

Monolithic lithium niobate bimorph X-ray mirrors: design, modeling, and experimental validation

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ABSTRACT

Recent studies have introduced monolithic piezoelectric mirrors made of lithium niobate for X-ray beam control. We present prototypes of monolithic bimorph mirrors constructed from a single wafer of lithium niobate featuring symmetric, longitudinally continuous, shaped electrodes designed to modulate local curvature upon voltage application. This paper details their design, fabrication, and testing. Experimental results demonstrate a highly deterministic and linear central curvature response to the applied voltage ($R^2 \geq 0.9988$, $p < 0.05$), yielding actuation sensitivities of $1.1 \times 10^{-5} \text{ m}^{-1}/\text{V}$ and $1.3 \times 10^{-5} \text{ m}^{-1}/\text{V}$ for third- and fourth-order target profiles, respectively. Furthermore, we highlight critical fabrication challenges regarding domain inversion depth control and process-induced wafer deformation, providing key insights for future monolithic adaptive optics designs.

Keywords: adaptive X-ray optics, X-ray optics, mirrors, monolithic bimorph mirror, lithium niobate

1. INTRODUCTION

Adaptive X-ray optics have been utilized in synchrotron beamlines for more than three decades to optimize beam delivery.¹ By dynamically modulating the mirror surface profile, these systems shape wavefronts, correct aberrations, and enable on-demand tuning of focal distances. Modern adaptive optics elements typically achieve shape control by bonding or depositing a discrete array of lead zirconate titanate (PZT) piezoelectric actuators to the surface² or sides³ of an underlying silicon substrate. Applying a voltage alters the length of these actuators, enabling direct regulation of the local curvature. However, this multi-material architecture introduces significant fabrication complexities, thermal instabilities, and possibly, outgassing phenomena. When used for shape control, PZT materials show time-dependent creep and hysteresis that complicate fine actuation.⁴

To address these limitations, lithium niobate (LN, LiNbO_3) offers a compelling monolithic alternative. LN is a synthetic piezoelectric crystal characterized by intrinsic, natural polarization.⁵ Thermal treatment of LN near its Curie temperature can induce the formation of two domains with antiparallel polarization orientations.⁶ Consequently, the piezoelectric coefficients in these two layers become equal in magnitude but opposite in sign. When a voltage is applied across this treated substrate, one domain layer expands while the other contracts,

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inducing controlled, out-of-plane bending from a single material. By coating this domain-engineered LN substrate with thin metallic films that can serve simultaneously as electrodes and reflective surfaces, the substrate functions concurrently as both the active actuator and the optical mirror.^{7,8} The resulting monolithic system exhibits a linear actuation response that is notably free of hysteresis and creep,^{9,10} with the primary trade-off being a lower magnitude of mechanical actuation per unit voltage applied, compared to alternatives based on PZT.

In this study, we present the design and experimental characterization of two prototype monolithic bimorph mirrors fabricated from a single LN wafer. These mirrors feature symmetric, continuous, longitudinally shaped electrodes that we have recently proposed to modulate local curvature upon voltage application.¹¹ The two mirrors are designed to induce third- and fourth-order polynomial surface shape changes, respectively. This approach provides an alternative to conventional shape control based on segmented electrode arrays, inherited from multi-material PZT architectures.

2. DESIGN

The design process of a monolithic piezoelectric bimorph starts with the selection of its substrate properties. According to the linear theory of piezoelectricity, we can describe the response of the LN using the elastic stiffness, relative permittivity, and piezoelectric strain coefficient matrices.¹² Since the material is anisotropic, these properties depend on the rotation angle of the crystal cut.⁵ Thus, we can tailor the piezoelectric response of the mirror by selecting the orientation of the crystal axes relative to the substrate geometry. (A mathematical treatment of the LN crystal orientation and surface shape response was presented by the authors in Ref. 13.)

We model the substrate as a Kirchhoff plate¹⁴ without external loads applied. We assume that the polarization is inverted in half of the thickness, and that the voltage is applied to uniform, thin-film electrodes on the top and bottom surfaces of the substrate. The mirror curvature along the physical dimension j in the mirror plane, κ_j , can be written as¹³

$$\kappa_j = \frac{3Ud_{ij}}{h^2}, \quad (1)$$

where U is the applied voltage, h is the substrate thickness, and d_{ij} is the relevant piezoelectric strain coefficient in Voigt notation. Therefore, from the complete matrix of piezoelectric strain coefficients, we can focus only on the values along the tangential and sagittal directions of the mirror. The resulting actuated shape depends on the signs of these two strain coefficients and the applied voltage. Identical signs yield a local ellipsoid deformation, opposing signs yield a hyperbolic paraboloid (i.e. saddle shape), and a single zero coefficient yields a tangential or sagittal cylinder.

We focus on the cylindrical case and orient the crystal to have deflection only along the tangential direction of the mirror: a 74.3° rotated Y-cut of LN satisfies this condition. Taking advantage of the reduced dimensionality of the problem, we employ a Euler-Bernoulli beam model and incorporate continuous symmetrical electrodes that extend tangentially, on the top and bottom surfaces of the substrate, with a variable sagittal width, ruled by the parameter $\beta \in (0, 1]$. Designing β with longitudinal variation along the mirror enables customized control of the actuated deformation profile, scaled by the applied voltage. We assume that the substrate has two homogeneous polarization layers with thicknesses a_1 and a_2 , respectively, ($h = a_1 + a_2$). We treat the electric field as uniform between the top and bottom electrodes, oriented perpendicular to the surface, and null elsewhere. The tangential curvature, derived in,¹¹ is

$$\kappa_j = \frac{12Ud_{ij}\beta a_1 a_2}{h^4}. \quad (2)$$

Eq. 1 can be consistently recovered from Eq. 2 by substituting $\beta = 1$ and $a_1 = a_2 = h/2$. The tangential curvature of a target mirror profile $z(x)$ along the spatial coordinate x can be approximated by its second derivative, $z''(x)$, since the profile slope is typically close to zero for X-ray mirrors. The $\beta(x)$ required to obtain the target mirror profile is computed from Eq. 2:

$$\beta(x) = \frac{h^4}{12Ud_{ij}a_1a_2}|z''(x)|. \quad (3)$$

We apply this approach to realize third- and fourth-order polynomial mirror profiles, which implies designing first- and second-order electrode shapes, respectively (Fig. 1). The mirrors have half-width w , whereas the sagittal half-width of the electrodes ranges from w_1 to w_2 . For the first-order polynomial shape w_1 is null, while for the parabolic electrode w_1 is designed to be wider than the X-ray beam width, ensuring electrical continuity and preserving a uniform optical reflective surface. l is half of the total electrode length, which determines the clear aperture of the mirror. The electrode configurations depicted in Fig. 1 are symmetrically applied on the two opposing surfaces of the mirrors.

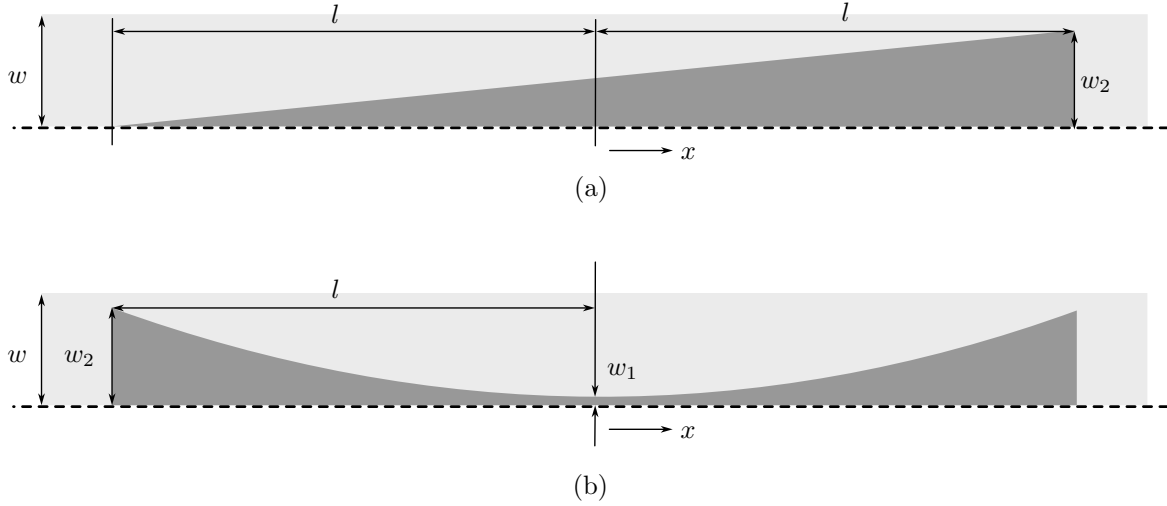


Figure 1: Top views, model of half of the monolithic bimorph mirrors with first- and second-order polynomial electrode shapes, (a) and (b), respectively. The electrode regions are shaded in darker gray. The coordinate origin $x = 0$ is at the mirror center, with $x \in [-l, l]$.

The corresponding fractional electrode widths, β_a for the first-order and β_b for the second-order, are

$$\beta_a = \frac{w_2}{2lw}(x+l), \quad (4)$$

$$\beta_b = \frac{1}{w} \left(w_1 + (w_2 - w_1) \left(\frac{x}{l} \right)^2 \right). \quad (5)$$

The analytical target profiles along the tangential direction are obtained by integrating Eq. 2 twice after substituting β_a , β_b , $a_1 = a_2 = h/2$ and imposing zero central slope and height:

$$z_a(x) = \frac{Ud_{ij}w_2}{4h^2w} \left(\frac{x^3}{l} + 3x^2 \right), \quad (6)$$

$$z_b(x) = \frac{Ud_{ij}}{2h^2w} \left(\frac{w_2 - w_1}{2l^2} x^4 + 3w_1 x^2 \right). \quad (7)$$

3. MODELING

For each case study, we developed a structural-electric coupled-field static finite element model (FEM) in ANSYS using SOLID227 elements to validate the analytical results. The substrate was modeled without external structural constraints as a composite geometry consisting of two distinct layers: a top domain-inverted layer and a pristine base polarization layer. We implemented the elastic stiffness, relative permittivity, and piezoelectric strain coefficients for the 74.3° rotated Y-cut following the procedure reported in Ref. 13. d_{ij} is $d_{21} = -6.6453 \text{ pm/V}$. The electrodes were modeled as ideal interfaces to apply the boundary conditions: the top electrode was biased with 100 V while the bottom one was grounded. We considered a substrate that is 80 mm long, 16 mm wide and 0.5 mm thick, matching the experimental demonstration, below. The numerical values of the design parameters appearing in Eqs. 4 and 5 are collected in Table 1.

Table 1: Numerical values for the design parameters of the polynomial-shaped electrodes.

	w	w_1	w_2	l
1 st -order (a)	8 mm	0 mm	7 mm	35 mm
2 nd -order (b)	8 mm	0.05 mm	7 mm	35 mm

A comparison between analytical and FEM results is shown in Fig. 2. For the first- and second-order polynomial electrode configurations featuring peak shape deformations of approximately $4 \mu\text{m}$ and $1 \mu\text{m}$, the analytical and numerical profiles agree to within root-mean-square errors (RMSEs) of 44 nm and 12 nm, respectively, evaluated across the electrode region.

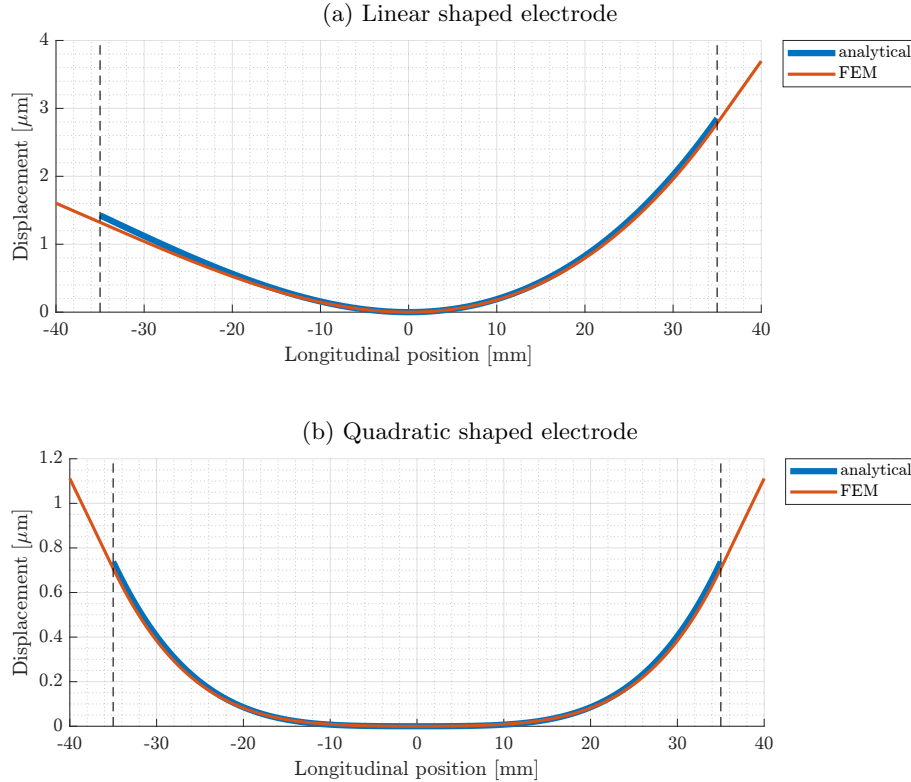


Figure 2: Mirror target displacements along the central meridian computed analytically and with FEM for the first- and second-order polynomial electrodes, (a) and (b), respectively. Vertical dashed lines mark the boundaries of the clear aperture, containing the electrodes. The LN orientation is 74.3° rotated Y-cut. The applied voltage is 100 V.

While the 74.3° rotated Y-cut is optimal for our application, material with this orientation is non-standard and may be difficult to acquire. With finite element analysis (FEA), we investigated the difference that using a 128° rotated Y-cut would have on our experiments, as shown in Fig. 3. This orientation features the highest piezoelectric strain coefficient among commercially available substrates at the expense of piezoelectric coupling in the sagittal direction.

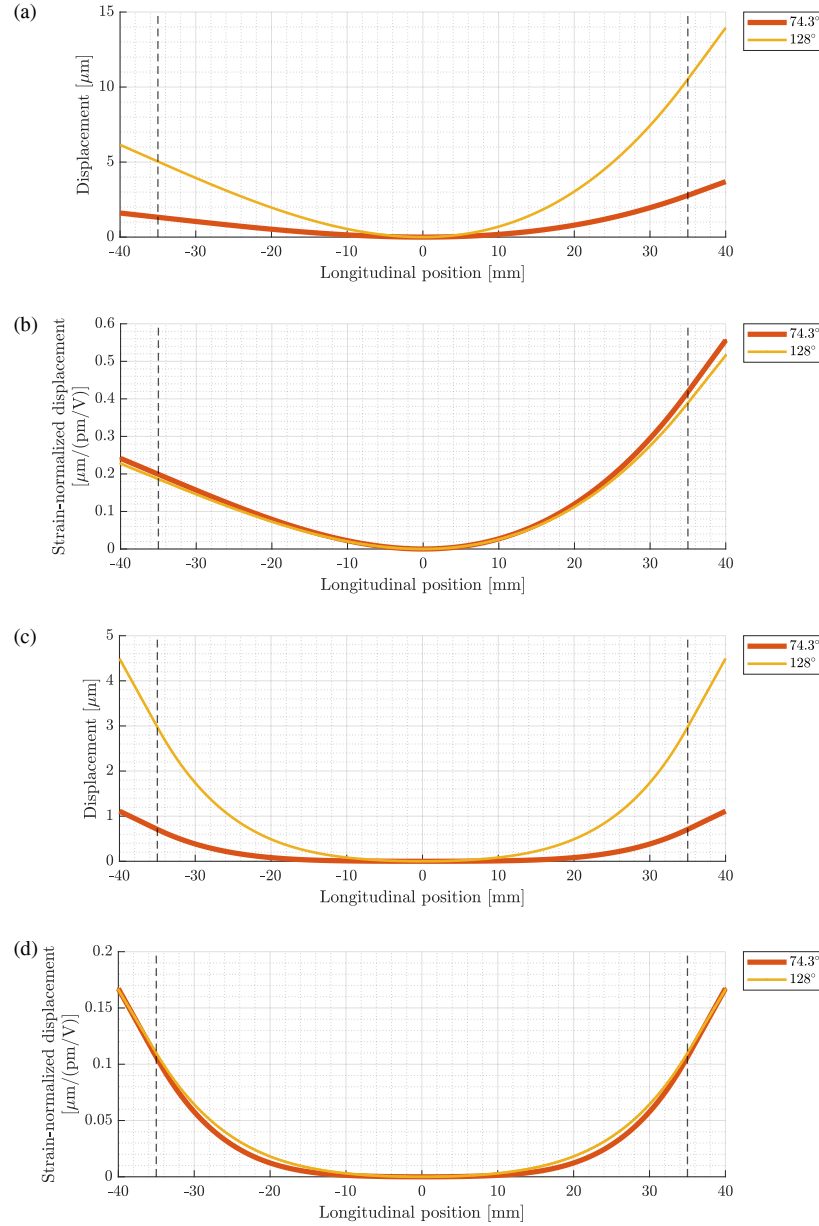


Figure 3: FEA comparison of central-meridian mirror displacements using 74.3° and 128° rotated Y-cuts of LN: (a, b) third-order and (c, d) fourth-order profiles showing absolute displacements under an applied voltage of 100 V. Plots (a) and (c) show absolute displacement; curves in (b) and (d) are normalized by the corresponding d_{ij} .

The maximum modeled displacement achieved with the 128° rotated Y-cut is four times higher than that obtained with the 74.3° rotated Y-cut (Figs. 3a and 3c), following the increased strength of d_{ij} , from -6.6453 pm/V

to -27.036 pm/V . By comparing the strain-normalized displacements in the two cases, we isolate the effect of the sagittal coupling on the target tangential profile (Figs. 3b and 3d). Although this coupling introduced a maximum relative deviation of 7% and 6.7% for the third- and fourth-order shape profiles, respectively, across the electrode region, these values were deemed acceptable for proof-of-concept prototypes.

4. FABRICATION

We started from a 100 mm diameter, 0.5 mm thick, LN wafer to fabricate the prototype mirrors described in Sec. 2. The wafer was heat treated in a Thermo Scientific Thermolyne FB1415M benchtop muffle furnace at 1100°C for 3 hours, with the lithium niobate wafer placed on an alumina ceramic sheet. The furnace was heated from room temperature (19°C) to the target temperature of 1100°C at a constant ramp rate of $5^\circ\text{C}/\text{min}$. The furnace was powered off and allowed to cool naturally to room temperature before the wafer was retrieved.

We fabricated the patterned electrodes using contact lithography and a lift-off process. First, we coated the wafer with photoresist and exposed it to deep UV light through a quartz photomask with chrome electrode patterns. After developing the exposed photosensitive polymer, a 50 nm chromium layer was deposited on both sides of the wafer by electron-beam physical vapor deposition (EB-PVD), with the thickness monitored using a quartz crystal microbalance. Finally, the sample was immersed in N-Methyl-2-pyrrolidone (NMP) to dissolve the remaining photoresist and lift off the excess metal, leaving the patterned electrodes.

The rectangular mirror substrates were cut from the LN wafer with a DISCO DAD3240 dicing saw. The wafer was mounted on a 0.120 mm thick adhesive dicing tape supported by a dedicated ring frame. A diamond blade operating at a spindle speed of 25000 RPM and a feed rate of 0.25 mm/s left a kerf 0.130 mm wide. Deionized cooling water was continuously supplied to the cutting zone to dissipate heat and remove debris. Following dicing, a die expander was used to mechanically separate the mirrors from the remaining wafer. The prototypes were then released from the adhesive tape by soaking in acetone. The manufactured mirrors are shown in Fig. 4.

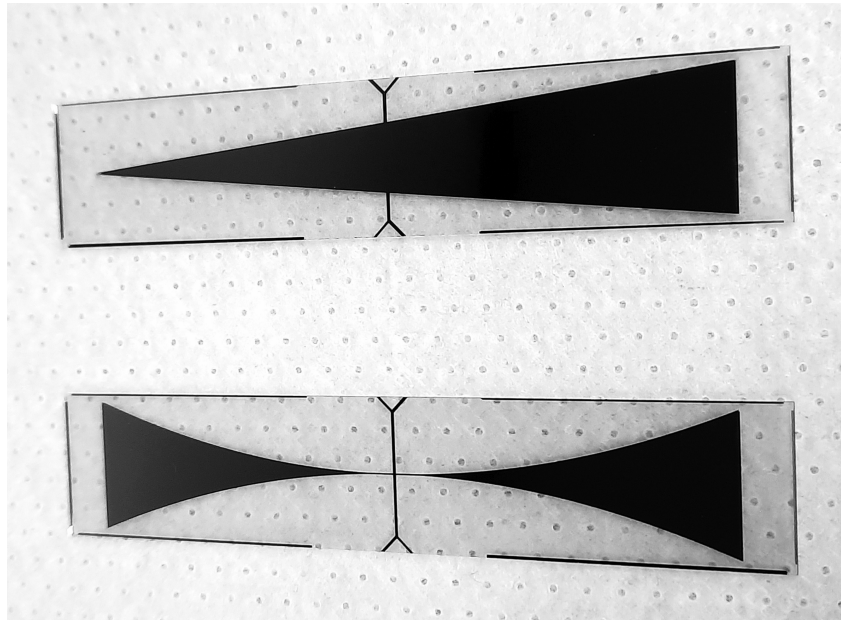


Figure 4: Photograph of the prototype mirrors with first-order (top) and second-order (bottom) polynomial-shaped chromium electrodes. The substrates are 80 mm long.

The electrode patterns include a 0.2 mm-wide wire spanning the width of the mirrors, as shown. Its central placement enabled the voltage to be applied by the clamped structural contacts of the mirror support, at the centered edge positions, affecting the target profile as little as possible in the tangential direction. No adhesives or bonding agents were used.

5. MEASUREMENT

During fabrication, we sought to measure the wafer shape before and after heat treatment. Surface measurements, using a Zygo DynaFiz Fizeau interferometer, were compromised by the thin, transparent substrate's reflections from the front and back surfaces. This necessitated an alternative metrology approach. Measurements were performed using a Zygo NewView 9000 3D optical profiler. However, the instrument's limited field of view required us to apply an automated stitching procedure, with 300 sub-images acquired over an 11-hour period.

Data recorded before and after heat treatment revealed substantial process-induced deformation. The peak-to-valley (PV) warp increased from an initial pre-treatment value of approximately $4\mu\text{m}$ to $180\mu\text{m}$, post-treatment. During measurements, the LN wafer was positioned horizontally on a three-sphere kinematic mount arranged in an isosceles triangle, with a 56.2 mm base aligned with the wafer's main flat and two 50.3 mm diagonal legs.

6. TESTING

The substrate warp, as characterized in Sec. 5, prevented a direct Fizeau interferometer measurement of the entire prototypes. A schematic drawing of the test setup is shown in Fig. 5. Consequently, the actuated profile along the central meridian was measured using a SmarAct PICOSCALE laser interferometer, with nanometer-level precision and a relative accuracy of 10^{-6} m/m. Two beam-focusing F01 sensor heads were mounted on a Newport ILS100PP linear stage moving tangentially at a speed of 1 mm/s, along the mirror's length. The stage provided a positioning accuracy of $\pm 2\mu\text{m}$ with unidirectional and bidirectional repeatability of $1\mu\text{m}$ and $\pm 1\mu\text{m}$, respectively. During scans, one sensor head targeted the mirror surface, while the second measured a stationary optical reference flat. Subtracting the reference signal eliminated translational stage-dependent errors from the measured profile. The stage position was continuously monitored during translation using a collimating C01 sensor head targeting a stage-mounted mirror. A fixed laser interferometer head targeted a stage-mounted mirror. The stage position was continuously monitored during translation using a collimating C01 sensor head targeting a stage-mounted mirror.

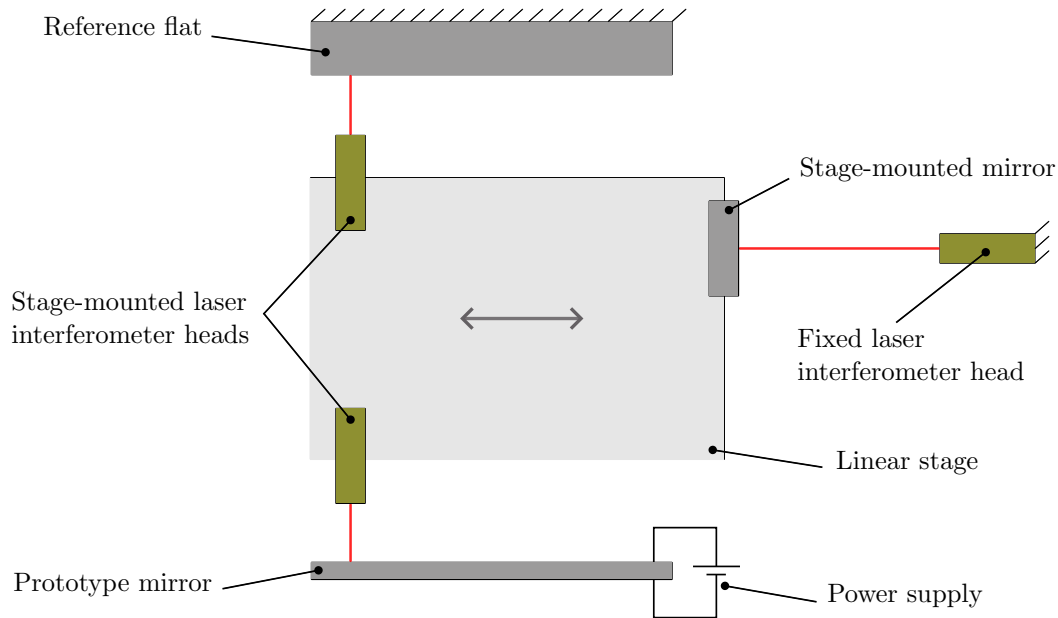


Figure 5: Top view, scheme of the test setup: the measurement is performed by scanning the prototype mirror along the tangential direction.

To bias the chromium electrodes, we connected a high-voltage power supply directly through the mechanical mount. A segmented fixture design maintained electrical isolation of the front and back electrodes. Mechanically, the mirror is supported at mid-length by two pairs of washers, coinciding with the V-shaped termination of

the electrode wires. Specifically, copper washers provided localized conductive contact, while Delrin® (acetal homopolymer) components electrically insulated the frame, allowing independent control of front and rear surface potentials. During testing, the mirror was mounted vertically so that gravity acted parallel to the optical surface without distorting the out-of-plane actuated profile. All measurements were conducted on an optical table under ambient laboratory conditions. The front surface was biased at operating potentials up to 300 V, while the rear surface was maintained at electrical ground. Fig. 6 shows the measured displacement profiles along the central meridian within the clear aperture for applied voltages ranging from 100 V to 300 V.

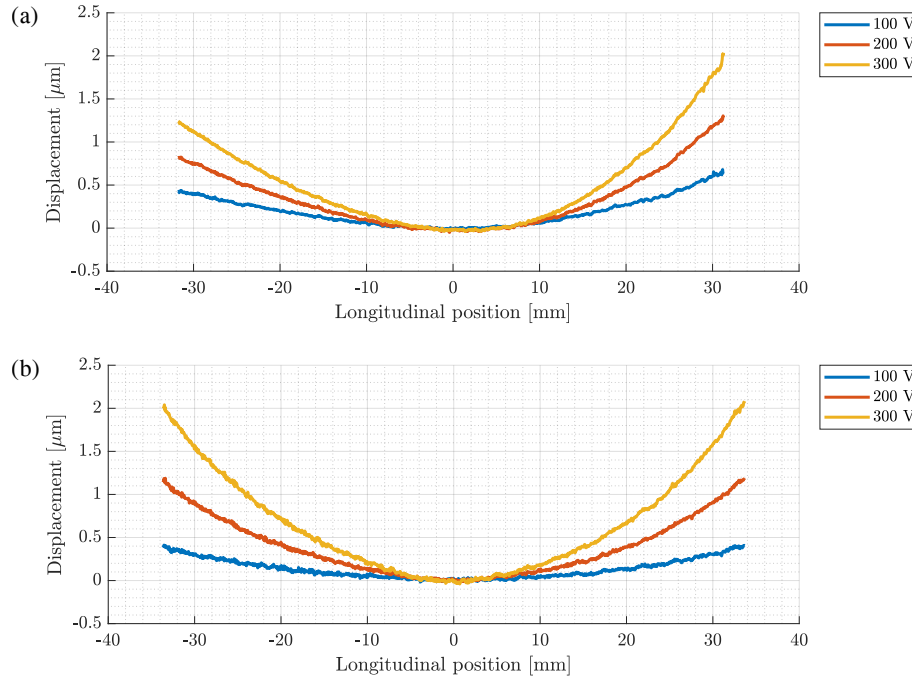


Figure 6: Measured displacement along the central meridian for first-order (a) and second-order (b) electrodes under applied voltages from 100 V to 300 V. The surfaces are measured 6 times, averaged and plotted with central slope and offset set to zero.

As expected, the plots show a clear monotonic trend, where increasing the applied voltage directly increases the deformation of the prototypes. Furthermore, the central curvature exhibits a highly significant linear dependence on the applied voltage. Linear regression of the central curvature with respect to the applied voltage yields an actuation sensitivity of $1.1 \times 10^{-5} \text{ m}^{-1}/\text{V}$ ($R^2 = 0.9999$, $p = 0.0026$) and $1.3 \times 10^{-5} \text{ m}^{-1}/\text{V}$ ($R^2 = 0.9988$, $p = 0.0218$) for the third- and fourth-order profiles, respectively, determined via a two-tailed Student's t -test.¹⁵

The measured displacement amplitudes are significantly lower than those predicted by the FEA models (Figs. 3a and 3c). FEA simulations incorporating clamp constraints showed that mechanical boundary conditions cannot account for this deviation. Our primary hypothesis for the discrepancy is incomplete polarization inversion through the target half-thickness ($a_1 \neq a_2$). Because the tangential curvature scales directly with the product of domain thicknesses ($a_1 a_2$, as shown in Eq. 2), a non-equal domain thickness ($a_1 \neq a_2$) significantly diminishes the internal bending moment per unit voltage applied. Reaching the necessary domain depth ($a_1 = a_2 = h/2$) may require higher temperatures or longer dwell times than our current furnace setup allowed.^{7,8}

We attempted to measure the inversion depth following the procedure of Hu *et al.* in Ref. 16. Post-dicing chemical etching was performed on remaining LN wafer scraps using a mixture of 60 mL HF (40% concentration) and 39 mL HNO₃ (100% concentration) for two hours at room temperature under continuous stirring. This process preferentially etches the domains, highlighting cross-sectional boundaries due to the differential etch rates between antiparallel polarization regions. Nevertheless, optical microscopy conducted before and after etching yielded insufficient contrast across the domain interface to measure the inversion depth.

Because this thickness could not be directly verified, we evaluated normalized displacement profiles to isolate the geometric shape-control capability from the overall actuation magnitude. When comparing normalized displacements between FEA predictions and experimental measurements in Fig. 7, the first-order electrode shows better agreement than the second-order design. The reasons for the greater discrepancy in the second case are currently under investigation.

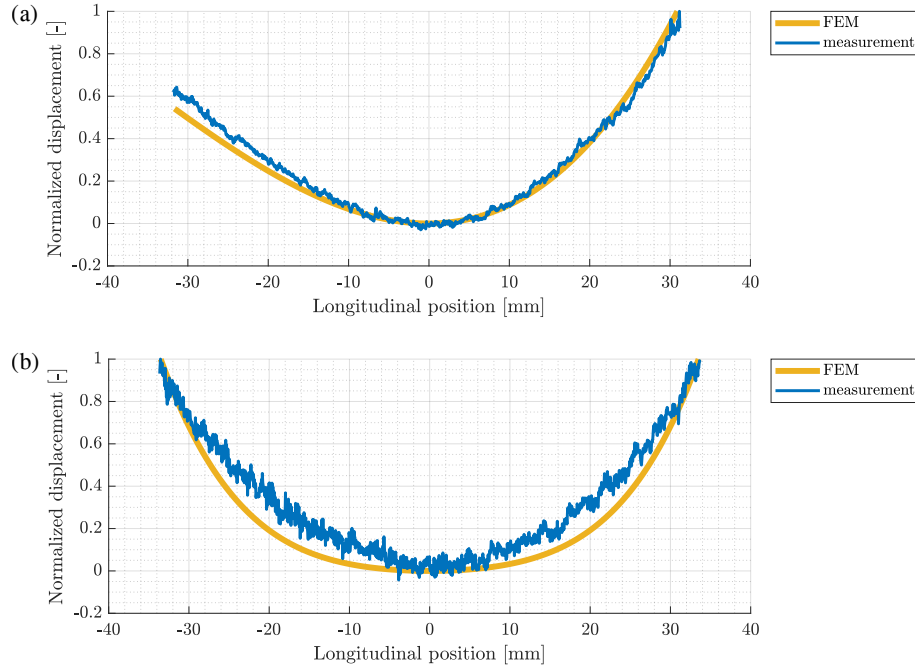


Figure 7: Comparison between FEM and measured displacements, each normalized to its maximum value, for the (a) first-order, and (b) second-order electrodes, with 100 V applied.

7. CONCLUSION

Polynomial shaped electrodes are an alternative approach to control or correct X-ray mirror surface shapes. They provide longitudinally continuous shaping with reduced complexity from fewer degrees of freedom. We designed, fabricated, and tested prototype monolithic LiNbO₃ bimorph X-ray mirrors with symmetric, longitudinally continuous electrodes shaped with first- and second-order polynomial profiles. Experimental characterization demonstrated a deterministic actuation behavior across both electrode designs. The central curvature exhibited a statistically significant linear response to the applied voltage ($R^2 \geq 0.9988$, $p < 0.05$). The extracted actuation sensitivities of $1.1 \times 10^{-5} \text{ m}^{-1}/\text{V}$ and $1.3 \times 10^{-5} \text{ m}^{-1}/\text{V}$ for the third- and fourth-order profiles, respectively, demonstrate that the electrode geometry can be exploited to tailor spatial deformation profiles while maintaining fine curvature modulation. Although controlling the domain inversion depth and mitigating wafer deformation during fabrication remain ongoing challenges, this work represents a step toward demonstrating the feasibility of shaped-electrode, monolithic LN actuators for adaptive X-ray optics.

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