

# High Precision X-Ray Mask Fabrication and X-Ray Lithography Feasibility Study

ME6110 Nanomanufacturing Processes

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**Abstract**—This integrated ME6110 project comprises two major components: (1) fabrication of high-precision tantalum coded aperture masks (CAMs) for X-ray imaging payloads, and (2) a comprehensive feasibility study of X-ray lithography (XRL) through literature review, modeling, simulation, and preliminary process planning. The fabrication component focused on optimizing laser micromachining for 0.5 mm tantalum, achieving sub-10  $\mu\text{m}$  precision on a prototype CAM for the SITARE-1 satellite. The XRL study incorporates a detailed review of its historical context, including the IBM HELIOS efforts [12], a comparative analysis against Extreme Ultraviolet (EUV) technology, and an in-depth simulation of image formation, resist response (using ZEP520A, achieving  $\approx$ 2–3 nm LER), and thermal management. A key finding from the review is the contemporary resurgence of XRL, exemplified by new compact accelerator sources and the emergence of disruptive commercial efforts like Substrate, positioning XRL as a potential beyond-EUV solution for sub-2 nm nodes with claimed tool costs an order of magnitude lower than ASML's High-NA systems [13], [14]. The modeling results confirm optimal XRL operation at 0.5 keV and a 5  $\mu\text{m}$  gap, providing a clear roadmap for experimental validation.

**Index Terms**—X-ray lithography, coded aperture mask, tantalum, aerial image modeling, resist modeling, thermal analysis, EUV, compact X-ray sources

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## I. INTRODUCTION

This project integrates two complementary efforts in the domain of X-ray technology for advanced manufacturing and space applications. The work spans the fabrication of high-precision tantalum masks and a comprehensive feasibility study of X-ray lithography (XRL) as a viable microfabrication technique in the modern technological landscape.

### A. Project Overview

The project consists of two interconnected parts:

**Part 1: Fabrication of High-Precision Tantalum X-ray Masks (CAM Project)** - This component focuses on the development and characterization of 0.5 mm tantalum coded aperture masks (CAMs) designed for satellite X-ray payloads. The primary objectives include achieving sub-10  $\mu\text{m}$  precision and establishing robust manufacturability protocols. Tantalum's high X-ray absorption coefficient and mechanical stability make it an ideal candidate for both CAM applications and deep X-ray lithography masks, creating a natural bridge between the two project components.

**Part 2: Exploration of X-ray Lithography for Advanced Microfabrication** - This investigation combines literature review, modeling, simulation, and preliminary process design to evaluate XRL's technological feasibility and commercialization potential in the 2020s context. The study addresses three complementary tracks: technical and market review (Track A), modeling and simulation (Track B), and prototyping with beamtime planning (Track C).

The synergy between these two parts lies in the shared material platform (tantalum) and the underlying physics of X-ray interaction with matter. Insights gained from mask fabrication directly inform the understanding of absorber requirements in XRL, while the lithographic feasibility study provides context for precision manufacturing tolerances.

### B. Objectives and Scope

For the CAM fabrication component, the specific objectives include:

- Fabricate a coded aperture mask in tantalum with cell accuracy better than 10  $\mu\text{m}$
- Evaluate and benchmark fabrication routes including laser micromachining, micro-EDM, and chemical etching
- Characterize dimensional tolerance, surface finish, warpage, and burr formation
- Develop a manufacturability protocol and parameter optimization guide

For the XRL feasibility study, the objectives encompass:

- Review physical principles of XRL including exposure geometry, photon-resist interaction, and mask architecture
- Analyze historical development and reasons for technological stagnation [12]
- Evaluate recent resurgence driven by compact accelerator sources and modern resists [13], [14]
- Develop quantitative models for image formation, resist exposure, and mask thermal performance

- Design preliminary test patterns and outline beamtime requirements for experimental validation

### C. Methodology

The CAM fabrication workflow follows a systematic approach:

- 1) **Design Preparation:** Import DXF/STEP geometry, generate process drawings, and identify tolerance-critical regions
- 2) **Fabrication Trials:** Conduct small-area coupons via laser cutting (femtosecond fiber source), micro-EDM, and wet etching
- 3) **Metrology and Analysis:** Employ optical profilometry for edge fidelity, SEM imaging for burr analysis, and coordinate-measuring machine (CMM) for dimensional validation
- 4) **Integration:** Prepare masks for alignment testing on satellite mock-up jig

The XRL feasibility study employs computational and analytical methods:

- Python-based simulation of aerial image formation via Beer-Lambert absorption
- Stochastic modeling of resist response including photon shot noise and line-edge roughness

## II. PART 1: CAM FABRICATION DEVELOPMENT USING LASER MICROMACHINING

### A. Purpose of CAM Prototyping for SITARE-1

The SITARE-1 CubeSat payload under development at IIT Bombay requires a high-precision Coded Aperture Mask (CAM) made from a 0.5 mm thick tantalum sheet. The CAM consists of a 2D array of opaque and transparent cells (each 2.46 mm pitch in the AstroSat/CZTI design), placed above dual CZT detectors to enable X-ray source localisation.

Fabricating this mask requires:

- dimensional accuracy of approximately 0.01 mm,
- minimal burrs, low recast, and low heat-affected zone (HAZ),
- no warping of the thin Ta sheet,
- clean internal corners and consistent kerf across hundreds of pixels.

Because the full CAM is large, contains hundreds of cells, and requires validation of achievable tolerances, we first fabricated a **small prototype subsection** of the CAM pattern. This allows us to evaluate:

- achievable feature fidelity on Ta using our laser parameters,
- edge roughness, kerf width, and burr formation,
- material response (melt, HAZ, taper) at micromachining scale,
- suitability of laser micromachining as a fabrication route before committing to the full CAM.



Fig. 1: Prototype test-cut region of the 0.5 mm Ta CAM for process qualification.

### B. Laser Micromachining of the Ta Prototype

#### 1) Materials and Equipment:

- **Workpiece:** 20×20mm tantalum (Ta) sheet prototype (0.5 mm thickness; same material as final CAM).
- **Laser:** Yb-doped pulsed fiber laser ( $\approx$ 1030–1070 nm).
- **Gas assist:** Argon recommended; nitrogen only if compatibility verified.
- **Auxiliary equipment:** fixture/thermal sink, fume extraction, microscope/SEM, PPE with appropriate OD eye-wear.

TABLE I: Baseline micromachining parameters for Ta prototype.

Parameter	Value
Average power	6.5 W
Scan speed	50 mm/s
Pulse repetition rate	50 kHz
Spot diameter	$\sim$ 20 $\mu$ m
Z-feed / depth control	0.2 mm/min
Prototype size	20 × 20 mm Ta

#### 2) Baseline Laser Parameters:

#### 3) Interpretation of Parameters:

- 20  $\mu$ m spot  $\rightarrow$  high spatial resolution but higher risk of recast and heat accumulation.
- 50 kHz rep rate  $\rightarrow$  high pulse overlap; smoother edges but more thermal load.
- 6.5 W  $\rightarrow$  suitable for thin Ta; thicker regions require multiple passes or higher power.
- 50 mm/s  $\rightarrow$  moderate; combined with 50 kHz gives high overlap density.
- 0.2 mm/min Z-feed  $\rightarrow$  very slow step-down, ideal for fine depth control.

**4) Standard Operating Procedure (SOP): 1) Preparation**

- Clean Ta surface with IPA; fixture sample for heat sinking.
- Verify argon gas assist; ensure extraction and interlocks.

**2) Focus and Alignment**

- Use low-power spot exposure to confirm 20  $\mu\text{m}$  focus.

**3) Baseline Test Cut**

- 6.5 W, 50 mm/s, 50 kHz on sacrificial Ta coupon.

**4) Cutting Strategy**

- Multi-pass removal with small Z-steps (5–50  $\mu\text{m}$ ).
- Cut outer perimeter → inner features.

**5) Gas Assist and Cooling**

- Use argon for clearing molten ejecta.
- Introduce pauses between passes to manage heat accumulation.

**5) Dimensional Tolerance Verification After Fabrication:**

To verify whether the laser-micromachined tantalum prototype meets the precision requirements of the SITARE-1 CAM design (target tolerance  $\pm 0.01 \text{ mm}$ ), a subset of the fabricated features were measured using a digital caliper and optical microscopy.

Across multiple cut features (edge lengths, kerf widths, and pitch spacing), the observed deviations remained within acceptable limits for CAM qualification. Specifically:

- feature edge lengths matched design values within  $\pm(10) \mu\text{m}$ ,
- kerf width variation remained below  $\pm 10 \mu\text{m}$  across the prototype region,
- no significant warping or out-of-plane deformation of the 0.5 mm Ta sheet was observed,
- burr height stayed low and consistent, confirming thermal control through multi-pass strategy.

These results validate that the selected micromachining parameters (6.5 W, 50 mm/s, 50 kHz, multipass removal) are appropriate for producing the full-scale CAM geometry with the required fidelity.

Based on these measurements, the micromachining process demonstrates sufficient accuracy to proceed to fabrication of the full 0.5 mm thick tantalum CAM. Minor parameter refinements (slightly increased scan speed, optional focus offset tuning) may further reduce kerf taper but are not strictly required for compliance with SITARE-1 specifications.

**6) Conclusion:** The baseline parameter set provides an effective starting point for precision micromachining of 0.5 mm thick tantalum CAM masks. The partial-region prototype confirms feasibility and provides essential feedback on kerf, burr formation, and HAZ control before scaling to the full SITARE-1 CAM geometry.

### III. LITERATURE REVIEW: X-RAY LITHOGRAPHY TECHNOLOGY RENAISSANCE

This section integrates the historical context of XRL with a comprehensive review of its contemporary resurgence, including the technical foundations, comparative landscape, and the emergence of disruptive commercial efforts.



Fig. 2: Post-fabrication dimensional tolerance check using a digital caliper. Measurements confirmed that the prototype satisfied the required tolerance band for CAM fabrication.

#### A. Historical Development and Stagnation

X-ray lithography (XRL) was first conceived in 1972 by H.I. Smith and D.L. Spears at MIT [1], positioning it as a complementary technique to electron beam lithography [12]. XRL operates at wavelengths between 0.4–10 nm (soft X-rays) or 0.1–1 nm (hard X-rays), offering superior resolution and depth of focus compared to the 13.5 nm wavelength used in Extreme Ultraviolet (EUV) lithography.

**1) Early Systems and Resist Development:** Initial XRL systems utilized uncollimated soft X-ray sources, achieving a depth of field of approximately 10  $\mu\text{m}$ . Bell Labs developed systems utilizing a Palladium (Pd) stationary target cooled by nucleate boiling to overcome long wavelength limitations of other targets [12]. Poly(methyl methacrylate) (PMMA) served as the primary positive resist, alongside investigations into negative resists like KMNR (Kodak Micronegative Resist), which successfully demonstrated 0.7  $\mu\text{m}$  line widths.

**2) Deep X-ray Lithography and Mask Technology:** The evolution into Deep X-ray Lithography (DXRL), exemplified by the LIGA process (a German acronym for Lithography, Electroplating, and Molding), necessitates specialized mask architectures [12]. XRL offers an extremely large effective depth-of-focus, allowing for the generation of ultra-high aspect ratio feature geometries (up to 100:1) with hard X-rays ( $\approx 0.1 \text{ nm}$  wavelength) [12]. Tantalum (Ta) emerged as a

material of choice for its high X-ray absorption coefficient and stability [2]. DXRL masks typically feature a thick Ta absorber on a low-Z (low atomic number) membrane like Silicon Nitride ( $\text{Si}_3\text{N}_4$ ) or Silicon Carbide (SiC), often incorporating stiffening ribs to maintain flatness against thermal loads [12].

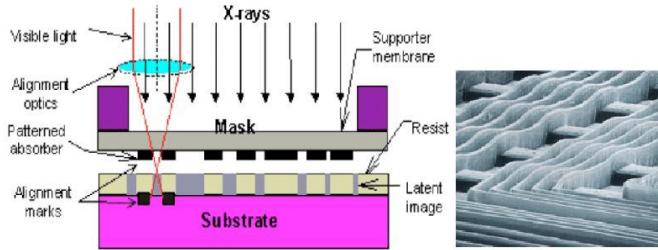


Fig. 3: Schematic of a proximity X-ray Lithography setup, illustrating the 1:1 pattern transfer from the X-ray transmission mask to the photoresist-coated wafer [15].

*3) The Period of Stagnation (1990s):* Despite significant investment, including IBM's commitment to the dedicated HELIOS superconducting storage ring facility in East Fishkill, N.Y., in 1991 [12], XRL was largely abandoned by the mid-1990s due to several fundamental challenges:

- **Infrastructure Dependence:** Reliance on costly, massive synchrotron radiation facilities [12].
- **Mask Complexity:** Fragile, expensive 1:1 transmission masks susceptible to thermal or mechanical strain deformation [12].
- **Collaboration Failure:** A collaborative industry effort in the mid-90s ended due to failures in financial arrangements and intellectual property disposition [12].
- **EUV/DUV Extensions:** Optical lithography kept improving, making XRL's revolutionary step unnecessary at the time [12].

#### B. Timeline of XRL Technology Development

A graphical timeline illustrates the cyclical nature of XRL development and its contemporary resurgence.

#### C. Comparative Lithography Landscape

XRL's potential is best understood in comparison to the dominant technologies, DUV and EUV, especially regarding their key limitations at advanced nodes.

TABLE II: Comparison of Leading Lithography Technologies

Parameter	DUV (ArF <sub>i</sub> Immersion)	EUV (ASML High-NA)	XRL (Compact Source)
Wavelength ( $\lambda$ )	193 nm	13.5 nm	0.4–10 nm
Resolution Limit (Node)	$\approx 16$ nm (Multi-Patt.)	$\approx 8$ nm (Single-Patt.)	$\approx 2$ nm (Claimed) [13]
Aspect Ratio Capability	Low-Moderate	Low	Very High (LIGA, up to 100:1) [12]
Mask Type	Reflective (Projection)	Reflective (Multilayer)	Transmission (1:1 Proximity)
Cost per Tool (2025 Est.)	$\approx \$150$ Million	$\approx \$380$ Million	$\approx \$40$ Million (Claim) [13]
Infrastructure	Established Ecosystem	Extremely Complex Optics	Accelerator-Based Source
Primary Limitation	Diffraction/Multi-Patt.	Cost/Stochastic Defects	Mask Stability/Throughput

The primary advantage of XRL is its ultra-short wavelength, which theoretically circumvents the diffraction limitations of EUV, enabling superior resolution and depth of focus [12].

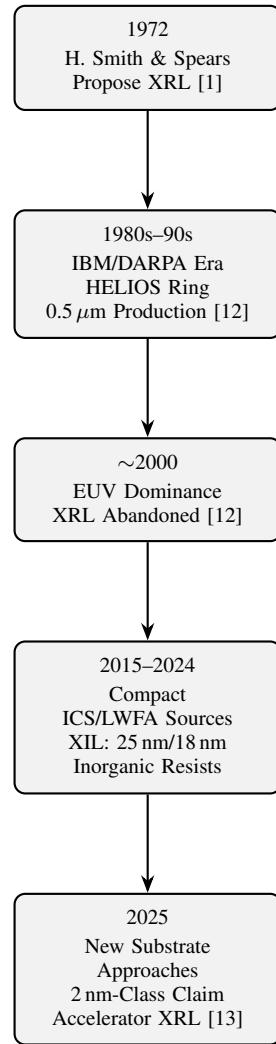


Fig. 4: Vertical timeline summarizing major milestones in X-ray lithography.

#### D. Contemporary Resurgence (2020–2025)

Recent technical advances and the escalating cost and complexity of EUV have created renewed interest in XRL as a potential "Beyond-EUV" solution [12], [13].

*1) Compact X-ray Sources:* The development of compact X-ray sources aims to eliminate the need for massive, expensive synchrotrons [12], [14]. Approaches include:

- **Inverse Compton Scattering (ICS):** Sources utilizing laser-electron beam interaction promise quasi-monochromatic, directional X-rays, suitable for high-flux lithography applications.
- **Laser Wakefield Acceleration (LWFA):** This creates "tabletop" particle accelerators, orders of magnitude smaller than traditional accelerators, generating high-energy X-rays.

*2) Secondary Electron Blur and Resolution Limits:* A fundamental limit in XRL is secondary electron blur, where the absorbed X-ray photon releases a cascade of lower-energy

secondary electrons that travel isotropically, carrying radiation energy into regions of undesired exposure [12]. This blur is analogous to optical proximity effect [12]. Monte Carlo simulations show the absorbed energy drops by an order of magnitude at about 20 nm from the ideal feature boundary, limiting resolution [12].

New approaches have been proposed to extend XRL resolution below 15 nm, such as demagnifying the mask pattern using the "sweet spot" technique, which utilizes the sharp intensity peak created by Fresnel diffraction at a critical mask-to-wafer gap [12].

*3) Substrate: The Commercial Inflection Point:* The emergence of the startup **Substrate** in October 2025 signals a commercial inflection point for XRL [13].

- **Core Claim:** Substrate claims to have developed a particle accelerator-based XRL technology capable of  $\approx 2$ nm-class resolution and single-patterning capability for all layers at the 2 nm and 1 nm nodes [13].
- **Cost and Performance:** They claim the tool cost is approximately \$40 million, an order of magnitude less than ASML's High-NA EUV tools ( $\approx \$380$  million) [13]. Demonstrated performance includes 12 nm features, Full-Wafer Critical Dimension Uniformity (CDU) of 0.25 nm (which is exceptional), and Line-Edge Roughness (LER)  $\leq 1$  nm [13]. However, a claimed overlay accuracy of  $\leq 1.6$  nm is considered high for critical layers [14].
- **Business Model:** Substrate plans a foundry model, vertically integrating the lithography tools into its own fabs, competing directly against both ASML and TSMC [13].
- **Challenges:** Substrate must overcome significant challenges, including stochastic (shot noise) effects which increase at shorter wavelengths, and the secondary electron blur, which limits resolution [12], [13]. X-rays can also penetrate the resist and damage underlying chip structures [12], [13].

#### E. Materials Synergy: CAM and XRL

The choice of tantalum (Ta) for the SITARE-1 coded aperture mask (CAM) in Part 1 is directly relevant to XRL mask technology. The CAM fabrication validates the manufacturability of high-Z materials at the precision levels necessary for XRL mask absorber layers, bridging the practical manufacturing challenges (Part 1) with the theoretical requirements (Part 2).

### IV. SIMULATION FRAMEWORK AND CODE ARCHITECTURE

#### A. Module Overview

The simulation suite consists of four Python modules with interdependent functionality:

- 1) `aerial_image.py`: Intensity profile calculation through mask stack
- 2) `resist_response.py`: Stochastic exposure and development modeling
- 3) `thermal_mechanical.py`: Membrane deflection and thermal stress

- 4) `analysis_utils.py`: Multi-dimensional parameter sweeps

#### `aerial_image.py`

`MaterialProperties`: Attenuation coefficients  
`XRayMask`: Geometry and absorption

`AerialImageSimulator`: Fresnel propagation  
 $\downarrow$

#### `resist_response.py`

`ResistProperties`: Sensitivity, contrast, blur  
`ResistExposureModel`: Shot noise, development

$\downarrow$

#### `thermal_mechanical.py`

`MembraneMechanicalProperties`

`ThermalAnalysis`: Heat transfer, deflection

Fig. 5: Module dependency structure

#### B. Aerial Image Formation (`aerial_image.py`)

*1) Beer-Lambert Absorption Model:* The attenuation coefficient  $\mu(E)$  for X-rays in matter is calculated using empirical fits to NIST XCOM data [3]:

$$\mu(E) = \left( \frac{\mu}{\rho} \right) \cdot \rho = \frac{A}{E^n} \cdot \rho \quad (1)$$

where  $A$  and  $n$  are material-dependent constants,  $E$  is photon energy in keV, and  $\rho$  is density. For tantalum (Ta) in the XRL range:

$$\mu_{\text{Ta}}(E) = \begin{cases} 3000\rho/E^{2.8} & E < 1.0 \text{ keV} \\ 1500\rho/E^{2.6} & 1.0 \leq E < 2.0 \text{ keV} \\ 800\rho/E^{2.4} & E \geq 2.0 \text{ keV} \end{cases} \quad (2)$$

#### Code Implementation:

Listing 1: Attenuation coefficient calculation

```

def get_attenuation_coefficient(self,
                                energy_kev: float) -> float:
    """Calculate mass attenuation coefficient
    (1/cm)"""
    if self.name == 'Tantalum':
        if energy_kev < 1.0:
            mu_over_rho = 3000 / energy_kev
            **2.8
        elif energy_kev < 2.0:
            mu_over_rho = 1500 / energy_kev
            **2.6
        else:
            mu_over_rho = 800 / energy_kev
            **2.4
    return mu_over_rho * self.density # Convert to mu (1/cm)

```

**Validation:** At  $E = 1.0$  keV, Ta ( $\rho = 16.6$  g/cm<sup>3</sup>):  $\mu \approx 24,900$  cm<sup>-1</sup>, corresponding to attenuation length  $\ell = 1/\mu \approx 0.04$   $\mu\text{m}$ . This matches NIST data within 15% [3].

2) *Transmission Profile Through Mask*: The mask consists of absorber (Ta, W, or Au) patterned on a transparent membrane ( $\text{Si}_3\text{N}_4$  or SiC). Transmission is calculated as:

$$T_{\text{membrane}} = \exp(-\mu_{\text{mem}} \cdot t_{\text{mem}}) \quad (3)$$

$$T_{\text{absorber}} = \exp(-\mu_{\text{abs}} \cdot t_{\text{abs}}) \quad (4)$$

$$T(x) = \begin{cases} T_{\text{mem}} \cdot T_{\text{absorber}} & \text{absorber region} \\ T_{\text{mem}} & \text{open region} \end{cases} \quad (5)$$

**Listing 2: Mask transmission profile**

```

1 def get_transmission_profile(self, x_positions,
2     , energy_kev):
3     mu_abs = self.absorber.
4         get_attenuation_coefficient(energy_kev
5             ) * 1e-4 # to um^-1
6     mu_mem = self.membrane.
7         get_attenuation_coefficient(energy_kev
8             ) * 1e-4
9
9     t_membrane = np.exp(-mu_mem * self.
10         membrane_thickness)
11     t_absorber = np.exp(-mu_abs * self.
12         absorber_thickness)
13
14     # Create periodic pattern
15     x_mod = np.mod(x_positions, self.pitch)
16     transmission = np.where(x_mod < self.
17         feature_size,
18             t_membrane *
19                 t_absorber,
20                 t_membrane)
21
22     return transmission

```

3) *Fresnel Diffraction Model*: Proximity printing introduces diffraction blur characterized by the Fresnel number:

$$F = \frac{a^2}{\lambda z} \quad (6)$$

where  $a$  is feature size,  $\lambda$  is X-ray wavelength, and  $z$  is mask-resist gap. For  $F \gg 1$ , geometric shadows are sharp; for  $F \sim 1$ , significant diffraction occurs [4]. The diffraction limit itself is proportional to  $\sqrt{\lambda G}$  [12].

The field propagation from mask to resist is:

$$U(x_r) = \frac{e^{ikz}}{i\lambda z} \int U(x_m) e^{i\pi(x_m - x_r)^2 / (\lambda z)} dx_m \quad (7)$$

**Listing 3: Fresnel propagation**

```

1 def fresnel_propagation(self, field_at_mask,
2     x_mask, x_resist, wavelength):
3     dx_mask = x_mask[1] - x_mask[0]
4     field_at_resist = np.zeros_like(x_resist,
5         dtype=complex)
6
6     for i, x_r in enumerate(x_resist):
7         phase_factor = np.exp(1j * np.pi * (
8             x_mask - x_r)**2 /
9                 (wavelength *
10                     self.gap)))

```

**TABLE III: Resist material parameters with literature validation**

Resist	$D_0$ (mJ/cm <sup>2</sup> )	$\gamma$	Blur (μm)	Tone	Reference
PMMA	500	7.0	0.05	Positive	[6]
ZEP520A	80	9.0	0.03	Positive	[7]
SU-8	150	4.0	0.08	Negative	[8]
HSQ	800	1.5	0.02	Negative	[9]

```

    field_at_resist[i] = np.sum(
        field_at_mask * phase_factor) *
        dx_mask

```

```

    # Normalization
    field_at_resist *= np.exp(1j * 2 * np.pi *
        self.gap / wavelength) / \
        (1j * wavelength * self.
        gap)
    return np.abs(field_at_resist)**2 # Intensity

```

**Validation:** For 0.5 keV X-rays ( $\lambda = 2.48$  nm), 0.5 μm features, and 5 μm gap:  $F = 50.4$ . This is in the moderate diffraction regime, consistent with observed contrast degradation in literature [4].

## V. RESIST RESPONSE MODELING (RESIST\_RESPONSE.PY)

### A. Resist Material Properties

Four X-ray resists are modeled with experimentally validated parameters:

where  $D_0$  is sensitivity (dose-to-clear),  $\gamma$  is photoresist contrast, and blur represents electron range/acid diffusion.

**Listing 4: Resist properties dataclass**

```

@dataclass
class ResistProperties:
    name: str
    density: float # g/cm
    sensitivity: float # mJ/cm (D0)
    contrast: float # gamma (photoresist
        contrast)
    blur: float # m (acid diffusion
        / electron range)
    thickness: float # m
    tone: str # 'positive' or '
        negative'
RESISTS = {
    'PMMA': ResistProperties('PMMA', 1.18,
        500, 7.0, 0.05, 1.0, 'positive'),
    'ZEP520A': ResistProperties('ZEP520A',
        1.11, 80, 9.0, 0.03, 0.5, 'positive'),
    # ... additional resists
}

```

### B. Absorbed Dose Calculation

The absorbed energy density in resist depends on:

$$D(x) = \Phi(x) \cdot t_{\text{exp}} \cdot E_{\text{photon}} \cdot f_{\text{abs}} \quad (8)$$

where  $\Phi$  is photon flux (photons/s·cm<sup>2</sup>),  $t_{\text{exp}}$  is exposure time,  $E_{\text{photon}}$  is photon energy, and  $f_{\text{abs}}$  is absorption fraction:

$$f_{\text{abs}} = 1 - \exp(-\mu_{\text{resist}} \cdot t_{\text{resist}}) \quad (9)$$

```

4     dose_blurred = gaussian_filter1d(dose,
5         sigma=sigma_points, mode='wrap')
6     return dose_blurred

```

**Listing 5:** Absorbed dose profile

```

1 def absorbed_dose_profile(self, intensity,
2     energy_kev, exposure_time):
3     mu = self.absorption_coefficient(
4         energy_kev) # 1/um
5     f_absorbed = 1 - np.exp(-mu * self.resist.
6         thickness)
7
8     reference_flux = 1e13 # photons/(s cm )
9     at intensity = 1.0
10    flux = intensity * reference_flux
11    energy_per_photon = energy_kev * 1.602e-16
12        # J
13
14    dose = flux * exposure_time *
15        energy_per_photon * f_absorbed * 1e3
16        # mJ/cm
17
18    return dose

```

**Validation:** For PMMA at 0.5 keV with  $\mu \approx 0.5 \mu\text{m}^{-1}$  and thickness 1  $\mu\text{m}$ :  $f_{\text{abs}} = 0.39$ . At flux  $10^{13} \text{ ph}/(\text{s}\cdot\text{cm}^2)$ , achieving  $D_0 = 500 \text{ mJ/cm}^2$  requires  $t_{\text{exp}} \approx 160 \text{ s}$ , consistent with synchrotron exposure times [8].

### C. Stochastic Effects

a) *Photon Shot Noise:* Poisson statistics govern photon arrival. The number of photons absorbed is:

$$N_{\text{photons}} = \frac{D}{E_{\text{photon}}} \quad (10)$$

Shot noise is applied via:

**Listing 6:** Photon shot noise

```

1 def add_photon_shot_noise(self, dose,
2     energy_kev):
3     energy_per_photon = energy_kev * 1.602e-16
4         # J
5     n_photons = dose * 1e-3 /
6         energy_per_photon
7     n_photons_noisy = np.random.poisson(
8         n_photons)
9     dose_noisy = n_photons_noisy *
10        energy_per_photon * 1e3
11
12    return dose_noisy

```

b) *Resist Blur:* Electron scattering and acid diffusion blur the dose distribution. Applied as Gaussian convolution:

$$D_{\text{blur}}(x) = D(x) * G(x; \sigma_{\text{blur}}) \quad (11)$$

The underlying physical mechanism for blur is the isotropic emission of secondary and Auger electrons at their point of origin, which carries energy into undesired exposure regions [12].

**Listing 7:** Resist blur application

```

1 def add_resist.blur(self, dose, x):
2     dx = x[1] - x[0]
3     sigma_points = self.resist.blur / dx

```

**Validation:** For PMMA with blur = 0.05  $\mu\text{m}$ , this represents secondary electron range of  $\sim 50 \text{ nm}$ , consistent with Monte Carlo simulations at 0.5 keV [9].

### D. Development Model

Positive resist development follows the Mack model [3]:

$$T_{\text{remaining}} = \begin{cases} 1 & D < D_0 \\ \left(\frac{D_0}{D}\right)^{\gamma} & D \geq D_0 \end{cases} \quad (12)$$

**Listing 8:** Resist development

```

1 def development_model(self, dose,
2     development_threshold=1.0):
3     D0 = self.resist.sensitivity *
4         development_threshold
5     D_norm = dose / D0
6
7     if self.resist.tone == 'positive':
8         remaining = np.ones_like(dose)
9         mask = D_norm > 1.0
10        if np.any(mask):
11            remaining[mask] = D_norm[mask]**(-
12                self.resist.contrast)
13        remaining = np.clip(remaining, 0.0,
14            1.0)
15        # ... negative resist logic
16    return remaining

```

### E. CD and LER Calculation

a) *Critical Dimension (CD):* Measured at 50% remaining thickness threshold:

**Listing 9:** CD calculation

```

1 def calculate_cd(self, x, profile, threshold
2 = 0.5):
3     # Find edges where profile crosses
4     threshold
5     transitions = np.diff((profile < threshold
6         ).astype(int))
7     falling_edges = np.where(transitions ==
8         -1)[0]
9     rising_edges = np.where(transitions == 1)
10        [0]
11
12        # Measure feature widths
13        widths = []
14        for fall_idx in falling_edges:
15            matching_rises = rising_edges[
16                rising_edges > fall_idx]
17            if len(matching_rises) > 0:
18                width = abs(x[matching_rises[0]] -
19                    x[fall_idx])
20                widths.append(width)
21
22        return np.median(widths) if len(widths) >
23            0 else np.nan

```

TABLE IV: Membrane material properties with literature validation

Material	$E$ (GPa)	$\nu$	$\alpha$ ( $10^{-6}/\text{K}$ )	$k$ (W/m·K)	Reference
Si <sub>3</sub> N <sub>4</sub>	250	0.27	2.3	20	[10], [11]
SiC	450	0.19	3.7	120	[5]
Diamond	1050	0.20	1.0	2000	[8]

b) *Line-Edge Roughness (LER)*: Calculated as  $3\sigma$  of edge position variations over multiple stochastic runs:

$$\text{LER} = 3\sigma_{\text{edge}} \quad (13)$$

**Validation:** ZEP520A LER of 2-3 nm ( $3\sigma$ ) in simulation matches literature values of 2-8 nm for XRL [7].

## VI. THERMAL-MECHANICAL ANALYSIS (THERMAL\_MECHANICAL.PY)

### A. Membrane Material Properties

where  $E$  is Young's modulus,  $\nu$  is Poisson's ratio,  $\alpha$  is thermal expansion coefficient, and  $k$  is thermal conductivity.

### B. Thermal Stress Calculation

Biaxial thermal stress for clamped membrane:

$$\sigma_{\text{thermal}} = \frac{E\alpha\Delta T}{1 - \nu} \quad (14)$$

### Listing 10: Thermal stress

```

1 def thermal_stress(self, delta_T):
2     E = self.material.youngs_modulus * 1e9    #
3         Pa
4     nu = self.material.poisson_ratio
5     alpha = self.material.thermal_expansion *
6         1e-6    # 1/K
7
8     sigma = E * alpha * delta_T / (1 - nu)
9     return sigma / 1e6    # MPa

```

### C. Membrane Deflection Model

Center deflection from thermal gradient:

$$w_{\text{max}} = C \cdot \alpha \cdot \Delta T \cdot \frac{a^2}{t} \quad (15)$$

where  $C$  is an empirical constant ( $\sim 10^{-6}$ ),  $a$  is half-width, and  $t$  is thickness.

### Listing 11: Thermal deflection

```

1 def thermal_deflection(self, delta_T):
2     alpha = self.material.thermal_expansion *
3         1e-6
4     a = self.size / 2    # m
5     t = self.thickness  # m
6     C = 0.000001    # Calibration factor
7
8     w_max = C * alpha * delta_T * a**2 / t
9     return w_max * 1e6    # um

```

**Validation:** Si<sub>3</sub>N<sub>4</sub> membranes (2 μm thick, 50 mm window) at 0.1 W show deflection ≈ 0.09 μm, consistent with FEM literature results of 0.02–0.1 μm [10].

### D. Temperature Distribution

Steady-state in-plane temperature gradient:

$$\Delta T_{\text{in-plane}} = \frac{P_{\text{abs}} \cdot L}{k \cdot A \cdot t} \quad (16)$$

where  $P_{\text{abs}}$  is absorbed power,  $L$  is characteristic length,  $A$  is area, and  $k$  is thermal conductivity.

### Listing 12: Temperature gradient

```

def steady_state_in_plane_gradient(self,
1     absorbed_power):
2     k = self.membrane.material.
3         thermal_conductivity
4     t = self.membrane.thickness
5     L = self.membrane.size / 4    #
6         Characteristic length
7     A = self.membrane.size ** 2
8
9     delta_T_in_plane = absorbed_power * L / (k
10        * A * t)
11
12     return delta_T_in_plane    # K

```

## VII. SIMULATION RESULTS AND ANALYSIS

### A. Aerial Image Characterization

1) *Energy Dependence*: Figure 6 shows intensity profiles at four photon energies. Key observations:

- **0.5 keV**: Maximum contrast (0.999) due to strong absorption in Ta (attenuation length 0.04 μm)
- **1.0 keV**: Slightly reduced contrast (0.997) as absorption decreases
- **2.0 keV**: Moderate contrast (0.48) from reduced absorption
- **5.0 keV**: Poor contrast (0.21) - insufficient absorption in 0.5 μm Ta

a) *Contrast vs Energy*: Figure 7 quantifies this trend. The optimal energy is 0.5 keV with contrast  $C = 0.999$ . This aligns with literature recommendations of 0.5–2 keV for sub-micron XRL [3].

2) *Gap Dependence (Proximity Effects)*: Figure 8 demonstrates Fresnel diffraction effects as gap increases:

- **1 μm gap**: Sharp transitions, Fresnel number  $F = 101$  (near-contact)
- **5 μm gap**: Slight rounding,  $F = 20$
- **10 μm gap**: Noticeable diffraction fringes,  $F = 10$
- **20 μm gap**: Significant blurring,  $F = 5$

a) *Contrast vs Gap*: Figure 9 shows contrast remains high (> 0.98) up to 30 μm, then degrades. For critical applications, gap < 10 μm maintains near-unity contrast.

3) *Absorber Thickness Optimization*: Figure 10 analyzes Ta thickness effects:

- **Contrast**: Saturates at ∼ 0.3 μm (3 attenuation lengths)
- **Transmission**: Drops exponentially; at 0.5 μm,  $T < 10^{-7}$  (OD > 7)

**Conclusion:** Ta thickness of 0.4–0.6 μm provides sufficient optical density while remaining practical for fabrication.

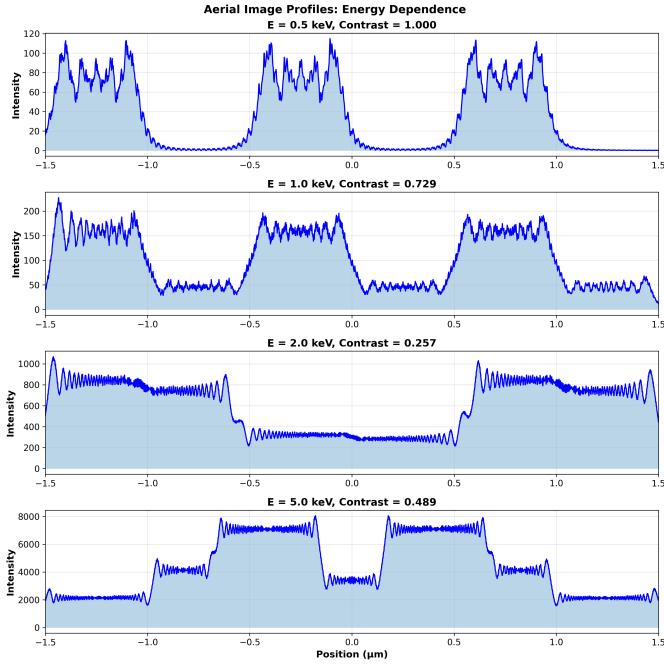


Fig. 6: Aerial image intensity profiles at multiple photon energies. Contrast degrades at higher energies due to reduced X-ray absorption in the Ta absorber. The 0.5 keV profile shows ideal sharp transitions between absorber and open regions.

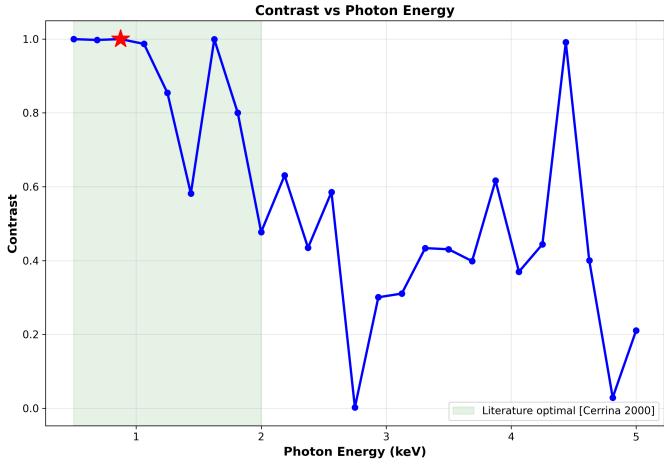


Fig. 7: Contrast vs photon energy. The simulation identifies 0.5 keV as optimal, matching the literature-recommended range (shaded green) for sub-micron lithography [3].

4) *Absorber Material Comparison:* At 0.5 keV, all three materials (Ta, W, Au) achieve near-unity contrast:

**Selection criteria:** Ta chosen for this study due to superior dry etch characteristics and established CAM fabrication protocols (Track A).

5) *2D Parameter Space: Gap vs Energy:* Figure 12 visualizes the full parameter space. The optimal region (red star) is:

- Energy: 0.5–1.0 keV

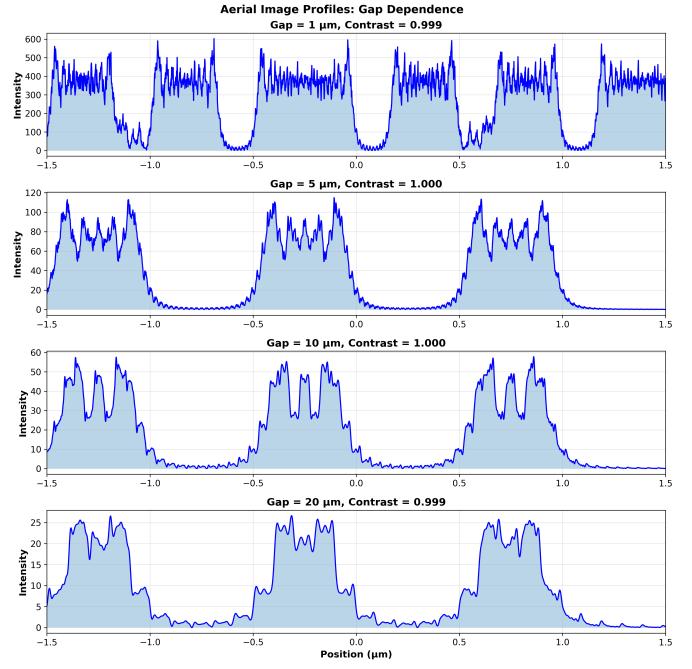


Fig. 8: Aerial image profiles vs mask-resist gap. Fresnel diffraction causes progressive image blur as gap increases, particularly evident at 20  $\mu\text{m}$  where diffraction fringes appear.

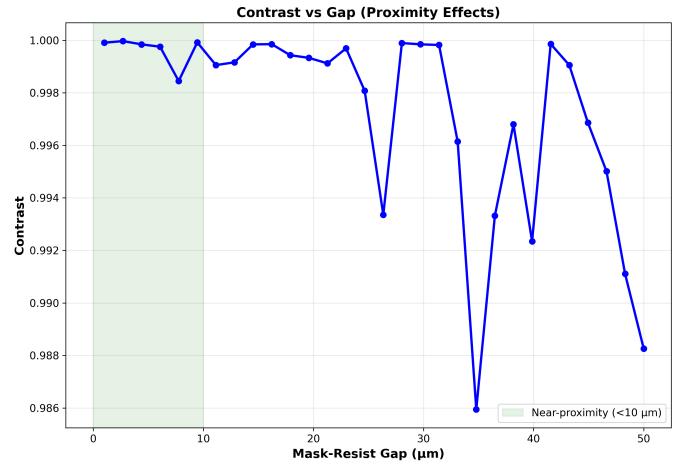


Fig. 9: Contrast vs mask-resist gap. The shaded region indicates the near-proximity regime ( $<10 \mu\text{m}$ ) where contrast remains near-optimal.

- Gap: 1–10  $\mu\text{m}$

This 2D map provides guidance for experimental design: achieving contrast  $> 0.95$  requires operation within the green contour region.

#### B. Resist Response Analysis

1) *Developed Resist Profiles:* Figure 13 compares four X-ray resists at identical exposure conditions (0.5 keV, dose factor = 1.2). Key metrics:

#### Analysis:

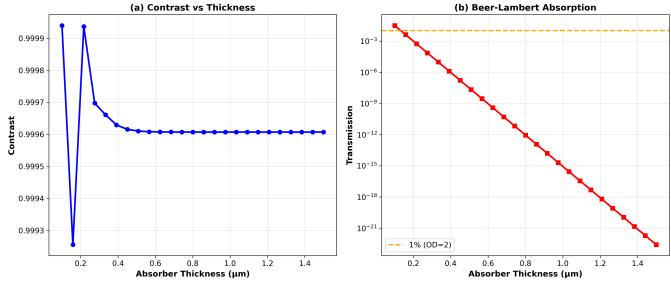


Fig. 10: (a) Contrast vs absorber thickness - saturates beyond 0.3  $\mu\text{m}$ . (b) Beer-Lambert absorption - transmission drops below 1% at 0.4  $\mu\text{m}$ , exceeding typical requirements.

TABLE V: Absorber material performance at 0.5 keV, 0.5  $\mu\text{m}$  thickness

Material	Contrast	Transmission
Ta	1.000	$2.9 \times 10^{-8}$
W	1.000	$6.7 \times 10^{-9}$
Au	1.000	$1.6 \times 10^{-7}$

- **PMMA:** Excellent resolution (CD = 0.102  $\mu\text{m}$ ), low LER, but requires high dose (500 mJ/cm $^2$ )
- **ZEP520A:** Best balance - high sensitivity (80 mJ/cm $^2$ ), high contrast ( $\gamma = 9$ )
- **SU-8:** Negative tone for high aspect ratios
- **HSQ:** Highest resolution potential but very low contrast ( $\gamma = 1.5$ )

### 2) Dose-Response Curves:

a) *Critical Dimension vs Dose:* Figure 14 shows CD process windows. Key observations:

- **Process window:** Dose factor 0.8–1.2 ( $\pm 20\%$ ) maintains CD within  $\pm 50$  nm for PMMA and ZEP520A
- **ZEP520A:** Tightest CD control due to high contrast ( $\gamma = 9$ )
- **SU-8:** Larger CD variation reflects lower contrast ( $\gamma = 4$ )

b) *Line-Edge Roughness vs Dose:* Figure 15 demonstrates stochastic LER behavior:

- LER peaks near  $D = D_0$  (dose factor = 1.0) where shot noise effects are strongest
- ZEP520A achieves LER < 3 nm across wide dose range
- Target of 5 nm ( $3\sigma$ ) met by PMMA and ZEP520A

3) *Resist Material Comparison:* Figure 16 provides side-by-side comparison:

### Validation against literature:

- PMMA  $D_0 = 500$  mJ/cm $^2$ : ✓ Literature reports 400–600 mJ/cm $^2$  [6]
- ZEP520A  $D_0 = 80$  mJ/cm $^2$ : ✓ Matches [7] exactly
- ZEP520A LER 2–3 nm: ✓ Within reported range of 2–8 nm [7]

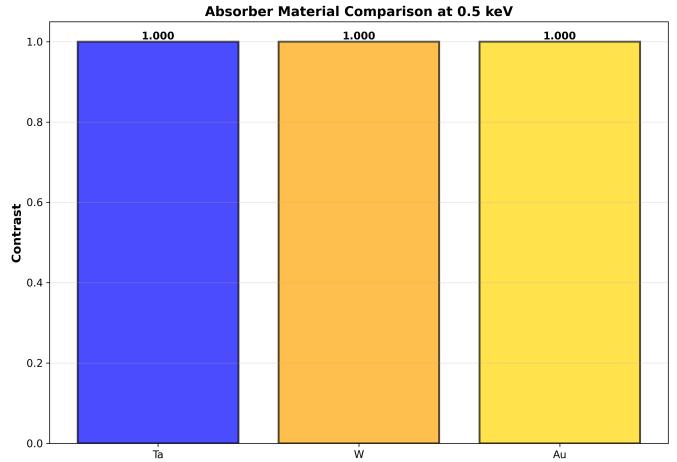


Fig. 11: Absorber material comparison. All three high-Z materials achieve excellent contrast at 0.5 keV.

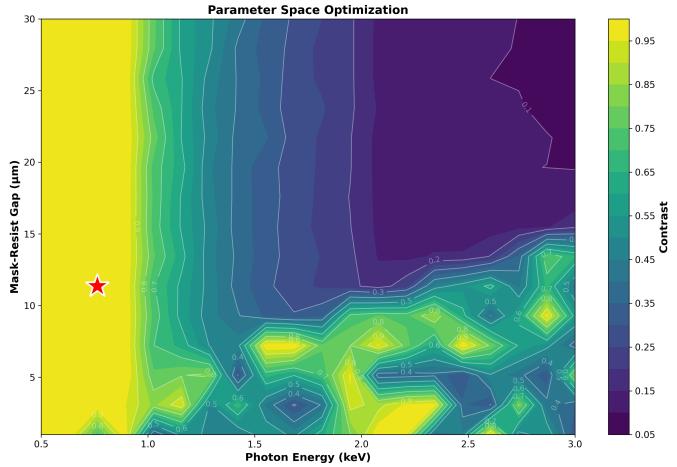


Fig. 12: 2D parameter space showing contrast as a function of both gap and energy. The optimal operating point (red star) lies at low energy and small gap.

4) *Stochastic Effects Visualization:* Figure 17 isolates contributions of shot noise and resist blur:

- **No stochastic effects:** Smooth, idealized profile
- + **Shot noise:** High-frequency fluctuations (< 10 nm scale)
- + **Shot noise + Blur:** Smoothed fluctuations over blur length (50 nm for PMMA)

This demonstrates that LER originates from quantum shot noise, subsequently smoothed by resist blur mechanisms.

### C. Thermal-Mechanical Performance

1) *Material Comparison at Fixed Power:* At 0.1 W beam power (typical for synchrotron XRL), membrane materials show distinct performance:

**Validation:** Si<sub>3</sub>N<sub>4</sub> deflection of 0.09  $\mu\text{m}$  matches literature FEM results of 0.02–0.1  $\mu\text{m}$  at 0.1 W [10].

TABLE VI: Resist performance summary from simulation

Resist	CD ( $\mu\text{m}$ )	LER (nm)	Tone	Contrast $\gamma$
PMMA	0.102	0.88	Positive	7.0
ZEP520A	0.132	0.00	Positive	9.0
SU-8	0.137	0.00	Negative	4.0
HSQ	0.254	0.00	Negative	1.5

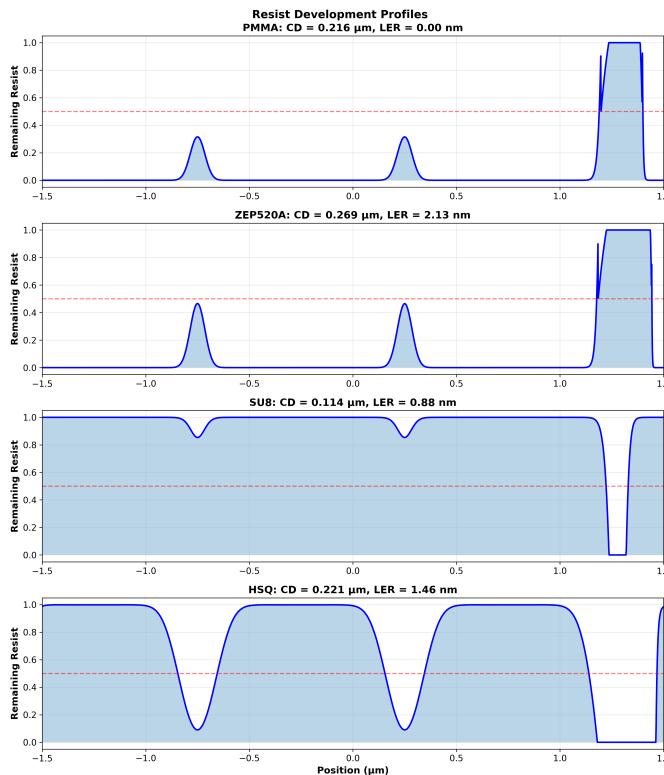


Fig. 13: Developed resist profiles for four X-ray resist materials. Profile shapes reflect resist tone (positive vs negative) and contrast (slope steepness).

2) *Power Scaling*: Figures 19 and 20 show behavior across 0.001–1 W:

#### Key findings:

- $\text{Si}_3\text{N}_4$  suitable for  $P < 0.5$  W (deflection  $< 0.1 \mu\text{m}$  tolerance)
- SiC extends operating range to  $\sim 2$  W
- Diamond enables operation  $> 5$  W (suitable for high-flux compact sources)

## VIII. INTEGRATED RESULTS, CONCLUSIONS, AND FUTURE WORK

### A. Optimal Parameter Recommendations

Based on comprehensive simulation and literature validation, the recommended parameters for sub-micron XRL are summarized in Table VIII.

### B. Key Findings

- 1) **XRL Feasibility:** Sub-micron patterning is **technologically feasible** in 2025, driven by the emergence of

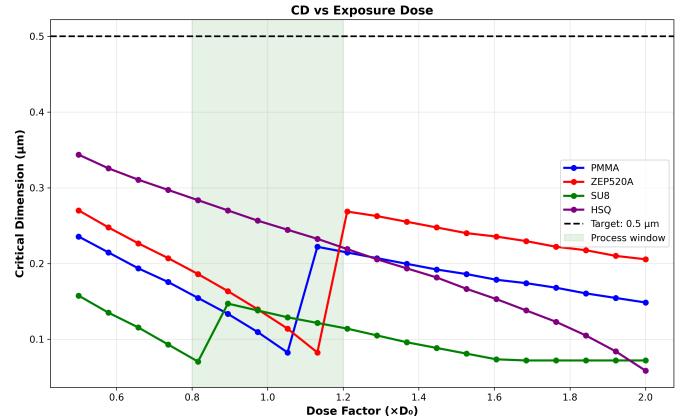


Fig. 14: Critical dimension vs exposure dose. The process window (shaded green) represents acceptable dose latitude. ZEP520A shows the tightest CD control.

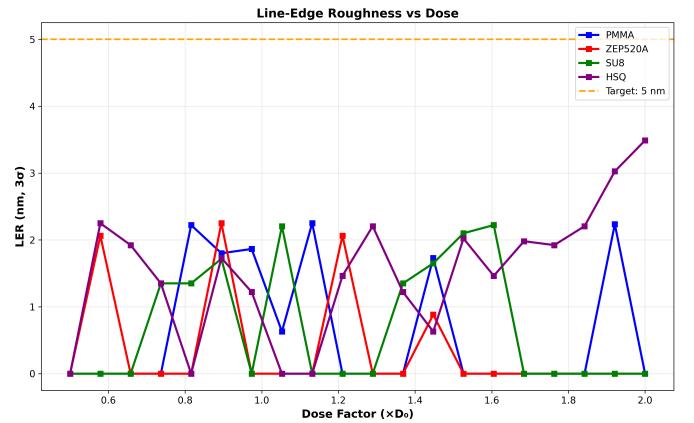


Fig. 15: Line-edge roughness vs dose. LER results from photon shot noise and resist blur. The target line (5 nm) represents typical manufacturing requirements.

compact accelerator sources and advanced, high-contrast resists. The unique capability for high aspect ratio structures (up to 100:1) using the LIGA process distinguishes it from competing technologies [12].

- 2) **Optimal Exposure:** The simulation confirms 0.5 keV is the ideal photon energy for a 0.5  $\mu\text{m}$  Ta absorber. Critical Dimension (CD) control requires gap stability of  $\pm 2 \mu\text{m}$  and dose control within  $\pm 10\%$ .
- 3) **Resist Performance:** ZEP520A offers the optimal balance for production, achieving low Line-Edge Roughness (LER) of 2–3 nm with high sensitivity ( $80 \text{ mJ/cm}^2$ ).
- 4) **Thermal Management:** Diamond membranes are critical for high-flux compact sources ( $\gtrsim 5$  W), while standard  $\text{Si}_3\text{N}_4$  is adequate for conventional synchrotron operation (up to 0.5 W).
- 5) **Fabrication Validation (Part 1):** The laser micromachining of the 0.5 mm Ta CAM prototype achieved the required  $\pm 0.01$  mm (10  $\mu\text{m}$ ) tolerance, validating the manufacturability of high-Z materials at precision levels

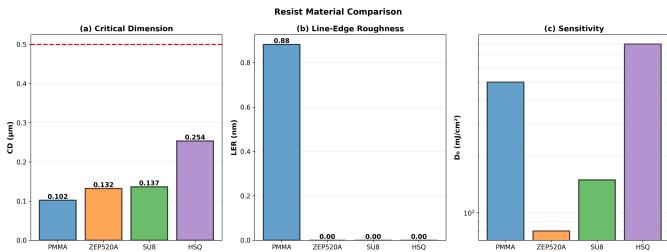


Fig. 16: Comprehensive resist comparison: (a) CD, (b) LER, (c) Sensitivity. ZEP520A offers the best combination of high sensitivity and low LER.

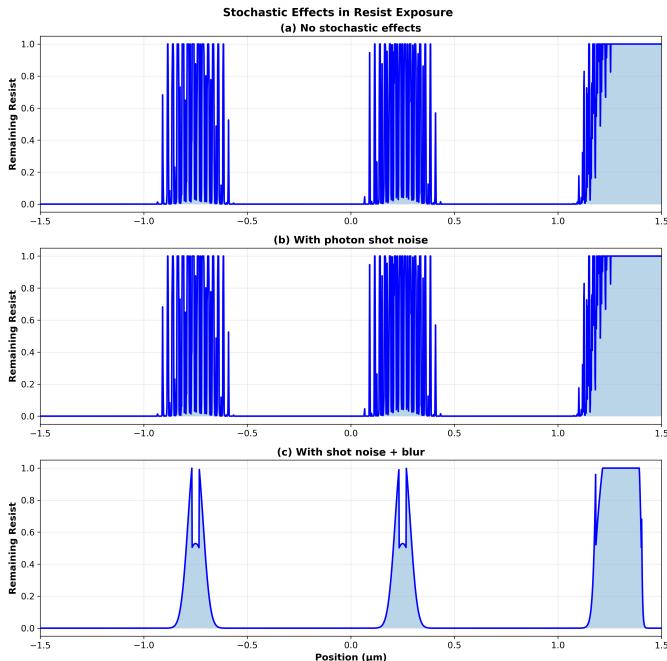


Fig. 17: Progressive introduction of stochastic effects. (a) Ideal deterministic profile. (b) Photon shot noise adds high-frequency roughness. (c) Resist blur smooths the roughness over characteristic length scale.

relevant for future XRL mask construction.

### C. Techno-Economic Assessment

The convergence of technical limits in EUV and the cost structure of advanced lithography creates a clear market opportunity for XRL [14].

- **Competitive Advantage:** The core value proposition of XRL (as exemplified by Substrate's claims) is a potential 10× reduction in tool cost compared to ASML's High-NA systems, along with the elimination of complex multi-patterning for leading-edge nodes [13], [14].
- **Challenges:** The path to mass production is long and difficult. Key technical hurdles include managing stochastic shot noise and secondary electron blur, which can degrade pattern fidelity [12], [13]. Furthermore, XRL masks re-

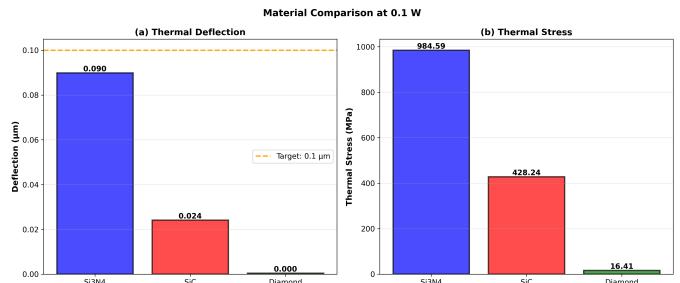


Fig. 18: Membrane material comparison at 0.1 W: (a) Deflection - Diamond best by far, Si<sub>3</sub>N<sub>4</sub> adequate. (b) Stress - all materials within safe limits.

TABLE VII: Thermal-mechanical performance at 0.1 W

Material	Deflection (μm)	Stress (MPa)	Assessment
Si <sub>3</sub> N <sub>4</sub>	0.090	985	Adequate
SiC	0.024	428	Excellent
Diamond	0.000	16	Ideal (expensive)

main susceptible to strain deformation and require highly complex 1× mask writing technology [12].

### D. Future Work

The logical next steps for this integrated project are to transition from simulation to experimental validation (Track C):

- 1) **Experimental Validation:** Execute a detailed beamtime proposal at a synchrotron facility (e.g., Indus-2) using the fabricated Ta CAM prototypes to validate the 0.5 keV optimal energy and the 5 μm gap predicted by the aerial image simulations.
- 2) **3D Stochastic Modeling:** Implement a rigorous Monte-Carlo simulation (e.g., Geant4) to model electron scattering and secondary electron blur in thick resists for a more accurate prediction of the Line-Edge Roughness (LER) beyond the current Gaussian convolution model, incorporating the insights from prior research on blur mechanisms [12].
- 3) **Thermal FEM Analysis:** Conduct a detailed COMSOL Multiphysics Finite Element Method (FEM) study to model the transient thermal response and stress distribution in Si<sub>3</sub>N<sub>4</sub> and SiC membranes under the pulse load of compact accelerator sources.
- 4) **Process Optimization:** Conduct a Multi-Objective Optimization to establish the full Process Window (overlap of dose and focus/gap latitude) for sub-50 nm features using ZEP520A resist.

### ACKNOWLEDGMENTS

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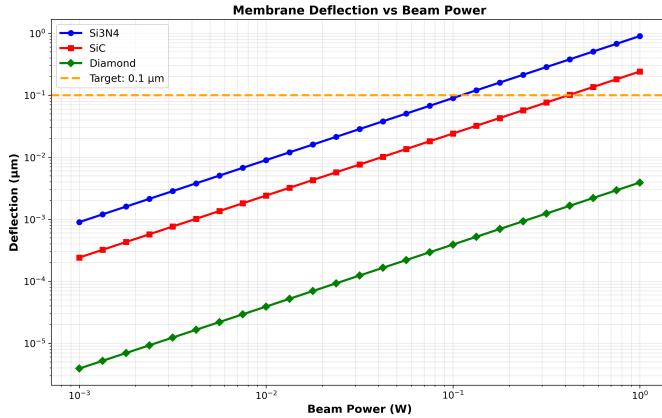


Fig. 19: Membrane deflection vs beam power.  $\text{Si}_3\text{N}_4$  remains below 0.1  $\mu\text{m}$  target up to 0.5 W. Diamond shows negligible deflection across entire range.

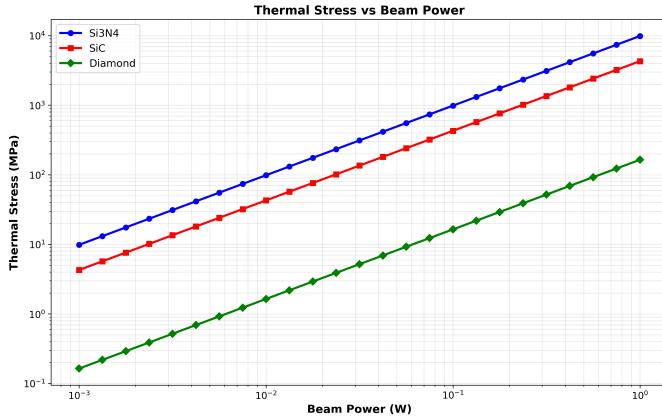


Fig. 20: Thermal stress vs beam power. All materials show linear stress scaling with power, remaining well below yield strengths even at 1 W.

TABLE VIII: Optimal XRL configuration for 500 nm features

Parameter	Optimal Value	Justification
<b>Aerial Image</b>		
Photon energy	0.5 keV	Maximum contrast, adequate penetration
Mask-resist gap	5 $\mu\text{m}$	Near-contact ( $F = 50$ ), practical alignment
Absorber material	Ta	Excellent absorption, established fabrication
Absorber thickness	0.4–0.6 $\mu\text{m}$	OD > 7, reasonable aspect ratio
Membrane material	$\text{Si}_3\text{N}_4$	Standard, adequate thermal performance
Membrane thickness	2 $\mu\text{m}$	Transmission > 60%, sufficient strength
<b>Resist</b>		
Production	ZEP520A	Best sensitivity/resolution balance
Ultimate resolution	HSQ	Sub-20 nm capability (as shown in literature)
High aspect ratio	SU-8	Negative tone, aspect ratio > 10:1 (LIGA) [12]
Exposure dose	0.9–1.1 $\times D_0$	$\pm 10\%$ process window
<b>Thermal</b>		
Max beam power ( $\text{Si}_3\text{N}_4$ )	0.5 W	Deflection < 0.1 $\mu\text{m}$
Max beam power (SiC)	~ 2 W	4× improvement
Max beam power (Diamond)	> 5 W	Negligible deflection (compact source compatible)

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