Designing and Analyzing the Phase Response of Metasurfaces

White Paper Version 2.0

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Related Documents

This white paper is part of a series on optical simulation and design from LightTrans International GmbH:

- **Surrogate Model White Paper:** *Surrogate Modeling: Enabling Practical Metalens Design and Simulation* [1] — Describes the precomputed Jones matrix responses that provide the input to the phase extraction methods discussed here.
- **PCA White Paper:** *The Periodic Cell Array (PCA) Approximation: The Foundation for Metalens Design and Modeling* [2] — Discusses the Periodic Cell Array approximation and why it is the logical starting point.
- **Metalens [PCA] Specification:** Describes the metalens twin that implements the design and modeling workflow [3].

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Executive Summary

This white paper establishes a rigorous framework for understanding, designing, and analyzing the phase response of metasurfaces.

The Problem: A metasurface is designed to impart a scalar phase profile. But the local meta-atom response is vectorial — it produces two generally different phases. Which one should we use?

The Solution: We define the **local common phase** $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$ as the quantity for a specified polarization $\boldsymbol{J}^{\text{in}}$, to associate with the phase profile. The quality of this representation depends on input polarization. We introduce a criterion σ^2 to measure this quality.

Key Steps:

- **Design stage:** For a given meta-atom type, we search the Poincaré sphere to find the optimal input polarization basis $\boldsymbol{J}_1, \boldsymbol{J}_2$ that minimizes σ^2 across the fabrication range. For pillars, $\boldsymbol{J}_1 = (1, 0)^T, \boldsymbol{J}_2 = (0, 1)^T$; for nanofins, $\boldsymbol{J}_1 = (1, i)^T, \boldsymbol{J}_2 = (1, -i)^T$.
- **Design using $\boldsymbol{J}_1$:** We select meta-atom geometries $\boldsymbol{p}(\boldsymbol{\rho})$ so that $\Psi_1 \approx \Delta\psi^{\text{profile}}(\boldsymbol{\rho})$.
- **Simulation:** Any incident field is decomposed into $V_1\boldsymbol{J}_1 + V_2\boldsymbol{J}_2$. The output consists of two modes with common phases Ψ_1 and Ψ_2 (evaluated at the actual local incidence direction).
- **Wavefront extraction:** $\Psi_1(\boldsymbol{\rho})$ is unwrapped and filtered to obtain the smooth imparted phase $\Delta\psi^{\text{meta}}(\boldsymbol{\rho})$. Residual phases capture all remaining effects.

This framework is the foundation for all metasurface design and analysis in VirtualLab Fusion.

Short Abstract (Document System)

This white paper establishes a rigorous framework for defining, extracting, and evaluating the phase response of metasurface meta-atoms, introducing the local common phase $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$ as the design-relevant quantity, a quality criterion σ^2 for input polarization selection, and optimal basis analysis $(\boldsymbol{J}_1, \boldsymbol{J}_2)$ for pillars (linear) and nanofins (circular).

1 Introduction

1.1 The Metasurface Phase Profile

A metasurface is designed to impart a scalar phase change to the incident wavefront. The user specifies a target phase profile $\Delta\psi^{\text{profile}}(\boldsymbol{\rho})$ — for example, a spherical focusing phase ($\boldsymbol{\rho} = (x, y)$):

$$\Delta\psi^{\text{profile}}(\boldsymbol{\rho}) = -k_0\sqrt{f^2 + |\boldsymbol{\rho}|^2} + \text{constant}. \tag{1}$$

The goal is to realize this profile as the additional phase added to the incident wavefront:

$$\psi^{\text{out}}(\boldsymbol{\rho}) = \psi^{\text{in}}(\boldsymbol{\rho}) + \Delta\psi^{\text{profile}}(\boldsymbol{\rho}). \tag{2}$$

Here, ψ^{in} is the incident wavefront phase, and ψ^{out} is the output wavefront phase after the metasurface.

1.2 The Challenge: Vectorial Response

However, the local response of a meta-atom is not scalar — it is vectorial. The output field is given by a multiplication with a Jones matrix $\mathbf{M}$ for each meta-atom. This produces two output phases, $\arg(J_x^{\text{out}})$ and $\arg(J_y^{\text{out}})$, which are generally different. The question arises:

Which phase should we associate with the metasurface phase profile?

1.3 The PCA Approximation

We utilize the Periodic Cell Array (PCA) approximation to determine the matrix $\mathbf{M}$ [2]. It assumes identical neighbors and applies the Rigorous Coupled Wave Analysis (RCWA) to obtain $\mathbf{M}$. The resulting matrix $\mathbf{M}$ depends on:

- The local geometry parameter $\boldsymbol{p}$ (e.g., pillar diameter d or nanofin rotation θ_r)
- The wavelength λ
- The local direction of incidence $\hat{\boldsymbol{s}}^{\text{in}}$

Thus, $\mathbf{M} = \mathbf{M}(\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}})$. For a detailed discussion of PCA — its justification, limitations, and application — see the PCA white paper [2].

1.4 Scope of This Paper

Given the matrix response $\mathbf{M}$ of a meta-atom, how do we define, extract, and evaluate its phase response for metasurface design and analysis? The surrogate model (see separate white paper [1]) provides $\mathbf{M}$ efficiently; here we discuss what to do with it.

2 Field Representation and Matrix Response

2.1 Incident Field Decomposition

The incident electric field components at a point $\boldsymbol{\rho} = (x, y)$ on the metasurface are expressed as:

$$E_x^{\mathrm{in}}(\boldsymbol{\rho}) = a_x^{\mathrm{in}}(\boldsymbol{\rho})\, e^{\mathrm{i}\psi^{\mathrm{in}}(\boldsymbol{\rho})}, \qquad E_y^{\mathrm{in}}(\boldsymbol{\rho}) = a_y^{\mathrm{in}}(\boldsymbol{\rho})\, e^{\mathrm{i}\psi^{\mathrm{in}}(\boldsymbol{\rho})}. \tag{3}$$

Here:

- $\psi^{\mathrm{in}}(\boldsymbol{\rho})$ is the **common wavefront phase** of the incident field. It is the same for both x and y components.
- $a_x^{\mathrm{in}}(\boldsymbol{\rho})$ and $a_y^{\mathrm{in}}(\boldsymbol{\rho})$ are the complex amplitudes **excluding** the common wavefront phase.

The transverse components are collected into a vector:

$$\boldsymbol{E}_\perp^{\mathrm{in}}(\boldsymbol{\rho}) = \begin{pmatrix} E_x^{\mathrm{in}}(\boldsymbol{\rho}) \\ E_y^{\mathrm{in}}(\boldsymbol{\rho}) \end{pmatrix} = \boldsymbol{a}_\perp^{\mathrm{in}}(\boldsymbol{\rho})\; e^{\mathrm{i}\psi^{\mathrm{in}}(\boldsymbol{\rho})} = \begin{pmatrix} a_x^{\mathrm{in}}(\boldsymbol{\rho}) \\ a_y^{\mathrm{in}}(\boldsymbol{\rho}) \end{pmatrix} e^{\mathrm{i}\psi^{\mathrm{in}}(\boldsymbol{\rho})}. \tag{4}$$

2.2 The Input Field Polarization in Design

In the design stage, we restrict to input fields with **uniform polarization**. Such fields can be expressed as:

$$\boldsymbol{a}_\perp^{\mathrm{in}}(\boldsymbol{\rho}) = \boldsymbol{J}^{\mathrm{in}} a^{\mathrm{in}}(\boldsymbol{\rho})\,, \tag{5}$$

with the Jones vector $\boldsymbol{J}^{\mathrm{in}} = (J_x^{\mathrm{in}}, J_y^{\mathrm{in}})^T$ and the scalar complex amplitude $a^{\mathrm{in}}(\boldsymbol{\rho})$. This restriction is by choice and could be skipped. Even if a metalens is designed for one specific uniform input polarization, the simulation model for the resulting metalens can deal with any input field.

2.3 Local Direction of Incidence

The spatial variation of $\psi^{\mathrm{in}}(\boldsymbol{\rho})$ determines the local direction of incidence. The spatial frequency vector is:

$$\boldsymbol{\kappa}(\boldsymbol{\rho}) = \nabla_\perp \psi^{\mathrm{in}}(\boldsymbol{\rho}) = k_0 n \begin{pmatrix} \sin\theta_x(\boldsymbol{\rho}) \\ \sin\theta_y(\boldsymbol{\rho}) \end{pmatrix}, \tag{6}$$

where $\nabla_\perp = (\partial_x, \partial_y)$ is the lateral gradient operator, $k_0 = 2\pi/\lambda$, and n is the refractive index of the incident medium.

2.4 Matrix Response of the Meta-Atom

The metasurface transforms the incident field to the output field via a local Jones matrix $\mathbf{M}$. This matrix depends on:

- The local meta-atom geometry $\boldsymbol{p}(\boldsymbol{\rho})$
- The wavelength λ
- The local direction of incidence $\hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})$

Thus, $\mathbf{M} = \mathbf{M}(\boldsymbol{p}(\boldsymbol{\rho}), \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho}))$.

The matrix applies locally to the incident Jones vector $\boldsymbol{J}^{\text{in}}$ and we obtain:

$$\boldsymbol{J}^{\text{out}} = \mathbf{M}(\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}}) \cdot \boldsymbol{J}^{\text{in}}. \tag{7}$$

2.5 The Central Question

Each component of $\boldsymbol{J}^{\text{out}}$ has its own phase: $\arg(J_x^{\text{out}})$ and $\arg(J_y^{\text{out}})$. These are generally different. The metasurface is intended to add a scalar phase profile $\Delta\psi^{\text{profile}}(\boldsymbol{\rho})$ to the incident wavefront. But the output field has **two** phases, not one. Which one corresponds to ψ^{out}?

This is the central question of this white paper.

3 Defining the Local Common Phase

3.1 The Common Phase as the Logical Choice

We need a single scalar phase that represents the meta-atom's contribution to the wavefront. We select the **common phase**:

$$\Psi = \arg\left(J_x^{\text{out}} + J_y^{\text{out}}\right). \tag{8}$$

This is the phase common to both field components in the sense that:

$$\begin{pmatrix} J_x^{\text{out}} \\ J_y^{\text{out}} \end{pmatrix} = e^{\mathrm{i}\Psi} \begin{pmatrix} |J_x^{\text{out}}|\, e^{\mathrm{i}(\arg(J_x^{\text{out}}) - \Psi)} \\ |J_y^{\text{out}}|\, e^{\mathrm{i}(\arg(J_y^{\text{out}}) - \Psi)} \end{pmatrix}. \tag{9}$$

3.2 Non-Common (Residual) Phases

The quantities

$$\Delta\phi_x = \arg(J_x^{\text{out}}) - \Psi, \qquad \Delta\phi_y = \arg(J_y^{\text{out}}) - \Psi \tag{10}$$

are the **non-common phases**. They represent polarization-dependent phase effects not captured by the common phase.

3.3 The Design Association

In metasurface design, we associate Ψ with the desired phase profile $\Delta\psi^{\text{profile}}$. At each position $\boldsymbol{\rho}$, we select $\boldsymbol{p}(\boldsymbol{\rho})$ such that:

$$\Psi\big(\boldsymbol{p}(\boldsymbol{\rho}), \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})\big) \approx \Delta\psi^{\text{profile}}(\boldsymbol{\rho}) \bmod 2\pi. \tag{11}$$

This is the design equation. But its success depends on the input polarization $\boldsymbol{J}^{\text{in}}$.

4 A Quality Criterion for the Common Phase

4.1 The Need for a Criterion

The quality of Ψ as a representation of the meta-atom's phase response depends on $\boldsymbol{J}^{\text{in}}$. For some polarizations, the non-common phases are small; for others, they are large. We need a quantitative measure.

4.2 Definition of σ^2 and Σ^2

For fixed $\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}}$ and a given $\boldsymbol{J}^{\text{in}}$, we compute $\boldsymbol{J}^{\text{out}} = \mathbf{M} \cdot \boldsymbol{J}^{\text{in}}$. The common phase is $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$.

For each component $\ell = x, y$, the phase difference with 2π modulo handling is:

$$\Delta\psi_\ell = \min_{q=0,\pm1}^{\dagger} \Big(\arg(J_\ell^{\text{out}}) - \big(\Psi + 2q\pi\big) \Big), \tag{12}$$

where $\min^\dagger$ denotes the minimum of the absolute value.

The non-common phase variance is defined as the weighted second moment:

$$\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p}) = \frac{|J_x^{\text{out}}|^2 (\Delta\psi_x)^2 + |J_y^{\text{out}}|^2 (\Delta\psi_y)^2}{|J_x^{\text{out}}|^2 + |J_y^{\text{out}}|^2}. \tag{13}$$

This expression is scale-invariant: multiplying $\boldsymbol{J}^{\text{in}}$ by a constant factor scales both numerator and denominator equally, leaving σ^2 unchanged.

To assess quality across the entire fabrication range, we sum over $\boldsymbol{p}$:

$$\Sigma^2(\boldsymbol{J}^{\text{in}}) = \sum_{\boldsymbol{p} \in \mathcal{P}_{\text{struct}}} \sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p}). \tag{14}$$

Here, $\mathcal{P}_{\text{struct}}$ denotes the discrete set of geometry parameters that can be manufactured (e.g., pillar diameters with 10 nm increment). A small Σ^2 indicates that Ψ is a good representation for all relevant geometries.

5 Finding the Optimal Input Polarization Basis

5.1 Search on the Poincaré Sphere

All polarization states are represented on the Poincaré sphere, parameterized by:

- ψ (azimuth) from 0 to $\pi/2$
- χ (ellipticity) from $-\pi/4$ to $\pi/4$

The corresponding Jones vector is:

$$\boldsymbol{J}(\psi, \chi) = \begin{pmatrix} \cos\psi \\ \sin\psi\, e^{i\chi} \end{pmatrix}. \tag{15}$$

We search over (ψ, χ) to find $\boldsymbol{J}_1$ that minimizes $\Sigma^2(\boldsymbol{J})$. The orthogonal polarization $\boldsymbol{J}_2$ is given by:

$$\boldsymbol{J}_2 = \begin{pmatrix} -\sin\psi\, e^{-i\chi} \\ \cos\psi \end{pmatrix}, \tag{16}$$

which is the antipodal point on the Poincaré sphere.

Both Ψ_1 and Ψ_2 (the common phases obtained with $\boldsymbol{J}_1$ and $\boldsymbol{J}_2$) have small σ^2 and are therefore well suited for design.

5.2 Special Cases

- **Pillars:** $\boldsymbol{J}_1 = (1, 0)^T$, $\boldsymbol{J}_2 = (0, 1)^T$, $\Psi_1 = \Psi_2$ (for orthogonal incidence).
- **Nanofins:** $\boldsymbol{J}_1 = \frac{1}{\sqrt{2}}(1, i)^T$ (LCP), $\boldsymbol{J}_2 = \frac{1}{\sqrt{2}}(1, -i)^T$ (RCP).

6 Design Stage: From Target Profile to Geometry

At this point, we have:

- The optimal basis $\boldsymbol{J}_1, \boldsymbol{J}_2$ for the meta-atom type
- The surrogate model providing $\Psi_1(\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}})$ and $\Psi_2(\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}})$ on demand:

$$\Psi_1 = \arg\left([\mathbf{M}\boldsymbol{J}_1]_x + [\mathbf{M}\boldsymbol{J}_1]_y\right), \qquad \Psi_2 = \arg\left([\mathbf{M}\boldsymbol{J}_2]_x + [\mathbf{M}\boldsymbol{J}_2]_y\right). \tag{17}$$

6.1 Design Equation

For each position $\boldsymbol{\rho}$, with local incident direction $\hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})$ (from $\nabla_\perp \psi^{\text{in}}$), we select:

$$\boldsymbol{p}(\boldsymbol{\rho}) = \underset{\boldsymbol{p} \in \mathcal{P}_{\text{struct}}}{\arg\min} \left| \Psi_1(\boldsymbol{p}, \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})) - \Delta\psi^{\text{profile}}(\boldsymbol{\rho}) \bmod 2\pi \right|. \tag{18}$$

Here, $\mathcal{P}_{\text{struct}}$ denotes the discrete set of geometry parameters that can be manufac-

tured (e.g., pillar diameters with 10 nm increment). This yields a discrete distribution $\boldsymbol{p}(\boldsymbol{\rho})$ and a corresponding common phase distribution $\Psi_1(\boldsymbol{\rho}) = \Psi_1(\boldsymbol{p}(\boldsymbol{\rho}), \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho}))$.

6.2 Quantization Error

Because $\mathcal{P}_{\text{struct}}$ is discrete due to fabrication constraints (e.g., pillar diameter cannot be changed continuously), we have a phase quantization error:

$$\delta\Psi^{\text{quanta}}(\boldsymbol{\rho}) = \Psi_1(\boldsymbol{\rho}) - \Delta\psi^{\text{profile}}(\boldsymbol{\rho}) \bmod 2\pi. \tag{19}$$

This error is inherent to fabrication constraints.

7 Simulation Stage: From Incident Field to Output Field

Now we have a designed metasurface: $\boldsymbol{p}(\boldsymbol{\rho})$ is known. In simulation, the incident field may be arbitrary — not necessarily the design polarization, not necessarily uniformly polarized, not necessarily the design incident direction, and can be of any wavelength. That enables the investigation of aberrations and other effects caused by the metasurface.

7.1 Decomposition into the Optimal Basis

For any incident field $\boldsymbol{E}_{\perp}^{\text{in}}(\boldsymbol{\rho})$, we decompose it into the optimal basis $\boldsymbol{J}_1, \boldsymbol{J}_2$ determined in Sec. 5:

$$\boldsymbol{E}_{\perp}^{\text{in}}(\boldsymbol{\rho}) = V_1(\boldsymbol{\rho})\boldsymbol{J}_1 + V_2(\boldsymbol{\rho})\boldsymbol{J}_2. \tag{20}$$

The coefficients are obtained by projecting the incident field onto the basis vectors. With $\boldsymbol{J}_1$ and $\boldsymbol{J}_2$ orthonormal ($\boldsymbol{J}_1^{\dagger}\boldsymbol{J}_1 = 1$, $\boldsymbol{J}_2^{\dagger}\boldsymbol{J}_2 = 1$, $\boldsymbol{J}_1^{\dagger}\boldsymbol{J}_2 = 0$), we have:[1]

$$V_1(\boldsymbol{\rho}) = \boldsymbol{J}_1^{\dagger} \cdot \boldsymbol{E}_{\perp}^{\text{in}}(\boldsymbol{\rho}), \qquad V_2(\boldsymbol{\rho}) = \boldsymbol{J}_2^{\dagger} \cdot \boldsymbol{E}_{\perp}^{\text{in}}(\boldsymbol{\rho}). \tag{21}$$

In matrix form, with $\boldsymbol{J}_1 = (J_{1x}, J_{1y})^T$ and $\boldsymbol{J}_2 = (J_{2x}, J_{2y})^T$:

$$\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} J_{1x}^* & J_{1y}^* \\ J_{2x}^* & J_{2y}^* \end{pmatrix} \begin{pmatrix} E_x^{\text{in}} \\ E_y^{\text{in}} \end{pmatrix}. \tag{22}$$

7.2 Output Field for Each Mode

For each mode, we evaluate the actual response at the actual local incidence direction $\hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})$ and with the designed geometry $\boldsymbol{p}(\boldsymbol{\rho})$.

For mode 1 (designed mode):

[1] $\boldsymbol{J}_1^{\dagger}$ denotes the conjugate transpose (Hermitian conjugate) of the Jones vector. For $\boldsymbol{J}_1 = (J_{1x}, J_{1y})^T$, we have $\boldsymbol{J}_1^{\dagger} = (J_{1x}^*, J_{1y}^*)$. The inner product $\boldsymbol{J}_1^{\dagger} \cdot \boldsymbol{E}_{\perp}^{\text{in}} = J_{1x}^* E_x^{\text{in}} + J_{1y}^* E_y^{\text{in}}$ ensures orthonormality for complex polarization states such as circular polarization.

$$\mathbf{M}(\boldsymbol{p}(\boldsymbol{\rho}), \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho}))\boldsymbol{J}_1 = e^{\mathrm{i}\Psi_1(\boldsymbol{\rho})} \begin{pmatrix} A_{1x}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{1x}(\boldsymbol{\rho})} \\ A_{1y}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{1y}(\boldsymbol{\rho})} \end{pmatrix}, \tag{23}$$

where:

- $\Psi_1(\boldsymbol{\rho}) = \arg\left([\mathbf{M}\boldsymbol{J}_1]_x + [\mathbf{M}\boldsymbol{J}_1]_y\right)$ is the common phase
- $A_{1x}(\boldsymbol{\rho}) = |[\mathbf{M}\boldsymbol{J}_1]_x|$, $A_{1y}(\boldsymbol{\rho}) = |[\mathbf{M}\boldsymbol{J}_1]_y|$ are the amplitudes
- $\delta\phi_{1x}(\boldsymbol{\rho}) = \arg([\mathbf{M}\boldsymbol{J}_1]_x) - \Psi_1(\boldsymbol{\rho})$, and similarly for y, are the non-common phases

For mode 2 (orthogonal mode):

$$\mathbf{M}(\boldsymbol{p}(\boldsymbol{\rho}), \lambda, \hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho}))\boldsymbol{J}_2 = e^{\mathrm{i}\Psi_2(\boldsymbol{\rho})} \begin{pmatrix} A_{2x}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{2x}(\boldsymbol{\rho})} \\ A_{2y}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{2y}(\boldsymbol{\rho})} \end{pmatrix}, \tag{24}$$

with analogous definitions.

7.3 Complete Output Field

The output field is obtained by combining the two modes, including the incident wavefront phase $\psi^{\text{in}}(\boldsymbol{\rho})$. Note that the incident amplitude $a^{\text{in}}(\boldsymbol{\rho})$ is already incorporated into $V_1(\boldsymbol{\rho})$ and $V_2(\boldsymbol{\rho})$ via the decomposition:

$$\boldsymbol{E}_{\perp}^{\text{out}}(\boldsymbol{\rho}) = e^{\mathrm{i}\psi^{\text{in}}(\boldsymbol{\rho})} \Bigg[V_1(\boldsymbol{\rho}) e^{\mathrm{i}\Psi_1(\boldsymbol{\rho})} \begin{pmatrix} A_{1x}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{1x}(\boldsymbol{\rho})} \\ A_{1y}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{1y}(\boldsymbol{\rho})} \end{pmatrix} \tag{25}$$

$$+ V_2(\boldsymbol{\rho}) e^{\mathrm{i}\Psi_2(\boldsymbol{\rho})} \begin{pmatrix} A_{2x}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{2x}(\boldsymbol{\rho})} \\ A_{2y}(\boldsymbol{\rho})\, e^{\mathrm{i}\delta\phi_{2y}(\boldsymbol{\rho})} \end{pmatrix} \Bigg]. \tag{26}$$

This expression is the basis for system-level simulation. The two modes evolve independently, each with its own common phase and residual phases. The field tracing engine propagates the complete field as given.

8 From Local Common Phase to Wavefront Phase

The common phase $\Psi_1(\boldsymbol{\rho})$ is not equal to $\Delta\psi^{\text{profile}}(\boldsymbol{\rho})$ because:

- $\Psi_1(\boldsymbol{\rho})$ is obtained modulo 2π (a consequence of the use of RCWA)
- $\hat{\boldsymbol{s}}^{\text{in}}(\boldsymbol{\rho})$ may differ from the design direction
- Quantization error $\delta\Psi^{\text{quanta}}$ is present
- The meta-atom response is angle-dependent

8.1 Unwrapping and Filtering

We apply an unwrapping and filtering operation Θ to obtain a smooth wavefront phase:

$$\Delta\psi_1^{\text{meta}}(\boldsymbol{\rho}) = \Theta\big\{\Psi_1(\boldsymbol{\rho})\big\}, \tag{27}$$

where $\Delta\psi_1^{\text{meta}}(\boldsymbol{\rho})$ is the smooth, unwrapped phase change imparted by the metasurface for mode 1. It is also the basis for aberration investigation for metalenses.

Similarly, for mode 2 we obtain:

$$\Delta\psi_2^{\text{meta}}(\boldsymbol{\rho}) = \Theta\big\{\Psi_2(\boldsymbol{\rho})\big\}. \tag{28}$$

For pillars, $\Delta\psi_1^{\text{meta}}$ and $\Delta\psi_2^{\text{meta}}$ are identical or very similar. For nanofins, they are approximately conjugates.

8.2 Total Residual Phases

The difference between the common phase and the smooth wavefront phase becomes part of the total residual:

$$\delta\phi_{1x}^{\text{total}}(\boldsymbol{\rho}) = \delta\phi_{1x}(\boldsymbol{\rho}) + \big(\Psi_1(\boldsymbol{\rho}) - \Delta\psi_1^{\text{meta}}(\boldsymbol{\rho})\big), \tag{29}$$

and analogously for y. These total residuals include:

- The original non-common phases
- The unwrapping/filtering residuals
- Any unwrapable phase features

For mode 2, analogous expressions hold.

8.3 Final Output Field for Simulation

The final output field is:

$$\boldsymbol{E}_{\perp}^{\text{out}}(\boldsymbol{\rho}) = e^{\mathrm{i}\psi^{\text{in}}(\boldsymbol{\rho})}\Bigg[V_1(\boldsymbol{\rho})e^{\mathrm{i}\Delta\psi_1^{\text{meta}}(\boldsymbol{\rho})}\begin{pmatrix}A_{1x}(\boldsymbol{\rho})e^{\mathrm{i}\delta\phi_{1x}^{\text{total}}(\boldsymbol{\rho})}\\ A_{1y}(\boldsymbol{\rho})e^{\mathrm{i}\delta\phi_{1y}^{\text{total}}(\boldsymbol{\rho})}\end{pmatrix} \tag{30}$$

$$+V_2(\boldsymbol{\rho})e^{\mathrm{i}\Delta\psi_2^{\text{meta}}(\boldsymbol{\rho})}\begin{pmatrix}A_{2x}(\boldsymbol{\rho})e^{\mathrm{i}\delta\phi_{2x}^{\text{total}}(\boldsymbol{\rho})}\\ A_{2y}(\boldsymbol{\rho})e^{\mathrm{i}\delta\phi_{2y}^{\text{total}}(\boldsymbol{\rho})}\end{pmatrix}\Bigg]. \tag{31}$$

This is the basis for system-level simulation. It shows clearly that the metasurface introduces wavefront phase responses, but also additional terms, which must be considered in the simulation for a full understanding of the performance of a metalens. All effects are fully accounted for in the field tracing engine.

9 Alternative Design Strategy: Single-Component Phase

Instead of using the common phase Ψ, one may design using the phase of a single output component, e.g., $\arg(J_x^{\text{out}})$.

9.1 Important Distinction

This approach works only for the specific input polarization used in design. Unlike the mode decomposition approach (which yields a well-defined response for any input polarization), the single-component approach does not provide a controlled response for arbitrary input polarizations.

9.2 Design Approach

1. Choose a fixed input polarization $\boldsymbol{J}^{\text{in}}$.
2. Compute $J_x^{\text{out}} = [\mathbf{M}\boldsymbol{J}^{\text{in}}]_x$.
3. Design such that $\arg(J_x^{\text{out}}) \approx \Delta\psi^{\text{profile}}$.

9.3 Simulation Approach

For an incident field with the same polarization $\boldsymbol{J}^{\text{in}}$, compute $\boldsymbol{E}_\perp^{\text{out}} = \mathbf{M}\boldsymbol{E}_\perp^{\text{in}}$ and apply a polarizer to keep only E_x^{out}.

9.4 Limitation

For any incident polarization different from $\boldsymbol{J}^{\text{in}}$, the response is uncontrolled and may cause stray light or aberrations.

10 Conclusion

This white paper has established a rigorous framework for designing and analyzing metasurfaces:

1. The incident field is decomposed into common wavefront phase ψ^{in} and complex amplitudes. In design, we restrict to uniform polarization $\boldsymbol{J}^{\text{in}}$.
2. The local common phase $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$ is the quantity to associate with the phase profile.
3. The quality criterion $\Sigma^2(\boldsymbol{J}^{\text{in}}) = \sum_{\boldsymbol{p}} \sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ identifies the optimal input polarization basis $\boldsymbol{J}_1, \boldsymbol{J}_2$.
4. **Design stage:** Select $\boldsymbol{p}(\boldsymbol{\rho})$ so that $\Psi_1 \approx \Delta\psi^{\text{profile}}$.
5. **Simulation stage:** Decompose any incident field into $V_1\boldsymbol{J}_1 + V_2\boldsymbol{J}_2$. The output consists of two modes with common phases Ψ_1 and Ψ_2.
6. **Wavefront extraction:** Unwrap and filter Ψ_1 to obtain $\Delta\psi_1^{\text{meta}}$ (the designed phase) and Ψ_2 to obtain $\Delta\psi_2^{\text{meta}}$. Total residuals capture all remaining effects.

7. **Special cases:** Pillars (linear basis, $\Psi_1 = \Psi_2$; orthogonal incidence), nanofins (circular basis, Ψ_1 and Ψ_2 are approximately conjugates).
8. An alternative single-component design strategy works only for a fixed input polarization.

Key Takeaway: The phase response of a metasurface is not uniquely defined. The common phase $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$ is the logical choice. The optimal basis (linear for pillars, circular for nanofins) provides the foundation for design. In simulation, any incident field is decomposed into this basis, and the output consists of two independent modes. Unwrapping and filtering yield the smooth wavefront phase per mode; total residuals capture all remaining effects.

A Complete Notation Reference

Symbol	Meaning
$\psi^{\text{in}}(\boldsymbol{\rho})$	Incident common wavefront phase
$\psi^{\text{out}}(\boldsymbol{\rho})$	Output common wavefront phase
$\Delta\psi^{\text{profile}}(\boldsymbol{\rho})$	Desired phase profile (user-specified)
$\Delta\psi_1^{\text{meta}}(\boldsymbol{\rho}), \Delta\psi_2^{\text{meta}}(\boldsymbol{\rho})$	Smooth imparted phases after unwrapping (modes 1 and 2)
Ψ	Local common phase of a single meta-atom: $\arg(J_x^{\text{out}} + J_y^{\text{out}})$
$\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$	Non-common phase variance (quality criterion)
$\Sigma^2(\boldsymbol{J}^{\text{in}})$	Summed variance over $\boldsymbol{p}$-space
$\boldsymbol{J}_1, \boldsymbol{J}_2$	Optimal input polarization basis
Θ	Unwrapping and filtering operation
$\boldsymbol{p}$	Structure parameter vector
$\mathcal{P}_{\text{struct}}$	Discrete set of geometry parameters (fabrication grid)
$\hat{\boldsymbol{s}}^{\text{in}}$	Local direction of incidence
λ	Wavelength
V_1, V_2	Complex coefficients of field decomposition
$A_{1x}, A_{1y}, \delta\phi_{1x}, \delta\phi_{1y}$	Amplitudes and non-common phases for mode 1
$A_{2x}, A_{2y}, \delta\phi_{2x}, \delta\phi_{2y}$	Amplitudes and non-common phases for mode 2
$\delta\phi_{1x}^{\text{total}}, \delta\phi_{1y}^{\text{total}}$	Total residual phases for mode 1 (includes unwrapping)
$\delta\phi_{2x}^{\text{total}}, \delta\phi_{2y}^{\text{total}}$	Total residual phases for mode 2

Table 1: Summary of notation.

B Document Version History

Version	Date	Changes
1.0	April 2026	Initial release
2.0	April 2026	Simplified notation: replaced $\underline{a}$ with J^{out}; simplified σ^2 to direct ratio form; harmonized with surrogate model paper

References

[1] Frank Wyrowski. *Surrogate Modeling: Enabling Practical Metalens Design and Simulation*. White Paper WP-META-SURROGATE. LightTrans International GmbH, 2026. link.

[2] Frank Wyrowski. *The Periodic Cell Array (PCA) Approximation: The Foundation for Metalens Design and Modeling*. White Paper WP-META-PCA. LightTrans International GmbH, 2026. link.

[3] LightTrans International GmbH. *Metalens [PCA]*. CS-MPCA01. Digital Twin Specification. Version 1.0. 2026. link.