifacts and pattern adhesion,
454 which can be attributed to inaccurate component segmentation caused by poorer
455 image quality. In addition, height histograms are provided to the right of each height
456 map. Both histograms display two distinct peaks corresponding to the heights of the
457 gold pattern and silicon substrate. The distance between the two peaks represent the
458 average height difference between the substrate and pattern, which are 37.53 and 36.86
459 nm for the full-pose and no-pose methods, respectively. Compared to the no-pose
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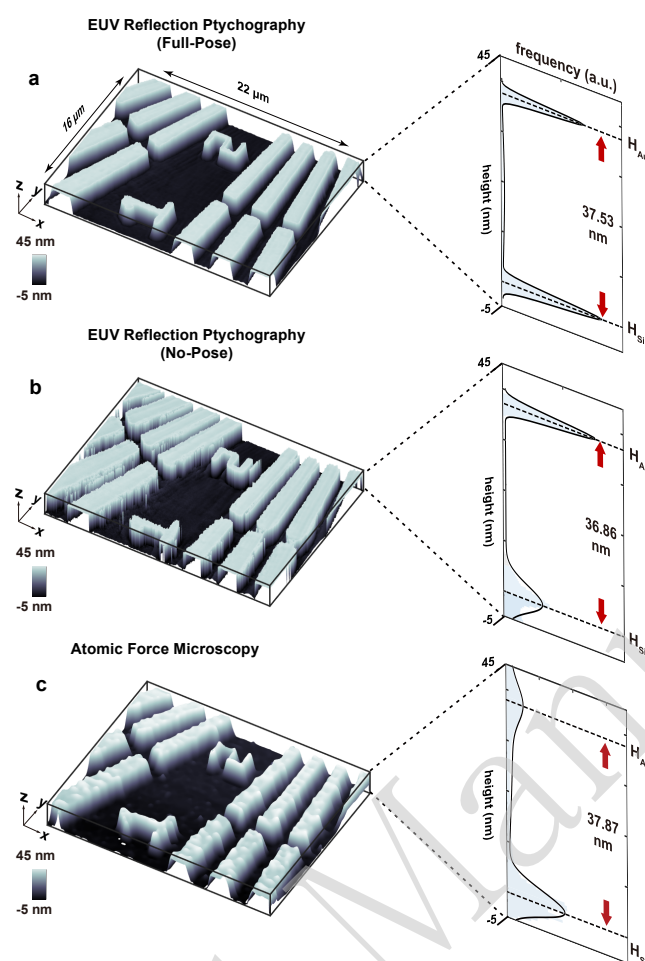


Fig. 3 Surface topography characterization. **a, b** Height maps in the area marked by a dotted square in Fig. 2a measured by EUV reflection ptychography with and without full-pose calibration. **c** Height maps measured by atomic force microscopy (AFM). Height histograms are provided to the right of each height map.

result, the peaks in the full-pose histogram are sharper, indicating clearer material differentiation. Fig. 3c shows the atomic force microscopy (AFM) measurement results and height distribution of the same sample region, with a peak-to-peak distance of 37.87 nm between the silicon and gold peaks. This height is closer to that measured by the full-pose method. Overall, we demonstrate that full-pose correction is critically important for surface topography characterization.

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2.3 Inspection of chip sample

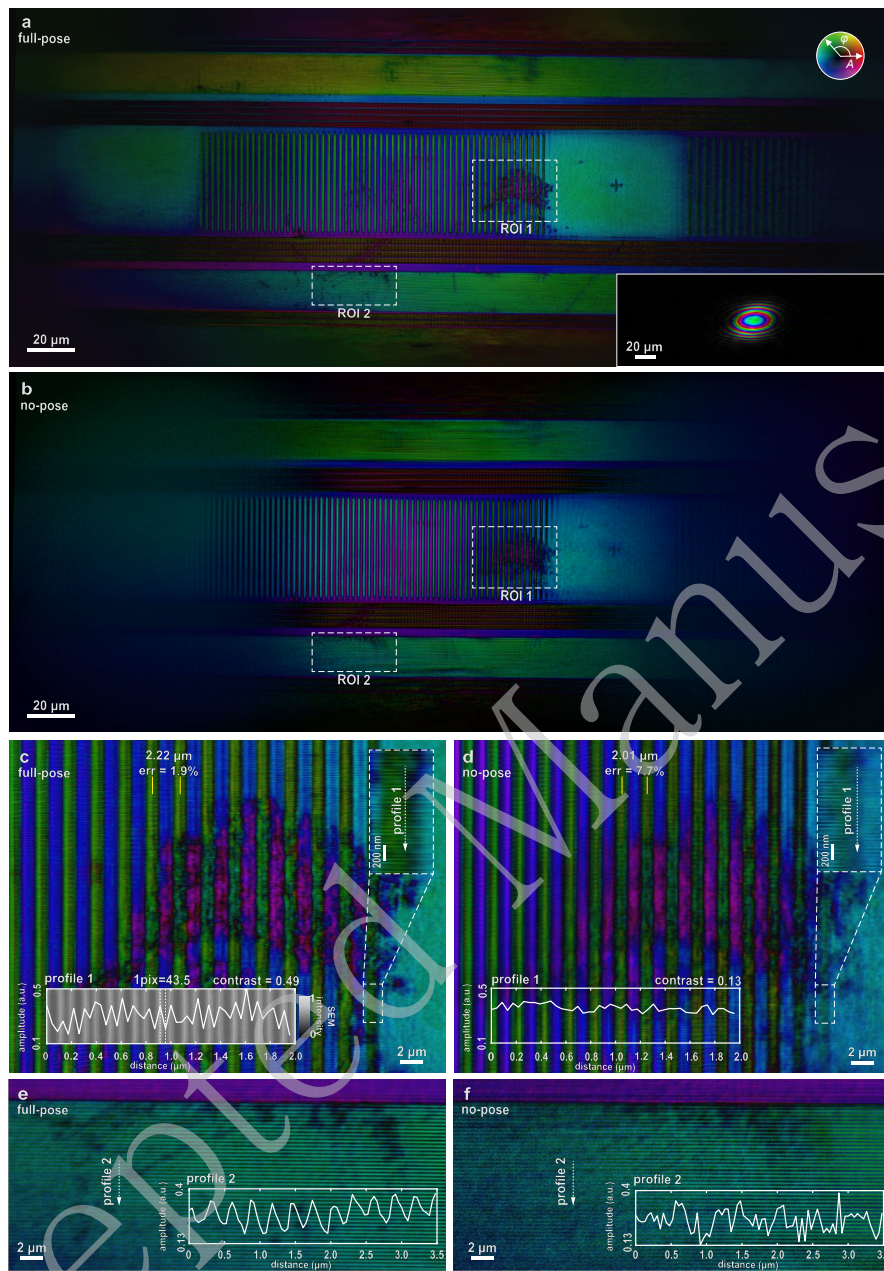
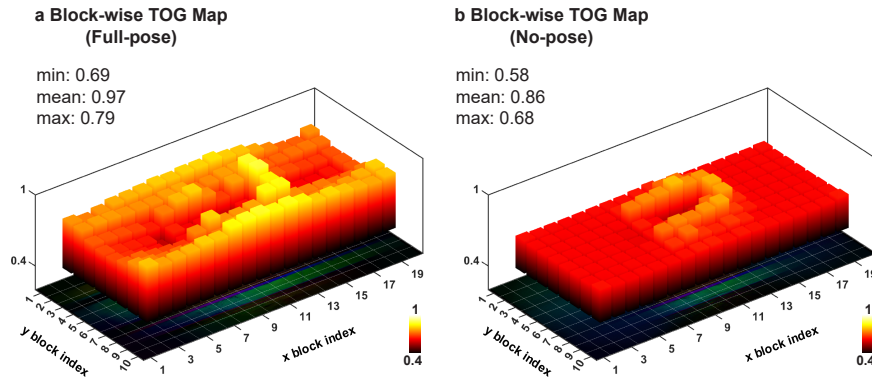


Fig. 4 Inspection on the chip sample. **a** Full-field pseudocolor result of the chip sample with full-pose calibration and probe image displayed in the bottom-right corner. **b** Full-field pseudocolor result with default parameters (no-pose calibration). **c**, **d** and **e**, **f** show magnified views of regions ROI 1 and ROI 2, respectively, reconstructed using full-pose calibration and default parameters (no-pose calibration). The SEM image of the grating area is used as the background of profile 1 in **c** for reference.

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612 **Fig. 5** Block-wise full-field image evaluation of the chip sample. **a** and **b** show the block-wise TOG
613 map corresponding to the reconstructed results with full-pose and no-pose calibration, respectively.

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Table 2 Calibrated pose parameter values on the chip sample with different strategies.

	d (mm)	θ ($^{\circ}$)	γ ($^{\circ}$)
No pose	50.00	[0.00, 70.00, 0.00]	[0.00, 0.00, 0.00]
Full pose	49.87	[-0.35, 71.67, 0.00]	[0.04, 3.45, 0.00]

625 This system was used to inspect chip samples to demonstrate its practical utility.
626 The sample height variation (within 100 nm) was well within the vertical measure-
627 ment range of our EUV reflection ptychography system, making it ideally suited for
628 characterization. An SEM image of the chip sample is presented in Fig. S10 in Section
629 S6. The system posture varies because the reinstallation of the clamping mechanism is
630 required for sample replacement, and system hardware such as the camera is reinstalled
631 between the two experiments. Consequently, the system parameters are reconstructed
632 synchronously with the image during the reconstruction process. Parameters with a
633 full-pose calibration and their default values (no pose) are listed in Table 2. Full-field
634 pseudocolor images of the chip sample and illumination probe are shown in Fig. 4 (a)
635 with full-pose calibration, and the non-pose reconstructed image is shown in panel b.

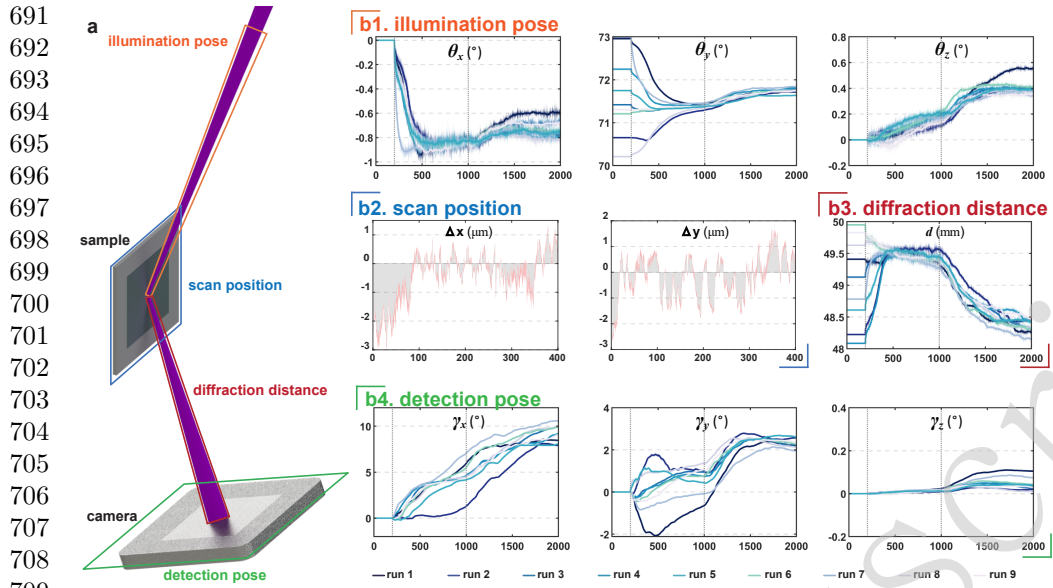
636 Edge regions exhibited reduced brightness and sharpness compared to that that
637 the center because of the low detection intensity at the FOV periphery. However, the
638 overall structure remained discernible. We magnified the two regions of interest (ROIs)
639 as shown in Figs. 4c–f. Images in Figs. 4c and 4e correspond to results obtained using
640 the full-pose strategy, whereas those in Figs. 4d and 4f correspond to results from
641 the default parameter set (no pose). In ROI1, the chip substrate, grating structures,
642 and contaminants are represented by blue, green, and purple regions, respectively,
643 indicating significant phase variations among these features. In the no-pose result, the
644 boundaries of the purple contaminant regions are noticeably ambiguous, and the green

grating structures in the lower right appear blurred. A comparison of Figs. S10 (b and c) shows that the contamination area in the EUV image with full-pose self-calibration is highly consistent with that in the SEM image. Magnified view in the dashed box highlights the details of the grating structure. Profile 1 shows an amplitude distribution perpendicular to the grating orientation. In the full-pose result, the grating exhibits high contrast (0.49) with the smallest amplitude change corresponding to one pixel (43.5 nm). Fig. S10 b shows an actual grating linewidth of 42.7 nm. The grating area of the SEM image is cropped and used as the background for Profile 1 in Fig. 4 (c) for reference. Although sampling aliasing causes some local contrast loss and slight shifts in peak-valley positions, the EUV ptychography profile accurately matches the grating structure observed in the SEM image. This confirms that the system resolution (half-pitch) reaches a diffraction limit of 43.5 nm. In contrast, the profile at the same location in the no-pose condition shows a significantly lower contrast (0.13).

We measured the distances between adjacent grating regions (marked by solid yellow lines) and obtained values of 2.22 and 2.01 μm using the full-pose and no-pose methods, respectively. Compared with the ground truth of 2.26 μm provided by SEM, the relative errors were 1.9% and 7.7%, respectively. ROI2 was located at the edge of the FOV, where the number of reflected photons was significantly lower than that of ROI1. In Fig. 4f, scratches and grating structures are overwhelmed by noise, whereas in Fig. 4 e, calibrated parameters significantly improve the SNR, which makes both scratches and grating clearly distinguishable. We conducted a full field image quality assessment of the reconstructed image of the chip to demonstrate the improvement achieved through full pose self calibration. Each image was evenly divided into 200 sub regions using a 10×20 grid, as indicated by the dashed lines. The TOG was calculated for every sub region except for those in the outermost border. The resulting TOG values are presented as heatmaps in Figs. 6a and b. Visually, the TOG values of the full pose reconstruction are significantly higher across the entire field of view compared to those of the no pose reconstruction. The statistical values of the segmented full-field TOGs such as the mean are shown in the figures. This blockwise full field evaluation effectively demonstrates the enhancement in image quality caused by full pose self calibration. Our method with full-pose self-calibration enhances the overall SNR of imaging and achieves the best resolution reported to date. Further, the higher-order diffraction signals from the chip sample are stronger than those from the Siemens star sample. The resolution in diffraction imaging depends not only on the NA of the system, but also critically on the SNR of the diffraction signals.

2.4 Consistency of full-pose self-calibration

Unambiguous and unique results are critical for industrial applications, necessitating self-calibration methods that deliver consistent calibration performances across varying conditions. Tests were performed on customized wafer sample data across nine independent runs for the evaluation. Convergence curves for different pose parameters are plotted in Figs. 6 (b), and Fig. 6 (a) describes system components that respond to the poses. For each run, initial estimates for d and θ_y were selected randomly from the ranges of 48–50 mm and 70–73 degrees, respectively. In general



711 **Fig. 6 Consistency test of full-pose self-calibration.** **a** System components corresponding to
712 different pose parameters. **b1–b4** Convergence of full-pose parameters in nine runs of the algorithm
713 with random initialized d and θ_y . **b1** Convergence curvature of the illumination pose parameters
714 θ_x, θ_y , and θ_z . **b2** Corrected position error Δx and Δy of 400 positions. The gray bars indicate
715 the mean value and pink bars represent the corresponding variation. **b3** Convergence curvature of
716 diffraction distance d . **b4** Convergence curvature of detection pose parameters γ_x, γ_y , and γ_z .

717 systems, random initialization is not performed, and the other parameters default to
718 zero.

719 The results confirm that parameter updates exhibit similar convergence trends
720 across runs, yielding final values of $\theta_x = -0.70 \pm 0.12^\circ$, $\theta_y = 71.74 \pm 0.11^\circ$, $\theta_z =$
721 $0.45 \pm 0.10^\circ$, $d = 48.32 \pm 0.17$ mm, $\gamma_x = 9.25 \pm 1.3^\circ$, $\gamma_y = 2.28 \pm 0.34^\circ$, and γ_z
722 consistently below 0.1° . The update behavior of most parameters changed significantly
723 before and after enabling scan position correction at the 1000th epoch. For example,
724 d converges to approximately 49.5 mm before epoch 1000, differing from its final
725 convergence value. This reflects the coupling effect between pose parameters and scan
726 position as discussed in Section S3, which justifies our segmented updating strategy.
727 The corrected position errors ($\Delta x_j, \Delta y_j$) are presented in Fig. 6b, and the gray and
728 pink bars represent the mean value and variation range of the position error across the
729 nine runs. This visualization confirms that the scan position correction is consistent
730 across the nine runs. In conclusion, our full-pose self-calibration method demonstrates
731 strong stability with respect to initial parameter states and consistently converges to
732 uniform calibration results across various scenarios.
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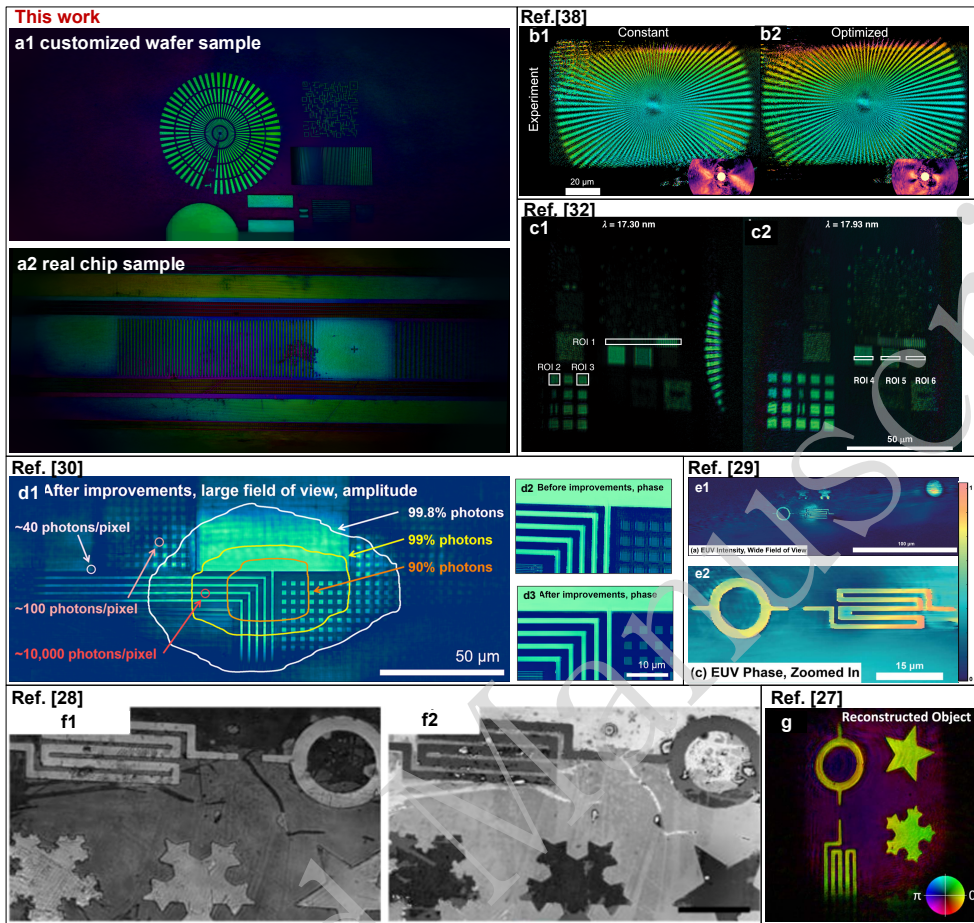
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Table 3 Features of reported reflection ptychography systems on a table-top EUV source

Reported systems	Reflection angle	Wavelength (nm)	method	System self-calibration			Real chip inspection	Half-pitch resolution (nm)
				Δr_j	d	θ		
Ref. [27]	moderate (45°)	29.5	ePIE	✓	✓	✓	150	
Ref. [28]	moderate (50.5°)	30	ePIE	✓	✓	✓	40	
Ref. [29]	high (70°)	29.3	ePIE& rPIE	✓	✓	✓	77.5	
Ref. [30]	high (65° - 69°)	29.3	mulptyRAAR	✓	✓	✓	65	
Ref. [32]	high (70°)	17.3	AD+SGD	✓	✓	✓	50	
Ref. [38]	high (70°)	17.5	AD+Adam	✓	✓	✓	550	
this work	high (70°)	17.9	AD+Adam	✓	✓	✓	43.5	

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3 Discussion



815 **Fig. 7** Representative imaging results of reported reflection ptychography systems based on EUV
 816 source. **a1** and **a2** show the full-field results with full-pose calibration in this work. **b1** and **b2** show
 817 the pseudocolor imaging results of a Siemens star sample without and with tilt-angle correction
 818 adapted from Senhorst *et al.* *Opt. Express* 32, 44017-44030 (2024) [38]. Copyright 2024 Author(s),
 819 licensed under a Creative Commons Attribution 4.0 License. **c1** and **c2** are pseudocolor imaging
 820 results adapted from Shao *et al.* *Light Sci. Appl.* 13, 196 (2024) [32]. Copyright 2024 Author(s),
 821 licensed under a Creative Commons Attribution 4.0 License. **d1–d3** are the amplitude and phase
 822 results adapted from Tanksalvala *et al.* *Sci. Adv.* 7, eabd9667 (2021) [30]. Copyright 2021 Author(s),
 823 licensed under a Creative Commons Attribution 4.0 License. **e1** and **e2** show the amplitude and
 824 phase results adapted with permission from Poter *et al.* *Optica* 4, 1552-1557 (2017) [29]. Copyright
 825 Optica Publishing Group. **f1** and **f2** show the amplitude and phase results adapted from Zhang *et al.*
 826 *Ultramicroscopy* 158, 98-104 (2015) [28]. Copyright 2015 Author(s), licensed under a Creative
 827 Commons Attribution 4.0 License. **g1** represent the pseudocolor result adapted with permission from
 828 Seaberg *et al.* *Optica* 1, 39-44 (2014) [27]. Copyright Optica Publishing Group.

We developed a table-top EUV reflection ptychography system for the simultaneous self-calibration of critical system parameters including the diffraction distance d , three-dimensional illumination angle θ , three-dimensional detection postures γ , and scan position. This framework demonstrates excellent imaging performance on both customized wafers and real chip samples characterized by robust and consistent self-calibration. The previously reported EUV reflective ptychography systems and their characteristics are summarized in Table 3. For the first time, we integrate the full-pose parameters of a reflection ptychography system into a unified self-calibration framework and demonstrate the universality of our imaging system using both simple (customized wafer) and complex (real chip sample) specimens. To provide an intuitive reference, Fig. 7 juxtaposes representative imaging results from the literature (drawn from the studies compared in Table 3) with those obtained in this study. We acknowledge that a direct quantitative comparison is challenging because of the differences in experimental hardware (e.g., driving laser sources and detectors) and reconstruction software. However, the visual comparison in Fig. 7 clearly demonstrates the significant advancements achieved by the proposed method.

The successful implementation of this approach relies on two elements: comprehensive modeling of the physical system and advanced computational techniques, which include specialized loss functions and robust optimizers. Modeling a full set of system parameters enables synthetic data to progressively approximate real-world physical systems, reducing discrepancy between simulated and actual data. This advancement stems from deeper physical insights and continuous refinements in numerical methods. However, well-designed loss functions and optimizers enable algorithms to maintain strong performance even when synthetic and real-world data cannot be aligned perfectly. The former approach aims to minimize mismatches, whereas the latter enhances robustness against such discrepancies. Our study demonstrates that combining both strategies leads to superior outcomes. This intelligent computing paradigm bridges the gap between physical principles and numerical simulations, paving the way for transformative progress in practical implementations of complex imaging systems. Our research not only advances EUV imaging capabilities but also inspires adaptations across broader imaging modalities and spectral regimes.

Compared to established techniques such as SEM and AFM, a key strength of EUV reflective ptychography is the chemical sensitivity inherent in its phase information. However, unlocking this capability requires angular scanning to acquire the phase-angle spectrum of the sample. Although experiments reported here were performed at a single angle, and thus, they do not fully exploit the material sensitive potential of the technique. We expect that the calibration strategy proposed in this work will still substantially improve the analysis efficiency and accuracy in multian-gle scanning scenarios. This stems from the computational efficiency of the automatic differentiation based correction framework and high fidelity imaging enabled by full pose self calibration.

However, practical deployment in online settings is limited by the computational speed of phase retrieval algorithms. Gradient based optimization schemes converge more slowly than the projection based methods. Therefore, future work should focus on integrating full pose learning into accelerated projection based frameworks while

875 leveraging graphics-processing-unit (GPU) accelerated parallel computing via compute
 876 unified device architecture. Such technical advances would enhance computational
 877 throughput, paving the way for EUV reflection ptychography to fulfill its potential in
 878 industrial metrology.

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880 4 Materials and method

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882 4.1 Derivation of mapping operator \mathbf{T}

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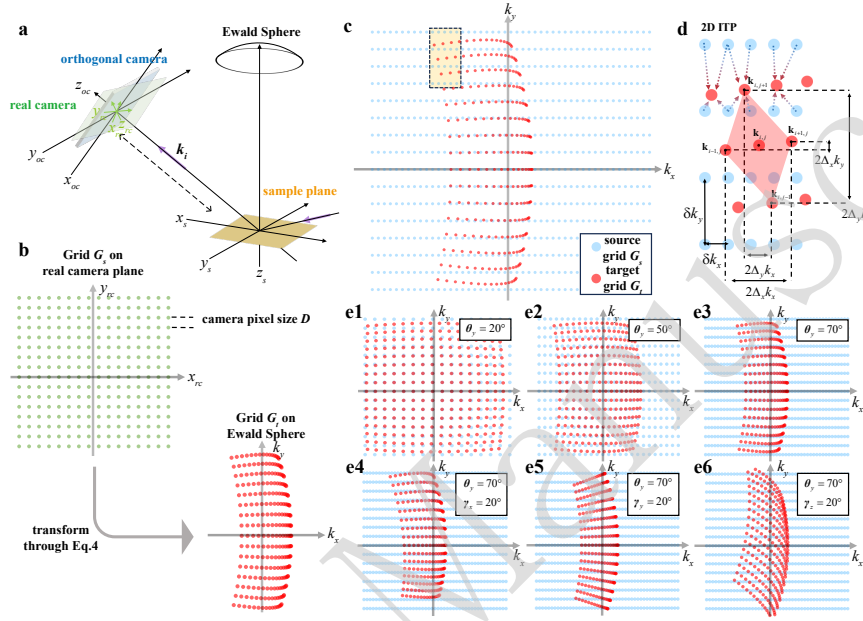
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905 **Fig. 8** Sampling grid transformation in the mapping operation \mathbf{T} . **a** Schematic of tilt detection
 906 in reflection ptychography. **b** Grid transformation from real camera plane to Ewald Sphere. The
 907 parameters are set to clearly demonstrate the effect of grid warping: wavelength = 17 nm, camera
 908 pixel size $D = 2200 \mu\text{m}$, diffraction distance $d = 50 \text{ mm}$, $\theta_y = 70^\circ$, and grid size 16×16 . **c** Uniform
 909 source and warped target grids on Ewald Sphere. The wavevector range of the source grid is about
 910 $[-120, 120] \text{ rad}/\mu\text{m}$ in both horizontal and vertical directions. **d** Zoom-in region marked by the dotted
 911 box in **c** illustrates the procedure of 2D interpolation and parameters used to calculate the Jacobian
 912 matrix. The Jacobian value at the (i,j) -th sampling point is determined by the coordinates of its four
 913 neighboring sampling points. **e1–e6** show grid settings with different pose parameters.

914 The mapping operator \mathbf{T} transforms the pattern from an Ewald sphere into a real
 915 detection plane via fast interpolation. We establish the transformation relationship of
 916 the sampling grid from the real camera coordinate system (x_{rc}, y_{rc}, z_{rc}) to the sample
 917 coordinate system (x_s, y_s, z_s) , as shown in Fig. 8 a. In a well-aligned setup, the
 918 camera should be orthogonal to the light emitted from the sample; however, achieving
 919 this in practice is challenging. We represent the sampling point \mathbf{p} in the actual camera
 920 coordinate system as $[\mathbf{p}]_{rc} = [x, y, 0]^T$. Considering possible three-dimensional rotation

of the camera, its representation in the orthogonal camera coordinate system (x_{oc}, y_{oc}, z_{oc}) is $[\mathbf{p}]_{oc} = \mathbf{R}_\gamma[\mathbf{p}]_{rc}$, where \mathbf{R}_γ represents the coordinate rotation operator as

$$\mathbf{R}_\gamma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \gamma_x & \sin \gamma_x \\ 0 & -\sin \gamma_x & \cos \gamma_x \end{bmatrix} \begin{bmatrix} \cos \gamma_y & 0 & \sin \gamma_y \\ 0 & 1 & 0 \\ -\sin \gamma_y & 0 & \cos \gamma_y \end{bmatrix} \begin{bmatrix} \cos \gamma_z & \sin \gamma_z & 0 \\ -\sin \gamma_z & \cos \gamma_z & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (3)$$

Further, we represent \mathbf{p} using the global sample coordinate system. Given distance d between the origins of coordinate systems (x_{oc}, y_{oc}, z_{oc}) and (x_s, y_s, z_s) , and a three-dimensional transformation with angle $\boldsymbol{\theta}$, the representation of the sampling point in the sample coordinate system is $[\mathbf{p}]_s = \mathbf{R}_\theta([\mathbf{p}]_{oc} + \mathbf{d})$, where $\mathbf{d} = [0, 0, d]^\top$. The coordinate relationship for far-field diffraction is established between the internal coordinates of the sample and reciprocal wavevector coordinates. Therefore, we transform the camera point \mathbf{p} into the corresponding wavevector coordinate $\mathbf{k} = k_0[\mathbf{p}]_s/|[\mathbf{p}]_s|$, where $k_0 = 2\pi/\lambda$. The probe illuminates the sample at a grazing angle, and therefore, the tilt phase causes a shift in the diffraction pattern during the Fourier transform. We add the illumination wavevector $\mathbf{k}_i = [\cos\theta_x \sin\theta_y, \sin\theta_x, \cos\theta_x \cos\theta_y]^\top$ in the wavevector coordinate transformation to counteract this shift: $\mathbf{k} = k_0[\mathbf{p}]_s/|[\mathbf{p}]_s| + \mathbf{k}_i$. In summary, the coordinate transformation for a sampling point can be expressed as

$$\mathbf{k} = k_0 \cdot \text{unit}[\mathbf{R}_\theta(\mathbf{R}_\gamma[\mathbf{p}]_{rc} + \mathbf{d})] + \mathbf{k}_i \quad (4)$$

where unit represents vector normalization $\cdot/|\cdot|$. When the sample thickness is negligible, we require only the first two dimensions (k_x and k_y) of \mathbf{k} to construct a two-dimensional sampling grid. We can derive the warped grid on the Ewald sphere using Eq. 4 by denoting the sampling grid of the real camera G_{rc} ; we call this the target grid G_t . An illustration of the grid transformation from G_{rc} to G_t is shown in Fig. 8 b. On the Ewald sphere, we have a uniform source grid G_s , as shown in Fig. 8 (c), which is determined by the sampling conditions on the sample plane. Thus, the complete mapping operator \mathbf{T} can be represented as

$$\mathbf{y} = |\det J| \cdot \text{ITP}(\mathbf{I}, G_s, G_t) \quad (5)$$

where ITP is a two-dimensional (2D) interpolation operator, \mathbf{y} and \mathbf{I} represent the images on tilt detection plane (target) and Ewald sphere (source), and $\det J$ represents the determinant of the Jacobian matrix defined by $\det J = \frac{\partial k_x}{\partial x} \frac{\partial k_y}{\partial y} - \frac{\partial k_x}{\partial y} \frac{\partial k_y}{\partial x}$. To avoid the dimensionality issue and cumbersome differentiation in the above equation, we numerically calculate the determinant using G_s and G_t as

$$\det J = \frac{\Delta_x k_x \Delta_y k_y - \Delta_y k_x \Delta_x k_y}{\delta k_{x_0} \delta k_{y_0}} \quad (6)$$

where Δ_x and Δ_y represent the center difference operations along the x- and y-directions, respectively, and δk_{x_0} and δk_{y_0} represent the sample intervals of the uniform grid G_s . These parameters used to calculate the Jacobian matrix are shown in Fig. 8 d. The multiplication operation with $|\det J|$ ensures the conservation of energy between

967 the source \mathbf{I} and target \mathbf{y} . Based on the above derivation, we can easily present the sam-
 968 pling grid settings for different pose parameters. Figs. 8 e1–e6 show the distributions
 969 of the source and target grids on the Ewald sphere for the different pose parameters.
 970

971 4.2 Algorithm implementation

972 In our forward model incorporating the coordinate mapping operator, sampling on
 973 the virtual detection plane requires an explicit definition. The coordinates of the vir-
 974 tual plane are represented in the wave vector k space. We employ an anisotropic grid
 975 with a sampling interval and dimensions $\delta\mathbf{k}$, \mathbf{M} to accurately match the distorted
 976 diffraction patterns in the reflection geometry: $\delta\mathbf{k} = 2\pi D [\cos\theta_{x_0}, \cos\theta_{y_0}]^\top / (\lambda d)$,
 977 $\mathbf{M} = [m, \text{round}(m \cos\theta_{x_0}/2 \cos\theta_{y_0})]^\top$ where D , m and $\theta_{x_0} = 0^\circ/\theta_{y_0} = 70^\circ$ repre-
 978 sent the camera pixel size, vertical dimension of the raw diffraction patterns, and
 979 default illumination angles, respectively. The resulting object-plane sampling interval
 980 is $2\pi/(\mathbf{M} \odot \delta\mathbf{k})$, which is defined as the standard sampling $\delta\mathbf{p}_{\text{st}}$. Such sampling results
 981 in a numerical aperture ratio of 2:1 between the y- and x-directions on the virtual
 982 plane, while the numerical aperture in the y-direction is consistent with the physical
 983 numerical aperture of the system in the y direction.
 984

985 Three regularization losses are applied beyond the data fidelity term: (1) Probe
 986 support: $\|\mathbf{M}_s \odot \mathbf{P}\|_2^2$ with binary mask \mathbf{M}_s , centering the probe and suppressing
 987 peripheral artifacts; (2) Total variation: $\|\nabla\mathbf{x}\|_1$ for image edge enhancement and noise
 988 suppression; (3) Pattern constraint: $\sum_j \|\mathbf{M}_p \odot \mathbf{I}_j\|_2^2$, where \mathbf{I}_j represents the virtual-
 989 plane predicted pattern and \mathbf{M}_p represents a binary mask constraining the energy in
 990 unmeasured regions.

991 Our algorithm is implemented using the open-source Python package PyTorch
 992 and executed on a server with Nvidia A100 GPU. In the experiment, high-resolution
 993 reconstruction follows a three-stage framework with low resolution (LR), medium res-
 994 olution (ML), and high resolution (HR) stages. In the LR stage, the images and system
 995 parameters are reconstructed using 512×512 data size with 2000 epochs. All pose
 996 parameters (d , $\boldsymbol{\theta}$ and $\boldsymbol{\gamma}$) are updated at the 200th epoch, whereas the scan positions
 997 remain fixed until the 1000th epoch. In the ML and RL stages, the variables are fur-
 998 ther refined to data sizes of 1024×1024 and 1900×1900 , each with 50 epochs.
 999 Camera edge pixels are discarded in the HR stage because of elevated noise levels. We
 1000 employ the Adam optimizer [47] with 10 batches per iteration throughout, resetting
 1001 the first-order and second-order momenta whenever new variables are activated. The
 1002 learning rates for the variables and regularization weighting coefficients are listed in
 1003 Tables 2 and 3. The pose parameters do not significantly change during the ML and
 1004 HR stages, indicating that they were successfully corrected during the LR stage.

1005 **Supplementary information.** This article has accompanying supplementary files.
 1006

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 1009 Haoyu Wu, Peixiang Xiong, Tianlei Jia and Tianhao Zhang.

1010 **Author contributions.** Y.C., H.X., Q.W., and Y.L. contributed equally to this
 1011 study. Y.C. conceived the idea. Y.C., Q.W., L.H., and S.L. performed the reflection
 1012

Table 4 Learning rate settings.

Variable	Learning rate
\mathbf{x}	1×10^{-2}
\mathbf{P}	1×10^{-2}
d	1×10^2
θ	1×10^{-3}
γ	5×10^{-4}
$\Delta \mathbf{r}_j$	5×10^{-3}

Table 5 Regularization coefficient settings.

Regularization	Weighting coefficient
Probe support	1×10^{-2} (LR)
	1×10^{-3} (MR)
	0 (HR)
Total variation	5×10^{-2} (LR)
	5×10^{-3} (MR)
	1×10^{-4} (HR)
Pattern constraint	5×10^{-2} (LR)
	1×10^{-3} (MR)
	0 (HR)

ptychography experiments and processed the data. H.X., Z.X., and J.L.^{1,3} prepared the EUV beam at 17.9 nm. Y. L., B. L., G. C., J. L.⁹, Y. W., and D. W. supported and developed the EUV source system. Y.C., F.W., and Y.S. prepared, revised, and finalized the manuscript. Z.F., X.Z., C.K. and Y.S. conceived the project. Y.S. supervised the study.

Data availability. Data and codes supporting this study are available from the corresponding author upon request.

Conflict of interest. The authors declare no conflicts of interest.

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