Scatterometry Using Speckle Correlations

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Chapter 1

Background

1.1 Material representation and acquisition

Representation Scattering materials are generally composed of small particles with varying refractive properties we describe through the bulk statistical properties of the material. We use three statistical properties to parameterize the scattering material. The extinction coefficient describes the extinction cross-section of the scattering particles per unit volume. It is therefore proportional to the density of scattering particles inside the material. The extinction coefficient is the sum of the absorption and scattering coefficients $\sigma_t = \sigma_a + \sigma_s$ which represent, respectively, the portion of light absorbed and scattered per unit length along the path. The material's phase function $\rho(\arccos(\hat{\mathbf{i}} \cdot \hat{\mathbf{v}}))$ describes the directionality of scattered light and determines the portion of light scattered towards direction $\hat{\mathbf{v}}$ when a scatterer is illuminated from direction $\hat{\mathbf{i}}$. A scatterer's phase function is dictated by its shape and refractive index. Phase functions for spherical particles can be computed analytically using Mie theory[7, 13, 17]. ρ is generally assumed to be isotropic. This means its value depends only on the inner product of the illumination and viewing directions, and not on the absolute directions. This may be relaxed by adding an anisotropy parameter $-1 \leq g \leq 1$ where $g = -1$ corresponds to fully backward scattering, $g = 0$ means light is scattered equally in all directions, and $g = 1$ is full forward scattering. The mean free path (MFP) of a material is defined as the average distance light travels inside the volume between two successive scattering events. The MFP is the inverse of the extinction coefficient $MFP = 1/\sigma_t$. When working with scattering volumes, it is common to express its geometric dimensions with respect to the MFP. For example, a volume with optical depth $OD = 4$ means its thickness is $4 \cdot MFP$. This means that light traveling through the medium is scattered four times in average.

Our work is primarily interested in the phase function ρ and will not discuss scattering coefficients.

Our work seeks to acquire ρ as a general function and does not assume common parameterizations such as the Henyey-Greenstein phase function [16].

Phase function from single scattering models A simple method for measuring phase functions is acquiring optically thin samples that scatter light once on average ($OD \approx 1$). This method is as simple as reflectometry: we illuminate a sample in direction $\boldsymbol{i}$ and measure the light received in direction $\boldsymbol{v}$, and the phase function is the portion of energy corresponding to scattering angle $\arccos(\hat{\mathbf{i}} \cdot \hat{\mathbf{v}})$. In the paraxial regime, we can apply the small-angle approximation to equate the scattering angle as the norm of the displacement vector between the illuminating and viewing directions $\boldsymbol{\tau} = \hat{\mathbf{v}} - \hat{\mathbf{i}}$, and $|\boldsymbol{\tau}| = \arccos(\hat{\mathbf{i}} \cdot \hat{\mathbf{v}})$. This method fails with increasing material thickness due to multiple scattering.

1.2 Speckle Correlations

Scattering refers to the propagation in media containing small, discrete scatterers with varying refractive properties. As light propagates through the medium, it interacts with multiple scatterers along its path, and each interaction changes its direction of travel. Scattering is common for a large variety of materials including biological tissues, the atmosphere, liquids, and cosmetics.

In this work, we increase the limited angular acquisition range from 8° to greater than 100° for a broader class of materials by combining the benefits of scatterometry and closed-form phase function computation from speckle correlations. Our scatterometer consists of two mutually coherent sources separated by a fixed, small elevation angle. Each beam illuminates a scattering medium, and scattered light is captured by a camera aperture. The image of each beam's scattered light is a speckle image, and both speckle images are correlated to find the single-scattered component proportional to the phase function. Because the medium scatters light spherically, we can capture speckle images with the beam pair located arbitrarily. By rotating the beam pair azimuthally with the sample at the center of rotation, we can measure speckle correlation over a broad range of scattering angles.

1.3 Related work

Material acquisition is the task of recovering the intrinsic properties of materials based on their appearance. It is of great importance in many applications. For example, tumors can be detected and classified as malignant or non-malignant [6]; important blood properties such as red and white blood counts can also be analyzed [5, 10]; in materials science, material acquisition is used to validate the fidelity and shelf life of material samples [29]; and the chemical compositions of nanodispersions can be inferred for particle sizing applications [28].

Inverse radiative transport [2] is studied heavily in graphics as well as the physical and biomedical sciences. While inverse radiative transport methods for scattering media fall into three main categories, methods using the *diffusion* approximation focus on optically thick media where high-order scattering is dominant. While this approximation simplifies inference and is suitable for both homogeneous and heterogeneous materials [12, 21, 27], it introduces parameter ambiguities. Similarity relations are hierarchical parameter relationships that allow scattering parameters to be altered without significantly altering the medium's spatial properties. These relations can be derived from transport equations to accelerate Monte Carlo simulations [34]. However, a radiance field computed via Monte Carlo simulations can be described by multiple, distinct sets of parameters, and finding mulutiple candidate solution sets is generally challenging. Parameter space warping and exploiting similarity relations have improved the efficiency of iterative solvers [36].

Rather than focusing purely on high-order scattering, another class of methods considers all paths of arbitrary lengths. Given a set of input images, they estimate material parameters whose combinations closely match the inputs when simulated using Monte-Carlo rendering [11, 26]. Differentiable rendering determines the effects of changes in scattering parameters by estimating derivatives of images. Traditionally, these estimtes have been approximate models that ignore complex light transport effects such as subsurface scattering and inter-reflections [19]. Differentiable Monte Carlo rendering overcomes these limiations by computing derivatives while accounting for all light transport effects [14, 15, 18, 24, 25]. Machine learning approaches offer lower computational complexity at the cost of reduced robustness and diminished physically accurate solutions. Encoder networks can be paired with Monte Carlo renderers to improve their generalization to scenes with unseen geometry and light sources [33, 9]. Energy losses in neural radiance fields are mitigated by efficient indirect illumination estimation via spherical harmonics [37]. While these approach are more general in nature and can handle arbitrarily thick materials, they are computationally expensive and require proper initialization.

The final class of methods are based on the *single scattering* approximation. The first approach assumes the medium is thin enough optically such that photons only scatter once when traveling through the medium. Since the scattering phase function is defined in terms of single-scattering, this allows the phase function to be observed directly. Although this method is as simple, it is limited to a narrow classes of materials such as gases and liquids of low viscosity [22]. Viscous liquids and thin solids can be acquired by illuminating materials with coherent light and computing the correlations of speckle images. Speckle image correlations are dominated by single-scattered light, and [1] showed that the phase function is proportional to the square root of the correlation and can be computed using a closed-form equation. However, this method is limited to measuring phase functions up to 8° due to aberrations.

1.4 Path-space framework

Given a volume containing quantity B randomly distributed scatterers with configuration O, the scattered field of incident light can be written as sums of contributions from all possible paths traveled within the medium. The set of all ordered sequences:

$$\vec{\mathbf{x}} = \mathbf{x_0} \rightarrow \mathbf{x_1} \rightarrow \dots \rightarrow \mathbf{x_{B+1}}, B \in [0, \infty) \tag{1.1}$$

Let μ be the change in complex amplitude for a chosen path segment. The speckle mean and covariance calculated for the set of enumerable paths passing through $\mathbf{x_1}...\mathbf{x_B}$ are:

$$m(\vec{\mathbf{x}}) = \mathbb{E}_O[u(\vec{\mathbf{x}})] = \mathbb{E}_O\left[\sum \mu(\vec{\mathbf{x}})\right], \tag{1.2}$$

$$C(\vec{\mathbf{x}}^1, \vec{\mathbf{x}}^2) = \mathbb{E}_O[u(\vec{\mathbf{x}}^1)u(\vec{\mathbf{x}}^2)^* - m(\vec{\mathbf{x}}^1)m(\vec{\mathbf{x}}^2)^*]. \tag{1.3}$$

Given two light sources and two sensors each located at $\mathbf{i_1}, \mathbf{i_2}, \mathbf{v_1}, \mathbf{v_2}$ respectively, the covariance can be written as volume integrals over all possible path pairs by swapping the order of the expectation and sum:

$$C^{\mathbf{i_1},\mathbf{i_2}}_{\mathbf{v_1},\mathbf{v_2}} = \int \int p(\vec{\mathbf{x}}^1, \vec{\mathbf{x}}^2)\mu(\vec{\mathbf{x}}^1)\mu(\vec{\mathbf{x}}^2)^* \, d\vec{\mathbf{x}}^1 \, d\vec{\mathbf{x}}^2 - m^{\mathbf{i_1}}_{\mathbf{v_1}} m^{\mathbf{i_2}*}_{\mathbf{v_2}} \tag{1.4}$$

where $p(\vec{\mathbf{x}}^1, \vec{\mathbf{x}}^2)$ is the probability all nodes on both $\vec{\mathbf{x}}^1$ and $\vec{\mathbf{x}}^2$ are included in the same particle configuration. Acquiring single-scattering speckle correlations requires choosing the source and sensor pairs locations and evaluating Equation 1.4 so measurements are beyond the memory effect range and the multi-scattering path contributions cancel due to random phase. This means $m^{\mathbf{i_1}}_{\mathbf{v_1}} m^{\mathbf{i_2}*}_{\mathbf{v_2}} \approx 0$, and only the integral must be computed.

Returning to the path space framework, given the volume in Figure **??**b, consider a single-scattering path containing only one particle: $\mathbf{i_1} \rightarrow \mathbf{x_b} \rightarrow \mathbf{v_1}$. Ignoring attenuation, the field produced by all scatterers can be expressed

$$u^{\mathbf{v_1}}_{\mathbf{i_1}} \propto \bar{s}^{\mathbf{v_1}}_{\mathbf{i_1}} \sum_{b=1}^{B} e^{jk(\mathbf{i_1} - \mathbf{v_1}) \cdot \mathbf{x_b}}. \tag{1.5}$$

where $\bar{s}^{\mathbf{v_1}}_{\mathbf{i_1}}$ is the square root of the scattering phase function since the phase function is defined for intensity, and amplitude is considered here. Another field $u^{\mathbf{v_1}}_{\mathbf{i_1}}$ will be produced by the other light-sensor

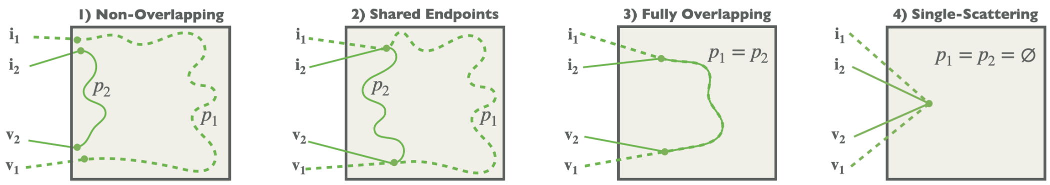


Figure 1.1: Scattered light paths can be generally categorized as one of four types, with only type 4 making significant contributions to speckle correlation. Paths types 1 and 2 have no overlap, meaning their phases are random and cancel in expectation. Paths of type 3 generally have non-zero correlation, but their contributions are smaller than those of type 4 (single-scattering paths).

pair. The correlation is then the expectation of the product of $u^{\mathbf{v}_1}_{\mathbf{i}_1}$ with $u^{\mathbf{v}_2*}_{\mathbf{i}_2}$ over all possible instantiations. The correlation in terms of a volume integral and the scattering coefficient σ_s is

$$C^{\mathbf{i}_1,\mathbf{i}_2}_{\mathbf{v}_1,\mathbf{v}_2} \propto \bar{s}^{\mathbf{v}_1}_{\mathbf{i}_1}\bar{s}^{\mathbf{v}_2}_{\mathbf{i}_2}\sigma_s \int_{\mathcal{V}} e^{jk((\mathbf{i}_1-\mathbf{v}_1)-(\mathbf{i}_2-\mathbf{v}_2))\cdot\mathbf{x}} d\mathbf{x}. \tag{1.6}$$

Single-scattering correlation is maximized when the complex exponential argument is zero. Define $\boldsymbol{\omega} = (\mathbf{i}_1 - \mathbf{v}_1) - (\mathbf{i}_2 - \mathbf{v}_2)$. If the sources and sensors are placed symmetrically about the z (depth) axis, only ω_z is nonzero. ω_z is minimized by choosing $\mathbf{i}_1, \mathbf{i}_2, \mathbf{v}_1, \mathbf{v}_2$ such that both $\mathbf{i}_1 - \mathbf{i}_2$ and $\mathbf{v}_2 - \mathbf{v}_1$ are as small as possible. The goal of our research is to find an imaging configuration that satisfies this condition.

1.5 Single-scattering approximation for speckle correlation

Consider a volume of scattering particles with configuration O. Define $I^{\hat{\mathbf{i}}}(\hat{\mathbf{v}})$ as the intensity scattered in direction $\boldsymbol{v}$ by a material illuminated from direction $\boldsymbol{i}$. Assuming the material is illuminated from two directions $\hat{\mathbf{i}}^1, \hat{\mathbf{i}}^2$, and light is observed from two directions $\hat{\mathbf{v}}^1, \hat{\mathbf{v}}^2$ the speckle covariance is

$$C^{\hat{\mathbf{i}}^1,\hat{\mathbf{i}}^2}_{\hat{\mathbf{v}}^1,\hat{\mathbf{v}}^2} \equiv \mathbb{E}_O\left[I^{\hat{\mathbf{i}}^1}(\hat{\mathbf{v}}^1)\cdot I^{\hat{\mathbf{i}}^2}(\hat{\mathbf{v}}^2)\right] - \mathbb{E}_O\left[I^{\hat{\mathbf{i}}^1}(\hat{\mathbf{v}}^1)\right]\cdot\mathbb{E}_O\left[I^{\hat{\mathbf{i}}^2}(\hat{\mathbf{v}}^2)\right] \tag{1.7}$$

where the expected value is evaluated over multiple instantiations of the medium $o \in O$. The memory effect states that two speckle fields created from similar illumination directions are shifted, correlated versions of each other. Namely, for a small displacement $\Delta = \hat{\mathbf{i}}^2 - \hat{\mathbf{i}}^1$, $I^{\hat{\mathbf{i}}^1}(\hat{\mathbf{v}}) \approx I^{\hat{\mathbf{i}}^2}(\hat{\mathbf{v}} + \Delta)$. The correlation is inversely proportional to material thickness and illuminator angular separation. Equation 1.7 is typically calculated by solving the wave equations numerically [30, 31, 35]. However, we are interested in closed-form expressions that relate correlations directly to material parameters.

Classical speckle theory suggests covariance can be written as an integral over the space of path-pairs p^1 from $\boldsymbol{i}^1$ to $\boldsymbol{v}^1$ and p^2 from $\boldsymbol{i}^2$ to $\boldsymbol{v}^2$ [32]. In classical ray tracing formulations, each path has a throughput since energy is lost along the path due to the extinction coefficient and scattering phase function. However, coherent light has a complex throughput whose phase is proportional to the path length. The large variation in path lengths leads to paths with random phases that ultimately cancel each other in expectation. This is supported by [3] who showed many paths can be omitted analytically, and efficient path sampling schemes can be utilized to only focus on paths that share their nodes. This reduced-path integral is evaluated using Monte-Carlo ray tracing algorithms [26, 11]. A majority of the longer path pairs contribute random phases, meaning single-scattering can be primarily attributed to single-scattering paths of the form $p^1 = \boldsymbol{i}^1 \rightarrow \mathbf{o} \rightarrow \boldsymbol{v}^1$, $p^2 = \boldsymbol{i}^2 \rightarrow \mathbf{o} \rightarrow \boldsymbol{v}^2$ [4]. This simplification is ray analog of the first Born approximation [23]. Rather than evaluating the full set of path pairs using Monte-Carlo sampling, this approximation means single-scattering paths can be evaluated in closed-form.

As shown previously, speckle correlation is maximized when the displacement between the two illumination directions and the two viewing directions are small. In terms of their 2D projections, $\hat{\mathbf{i}}^2 - \hat{\mathbf{i}}^1 = \hat{\mathbf{v}}^2 - \hat{\mathbf{v}}^1$. We parameterize these differences using 2D displacement vectors $\boldsymbol{\Delta}$ and $\boldsymbol{\tau}$:

$$\Delta \equiv \hat{\mathbf{i}}^2 - \hat{\mathbf{i}}^1 = \hat{\mathbf{v}}^2 - \hat{\mathbf{v}}^1, \quad \boldsymbol{\tau} \equiv \hat{\mathbf{v}}^1 - \hat{\mathbf{i}}^1 = \hat{\mathbf{v}}^2 - \hat{\mathbf{i}}^2. \tag{1.8}$$

where $\boldsymbol{\tau}$ is a parameterized scattering angle.

Using this notation, we can write the phase function at angle $\boldsymbol{\theta}$ as $\rho(|\boldsymbol{\theta}|)$. For illumination with wavenumber $k = 2\pi/\lambda$, [4] derived an closed-form expression for the single-scattering component of the correlation:

$$C(\boldsymbol{\tau}, \Delta) = \left(\rho(|\boldsymbol{\tau}|) L \sigma_s e^{-\sigma_t L} \operatorname{sinc}\left(\frac{kL}{2}(\boldsymbol{\tau} \cdot \Delta)\right)\right)^2. \tag{1.9}$$

where L is the scattering medium's thickness.

1.5.1 Phase function from speckle images

Validating extended range phase functions Phase functions can be validated by comparing correlations to results computed from full Monte-Carlo simulations. Monodispersions of microscopic silica beads are well-suited for validation because their scattering effects are well described by Mie theory. Alterman et al. validate their results by comparing closed-form correlations from Equation 1.9 to results to a Monte-Carlo simulator [3] that has been verified against an accurate wave solver [30]. We assess our results in two. First, we verify our acquisition setup and single-scattering computations by comparing acquired $3\mu m$ and $10\mu m$ monodispersions to Mie theory. We then validate results for non-monodisperse samples that are not easily characterized for simulation (e.g., mustard, milk, honey) by comparing our acquired phase functions to those acquired by Alterman et al. over angular ranges up to approximately 8 degrees [1]. Given extended-range verification against theory and limited-range validation with related work, we consider our extended-range measurements valid.

Chapter 2

Scatterometer design

In this chapter, we delve into the scatterometer design as well as the calibration and alignment process.

2.1 System design

Our scatterometer (detailed in Figures 2.1 and 2.2) consists of two mutually coherent, collimated beams of wavelength 532 nm separated vertically by a small angle of approximately 4° (assumed to be within the memory effect range for materials of interest). Both beams are attached to a stage that rotates the beams azimuthally about a scattering sample located on the stage's rotation axis. The intensity of scattered light is measured by a stationary camera as the beams are swept through a range of approximately 180°. The correlation of both beams' speckle images at a given azimuthal angle is proportional to the scattering phase function as a function of angle.

There are three primary components for acquisition. The first is the acquisition camera which we use to record speckle images. The second is the illuminator assembly which adjusts the angular illuminator separation and the azimuthal illumination direction relative to the acquisition camera. The third is the sample assembly which orients and positions the sample such that it is located on the azimuthal rotation axis of the illuminator assembly and maximal light is scattered towards the acquisition camera.

2.1.1 Acquisition camera

The acquisition camera must record high-contrast speckle images and assign directions to light arriving at the camera. A desirable camera and lens combination is one that maximizes angular resolution and light efficiency. Therefore, we choose a camera with a large sensor and small pixel pitch, and a fast lens focused at infinity with a long focal length.

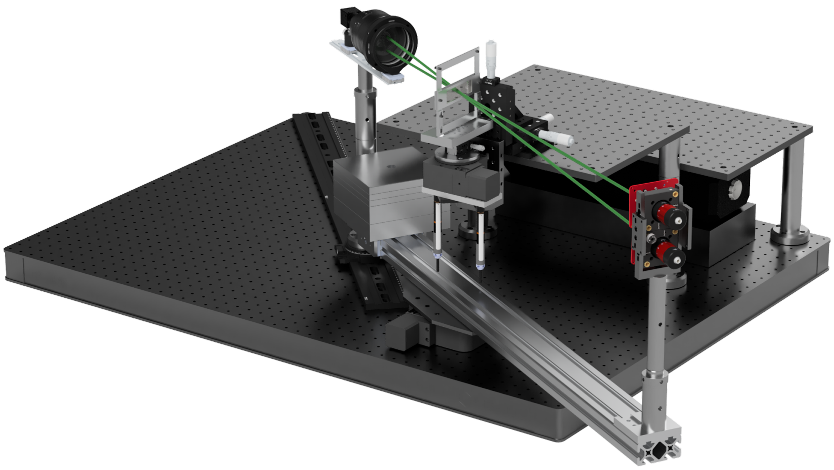


Figure 2.1: CAD rendering of speckle correlation scatterometer

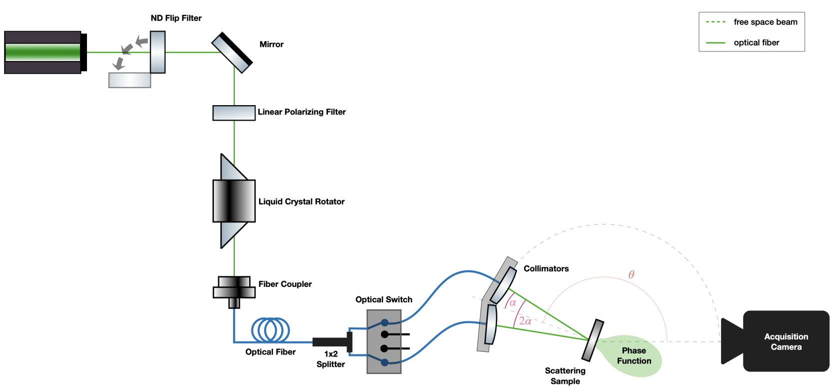


Figure 2.2: Light path diagram for speckle correlation scatterometer

Lens Focal Length Computing the speckle correlation from images produced by the two illuminators requires both beams to fall within the camera's FOV. Since we maximize single-scattered light by minimizing the illuminator separation, a lens with a small FOV corresponds to illuminators with a small angular separation. However, due to the finite size of the kinematic mounts, there is a minimum vertical separation. This minimum vertical separation and the FOV-limited angle between the beams define a triangle whose length is the distance from the illuminators' kinematic mounts to the scattering sample. An 85 mm lens allows a small beam angle 2.47° relative to horizontal and an overall setup size that complies with space constraints.

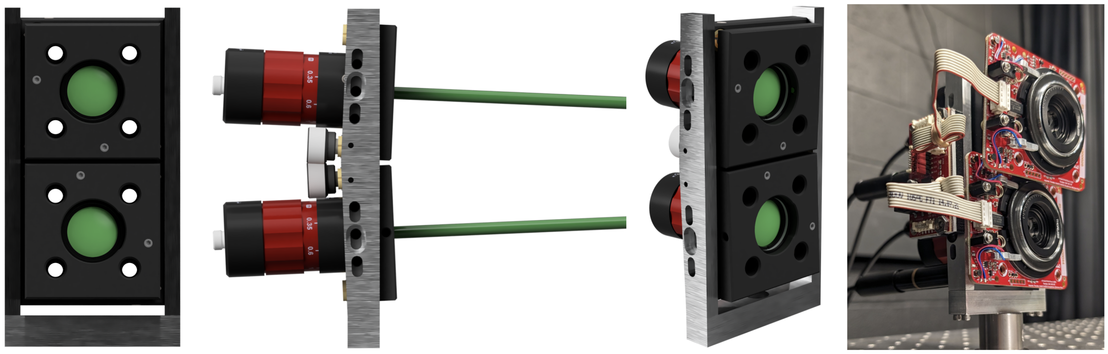
We use a FLIR Grasshopper scientific camera model GS3-PGE-91S6M-C with an AF-S Nikkor 85mm f/1.4G lens for acquisition.

Table 2.1: Acquisition camera specifications

Property	**Spec**
Camera Model	GS3-PGE-91S6M-C
Resolution	3376×2704
Megapixels	9.1
Pitch	3.69 μm
Sensor	Sony ICX814
Sensor Type	CCD
Sensor Size	12×10 mm
Spectrum	Mono
Lens Make	Nikkor
Lens Focal Length	85 mm
Lens Aperture	f/1.4
Lens Working Distance	∞

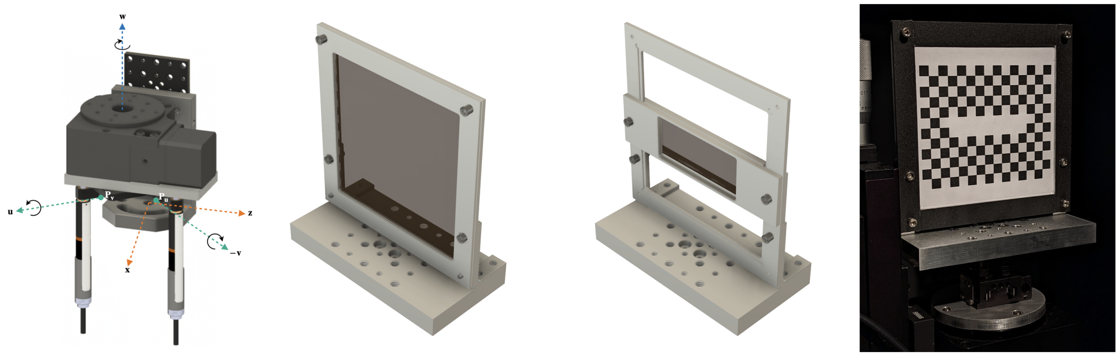
2.1.2 Illuminator assembly

The illuminator motion assembly controls the illumination beams' directions both in azimuth and elevation. The primary design considerations are high angular resolution and repeatability for fine control of the illumination configuration, and structural stability to minimize vibrations. Each illuminator is attached to a 2-axis kinematic mount that allows $\pm 5°$ in tip and $\pm 3°$ in tilt. Both kinematic mounts are attached to a custom collimator mount that minimizes their vertical separation while complying with the FOV constraint of $4.93°$ between the illuminators. The collimator mount is attached to the azimuthal rotation stage via an aluminum extrusion.



(a) (b) (c) (d)

Figure 2.3: (a) CAD front view of collimator mount; (b) CAD side view showing the relative orientations of illumination beams; (c) CAD perspective view; (d) Fully assembled collimator mount which controls vertical and angular illuminator separation. Beam diameter is also controlled using motorized iris diaphragms.



(a) (b) (c) (d)

Figure 2.4: (a) Sample motion assembly without sample mount; (b) Sample mount configured for calibration target (not drawn to scale with respect to (a)); (c) Sample mount configured for scattering sample on a microscope slide (not drawn to scale with respect to (a)); (d) Sample mount shown on top of sample assembly with calibration target installed

2.1.3 Sample assembly

The sample motion assembly is primarily used to rotate the scattering sample in order to maximize the amount of laser light transmitted through the air-glass interface as the illuminators' azimuthal position changes. This rotation is controlled by a small rotation stage which is mounted on an XYZ stage and an tip/tilt stage. These additional stages are used to control the rotation stage's orientation so it can made to be collinear with the illuminator assembly's azimuthal rotation axis. There is an additional translation stage mounted to the rotation stage's motion plate that is used to align the center of a mounted sample with the upper- and lower motion stages' rotation axes.

Sample Mount

The sample mount is a custom, dual purpose mount used to hold scattering samples during acquisition and checkerboard targets during calibration. It is designed such that the front face of a calibration target is in the same plane as the central plane of a scattering sample. It consists of a base and angle mounts used to attach a square aluminum frame that holds a 10×10 cm glass window in place through compression by tightening four thumbscrews. Scattering samples are mounted by removing the aluminum frame's front face and attaching an inset frame that holds microscope slides via compression.

Chapter 3

Scatterometer calibration and alignment

3.1 Calibration and alignment

3.2 Lower Stage Calibration

The goal of calibrating the lower assembly is to estimate its rotation axis and the 3D orientation of the illumination beams as a function of the azimuth angle θ. We do so by computing the 3D intersection of each illumination beam with a series of N planes whose poses we know. This process is repeated for all $\theta \in \Theta$ for a total of $2N|\Theta|$ points. From this set of points, we can estimate the illumination directions for

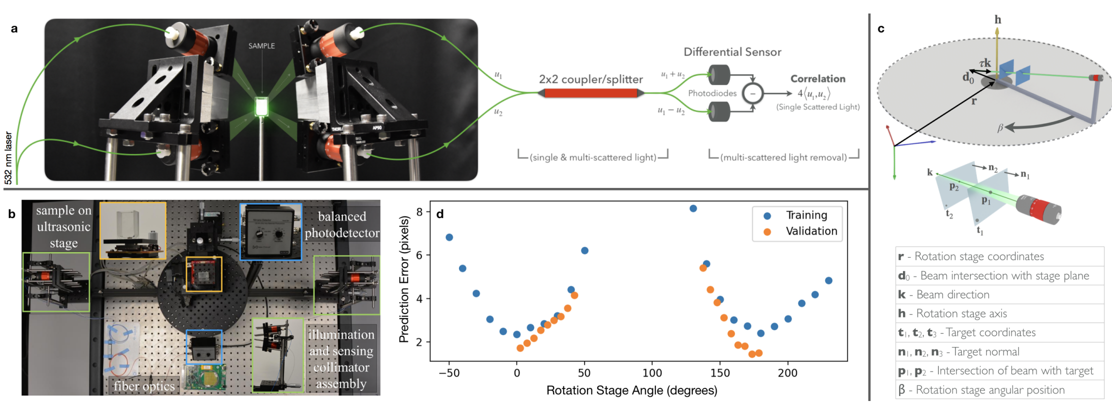


Figure 3.1: **a**: Speckle correlation computation pipeline. The sample is illuminated by two beams, and the correlation is computed using a differential sensor. **b**: Physical setup with sample placed on the circular breadboard. The illumination stand rotates about the sample while the sensing stand measures scattered light. The differential photodetector enables fast correlation computation. **c**: Geometry used to develop forward model for inverse problem estimation of 3D beam-plane intersection points. **d**: Mean estimation errors for training and validation phases showing angular dependence of error.

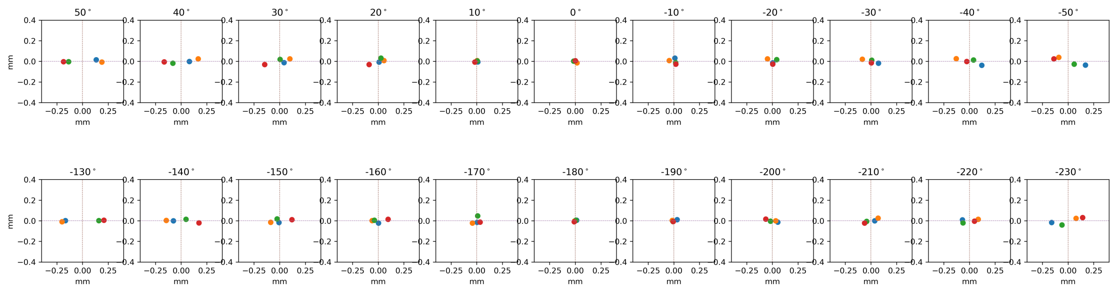


Figure 3.2: Perpendicular offsets of the four observed beam-plane intersections with respect to the estimated beam direction. Each plot is for an azimuthal angle $\theta \in \Theta$. The cause of increasing perpendicular offsets for increasing angle with respect to the plane normal and anti-normal is unknown.

both beams as a function of θ and the azimuth stage pose up to a rotational ambiguity about its rotation axis.

Azimuth Stage Rotation Axis Each beam is associated with a set of $N|\Theta|$ points. Define a set of difference vectors $\{\tilde{\boldsymbol{k}}_\theta\},\ |\{\tilde{\boldsymbol{k}}_\theta\}| = L$ as the differences between all N permute 2 points along a ray. We define a ray as a beam located at any particular $\theta \in \Theta$. Each $\tilde{\boldsymbol{k}}_\theta$ makes an angle $\pi/2 - \alpha$ with the rotation axis. However, the ${}_L P_2$ second order difference vectors are perpendicular to the azimuth rotation axis $\hat{\mathbf{h}}$, and we estimate $\hat{\mathbf{h}}$ as their null space.

Beam Direction for $\theta = 0$ Once we know the azimuth rotation axis, we can use it to estimate both illuminators' beam directions. For each $\theta \in \Theta$, we compute the centroid $\overline{\boldsymbol{p}}_\theta = \frac{1}{N} \sum p_n$. We subtract the centroid from the point set so it is zero mean and rotate it about $\hat{\mathbf{h}}$ by $-\theta$ so all points are aligned with $\theta = 0$. The beam direction $\boldsymbol{k}_0$ is simply the point set's principal component.

3.2.1 Stage Position & Beam Direction as a Function of θ

Assume a collimated beam fixed to a rotation stage with location $\boldsymbol{r}$ and rotation axis $\hat{\mathbf{h}}$. If the stage is rotated 360 degrees, the pencil of rays created by the rotated beam will form a paraboloid with axis $\hat{\mathbf{h}}$ and small radius ρ equal to the distance of closest encounter of the beam with the paraboloid axis. The locus of these points of closest encounter constitutes the beam's ray envelope. Note: Insert ray envelope theory The isoline of the ray envelope is

$$\boldsymbol{c}(\theta) = \boldsymbol{r} + \delta\hat{\mathbf{h}} + r(\theta)\boldsymbol{\rho}_0, \tag{3.1}$$

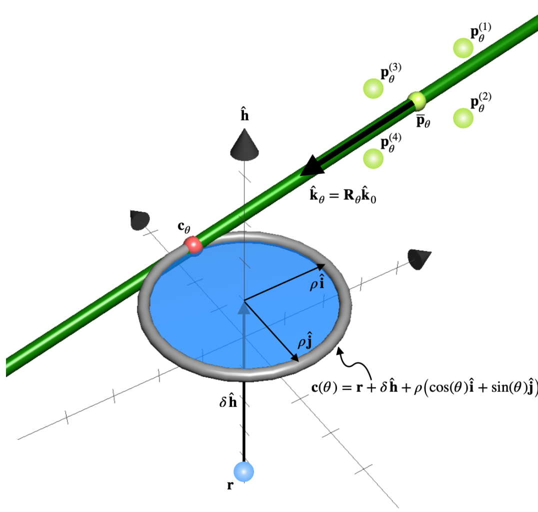


Figure 3.3: RT-5 Geometry - Frustrum top Surface

where δ is the height of the circle above the stage, $\boldsymbol{\rho}$ is a 2×1 vector. $r(\theta)$ is a 3×2 matrix consisting of a rotation of two basis vectors $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$ through an angle of θ about the rotation axis $\hat{\mathbf{h}}$ with each basis vector being perpendicular to $\hat{\mathbf{h}}$

$$r(\theta) = \boldsymbol{R}(\hat{\mathbf{h}}, \theta) \begin{bmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} \end{bmatrix}, \quad \boldsymbol{R}(\hat{\mathbf{h}}, \theta) \in \mathbb{R}^{3\times 3}. \tag{3.2}$$

If M points $\boldsymbol{p}_\theta^{(1)}, \boldsymbol{p}_\theta^{(2)}, \dots, \boldsymbol{p}_\theta^{(M)}$ are measured along the ray at a given rotation stage position $\theta \in \Theta$, then the beam with direction $\hat{\mathbf{k}}_\theta$ passes through their centroid $\overline{\boldsymbol{p}}_\theta$ with its pencil defined

$$\boldsymbol{l}_\theta(s) = \overline{\boldsymbol{p}}_\theta + s\hat{\mathbf{k}}_\theta \tag{3.3}$$

3.2.2 Azimuth Stage Location

Given the problem formulation, the objective is to find the circular conic section with perimeter $\boldsymbol{c}(\theta)$ by choosing $\boldsymbol{r}$ such that the circle's radius ρ is minimized. We achieve this by computing the minimum distance of each beam from the axis of rotation and minimizing the variance across all angles:

$$\min_{\boldsymbol{r}} g_2(\boldsymbol{r}) \tag{3.4}$$

$$\min_{\boldsymbol{r}} \sigma^2(\{\rho_\theta\}) \tag{3.5}$$

$$\min_{\boldsymbol{r}} \sum_{\theta \in \Theta} (\rho_\theta - \overline{\rho})^2 \tag{3.6}$$

where

$$\rho_\theta = \hat{\mathbf{n}}_\theta^\top(\overline{\boldsymbol{p}}_\theta - \boldsymbol{r}), \quad \hat{\mathbf{n}}_\theta = \frac{\hat{\mathbf{k}}_\theta \times \hat{\mathbf{h}}}{\|\hat{\mathbf{k}}_\theta \times \hat{\mathbf{h}}\|}, \quad \overline{\rho} = \frac{1}{|\Theta|}\sum \rho_\theta \tag{3.7}$$

We minimize the objective by computing its partial derivative with respect to $\boldsymbol{r}$. Firstly, we define

$$\overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}} = \frac{1}{|\Theta|}\sum \hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta, \quad \overline{\boldsymbol{n}} = \frac{1}{|\Theta|}\sum_\theta \hat{\mathbf{n}}_\theta, \tag{3.8}$$

and compute the partial derivative with respect to $\boldsymbol{r}$:

$$\frac{\partial g_2(\boldsymbol{r})}{\partial \boldsymbol{r}} = \sum_\theta (\rho_\theta - \overline{\rho})(\overline{\boldsymbol{n}} - \hat{\mathbf{n}}_\theta) \tag{3.9}$$

$$= \sum_\theta \Big[- (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta + (\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta + \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\hat{\mathbf{n}}_\theta - (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta + (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\overline{\boldsymbol{n}} - (\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\overline{\boldsymbol{n}} - \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\overline{\boldsymbol{n}} + (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\overline{\boldsymbol{n}} \Big] \tag{3.10}$$

$$= \sum_\theta \Big[- (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta + \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\hat{\mathbf{n}}_\theta + (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\overline{\boldsymbol{n}} - \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\overline{\boldsymbol{n}} \Big] + \sum_\theta \Big[(\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta - (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta - (\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\overline{\boldsymbol{n}} + (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\overline{\boldsymbol{n}} \Big] \tag{3.11}$$

We define

$$\boldsymbol{N}_\theta = \sum_\theta \hat{\mathbf{n}}_\theta \hat{\mathbf{n}}_\theta^\top, \quad \overline{\boldsymbol{N}}_\theta = \sum_\theta \hat{\mathbf{n}}_\theta \overline{\boldsymbol{n}}^\top, \quad \overline{\boldsymbol{N}} = \sum_\theta \overline{\boldsymbol{n}}\overline{\boldsymbol{n}}^\top, \tag{3.12}$$

set the partial derivative equal to zero, and rearrange it to the form $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$:

$$\sum_\theta \Big[\hat{\mathbf{n}}_\theta \hat{\mathbf{n}}_\theta^\top - \hat{\mathbf{n}}_\theta \overline{\boldsymbol{n}}^\top - \overline{\boldsymbol{n}}\hat{\mathbf{n}}_\theta^\top + \overline{\boldsymbol{n}}\overline{\boldsymbol{n}}^\top \Big]\boldsymbol{r} = \sum_\theta \Big[(\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta - \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\hat{\mathbf{n}}_\theta - (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\overline{\boldsymbol{n}} + \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\overline{\boldsymbol{n}} \Big] \tag{3.13}$$

$$\big(\boldsymbol{N}_\theta - \overline{\boldsymbol{N}}_\theta - \overline{\boldsymbol{N}}_\theta^\top + \overline{\boldsymbol{N}}\big)\boldsymbol{r} = \sum_\theta (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta - \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\sum_\theta \hat{\mathbf{n}}_\theta + \Big(- \sum_\theta \hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta + \sum_\theta \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}} \Big)\overline{\boldsymbol{n}} \tag{3.14}$$

$$\big(\boldsymbol{N}_\theta - 2\overline{\boldsymbol{N}}_\theta + \overline{\boldsymbol{N}}\big)\boldsymbol{r} = \sum_\theta (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta - \overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}|\Theta|\overline{\boldsymbol{n}} + \Big(- |\Theta|\overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}} + |\Theta|\overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}} \Big)\overline{\boldsymbol{n}} \tag{3.15}$$

$$\big(\boldsymbol{N}_\theta - 2\overline{\boldsymbol{N}}_\theta + \overline{\boldsymbol{N}}\big)\boldsymbol{r} = \sum_\theta (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta - |\Theta|\overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}}\overline{\boldsymbol{n}} \tag{3.16}$$

We solve equation 3.42 with the equality constraint $\hat{\mathbf{h}}^\top(\boldsymbol{r} - \boldsymbol{t}_2) = 0$. The resulting RT-5 location $\boldsymbol{r}$ is similar to the estimate in the first method with a displacement vector norm of only 0.001 mm, and the mean distance $\overline{\rho} = 0.42$mm (as expected).

3.2.3 Ray Envelope Center

Given $\boldsymbol{r}$ and $\{\rho_\theta\}_\Theta$, a point $\boldsymbol{c}_\theta$ is defined on each ray such that its distance from the RT-5 axis is equal to ρ_θ.

$$\boldsymbol{c}_\theta = \overline{\boldsymbol{p}}_\theta + t_\theta \hat{\mathbf{k}}_\theta \tag{3.17}$$

where

$$t_\theta = \frac{\boldsymbol{m}_\theta^\intercal B(\boldsymbol{r} - \overline{\boldsymbol{p}}_\theta)}{\boldsymbol{m}_\theta^\intercal B\hat{\mathbf{k}}_\theta}, \quad \boldsymbol{m}_\theta = \hat{\mathbf{n}}_\theta \times \hat{\mathbf{k}}_\theta \tag{3.18}$$

Given the set $\{\boldsymbol{c}_\theta\}_\Theta$, we solve the following minimization problem to choose the center of the circular ray envelope $\boldsymbol{r} + \delta\hat{\mathbf{h}}$ whose radius is $\overline{\rho}_\theta$:

$$\begin{aligned} &\min_\delta g_3(\boldsymbol{r}, \delta, \boldsymbol{c}_\theta) \\ &\min_\delta \sum_{\theta\in\Theta} \left(\|\boldsymbol{c}_\theta - \boldsymbol{r} - \delta\hat{\mathbf{h}}\|^2 - \overline{\rho}^2\right)^2. \end{aligned} \tag{3.19}$$

The partial derivative with respect to δ is

$$\frac{\partial g_3(\boldsymbol{r}, \delta, \boldsymbol{c}_\theta)}{\partial \delta} = 4|\Theta|\delta^3 + 3B\delta^2 + 2C\delta + D = 0 \tag{3.20}$$

where

$$B = 4\hat{\mathbf{h}}^\intercal \sum (\boldsymbol{r} - \boldsymbol{c}_\theta), \quad C = 2\sum \left[2(\boldsymbol{r} - \boldsymbol{c}_\theta)^\intercal \hat{\mathbf{h}}\hat{\mathbf{h}}^\intercal (\boldsymbol{r} - \boldsymbol{c}_\theta) + \|\boldsymbol{c}_\theta\|^2 - 2\mathbf{c}_\theta^\intercal \boldsymbol{r} + \|\boldsymbol{r}\|^2\right], \tag{3.21}$$

$$D = 4\hat{\mathbf{h}}^\intercal \sum (\boldsymbol{r} - \boldsymbol{c}_\theta)(\|\boldsymbol{c}_\theta\|^2 - 2\mathbf{c}_\theta^\intercal \boldsymbol{r} + \|\boldsymbol{r}\|^2) \tag{3.22}$$

The partial derivative is a third degree polynomial whose roots minimize the objective function $g_3()$. We find its roots via the roots() method from the numpy.polynomial.Polynomial class.

3.2.4 Ray Envelope Isoline

We find its radius and orientation defined by the vector $\boldsymbol{\rho}_0$ such that $\boldsymbol{c}(0) = \boldsymbol{r} + \delta\hat{\mathbf{h}} + \boldsymbol{\rho}_0$ is the point on the ray envelope corresponding to azimuthal position 0°. Given $\boldsymbol{r}$ and δ, and a set of points $\{\boldsymbol{c}_\theta\}$ defined by the intersections of rays with the ray envelope plane, we can solve for the least-squares optimal $\boldsymbol{\rho}_0$ using Equation 3.33:

$$\min_{\boldsymbol{\rho}_0} \sum_\theta \|R_\theta \boldsymbol{\rho}_0 - (\boldsymbol{c} - \boldsymbol{r} - \delta\hat{\mathbf{h}})\| \tag{3.23}$$

3.2.5 Training & Validation Datasets

The training set consists of 22 rotation stage positions in 10° increments spanning ±50° relative to the normal on both faces of a target, totaling 100° and a measurement for each target. The differences of these 3D point-plane intersections are computed as the initial beam direction estimates $\overline{\mathbf{k}}$. Given a learned model, the objective is to predict point-plane intersections for new planes and angles. The similar to training but with random target positions and a smaller angular sweep. Actual phase function measurements will be constrained to a 180° range. Therefore, the validation set consists of angles within this range, each offset from training angles by 5°.

3.3 Sample Motion Assembly Calibration

The goal in calibrating the sample motion assembly is estimating the primary rotation stage's pose as well as the translation and rotation axes of all stages used to position and orient the rotation stage.

Rotation Stage Pose Estimating the rotation stage pose is similar to the method used to estimate the azimuthal rotation axis. Rather than rotating a laser and computing beam-plane intersections, we we take photos of a series of N rotated planes and detect a 3D grid of M points on each plane. ${}_N P_2$ 1st-order difference vectors are computed for each of the M points in the grid totaling $M({}_N P_2)$ vectors that are in the plane of rotation. The rotation axis $\hat{\mathbf{w}}$ is perpendicular to the plane of rotation and is therefore the null space of the vector set.

Translation Stage Axes All translation stage axes are estimated by computing 3D coordinates of checkerboard corners at several positions along the translation stage's range of motion. Difference vectors are computed for all combinations of corresponding points on the planes, and the axis is the mean of all difference vectors. The vector is oriented to point in the direction of increasing stage position.

Tip & Tilt Stage Axes The sample assembly is oriented using a 2-axis tip/tilt kinematic stage. These axes are not used in any analytical expressions; they are simply used as a 2D basis for azimuthal rotation axis PID alignment. Their limited range of motion and image noise produce unstable estimates, so visually approximated estimates are sufficient as long as the axes are perpendicular.

3.4 Aligning Sample and Illuminator Assemblies

The sample and illuminator assemblies are aligned when their rotation axes are collinear.

3.4.1 Rotation

We define a plane $\mathbf{\Pi}$ with normal vector $\hat{\mathbf{h}}$ and origin $\boldsymbol{p}_{\hat{\mathbf{h}}}$. This plane defines a basis with projection matrix $\mathbf{\Pi} \in \mathbb{R}^{2\times 3}$ whose rows are in the null space of $\hat{\mathbf{h}}$. The sample assembly's rotation axis $\hat{\mathbf{w}}$ is aligned with the azimuthal axis when its projection $\mathbf{\Pi}\hat{\mathbf{w}} = \mathbf{0}$. For PID control we seek to express the alignment error vector $\boldsymbol{\epsilon} = \mathbf{\Pi}\hat{\mathbf{w}}$ in terms of two independent error components ϵ_u and ϵ_v controlled by u- and v-axis rotation respectively. Since rotation affects motion in a plane perpendicular to the axis, and the tip and tilt axes are perpendicular, we can express the alignment errors independently by defining a new error vector $\boldsymbol{\epsilon}'$ in terms of a modified basis $\boldsymbol{\Pi}' = \boldsymbol{\Pi}[\hat{\mathbf{u}}\ \hat{\mathbf{v}}]$. The new error vector is

$$\boldsymbol{\epsilon}' = \begin{bmatrix} \epsilon'_v \\ \epsilon'_u \end{bmatrix} = \boldsymbol{\Pi}'\hat{\mathbf{w}}. \tag{3.24}$$

Note the swapped order of the elements in the error vector due to perpendicularity: the u-axis error is the projection of $\hat{\mathbf{w}}$ onto the v-axis, and the v-axis error is the projection of $\hat{\mathbf{w}}$ onto the u-axis. This modified basis preserves the mapping of zero alignment error to the zero vector.

Although the tip and tilt axes are perpendicular, they are not independent since the square motion plate is actuated at opposite corners with a shared ball joint pivot point at another. Therefore, the alignment loop alternates between the u- and v-axis PID controllers with state error updates between each controller. The stage has limited range of motion due to space constraints, so we use the Zielger-Nichols "no overshoot" gain configuration.

Translation Once the two rotation axes are parallel, we use the x- and z-axis translation stages to make the collinear.

3.5 Aligning Calibration Target with Sample Motion Assembly Rotation Axis

The compact translation stage mounted on top of the RT-3 stage is used to position the calibration target locally such that the RT-3's rotation axis intersects the calibration target's surface at the height of a scattering sample. The error is computed by first defining a horizontal line on the calibration target whose height places it approximately midway along the height of a scattering sample. Define the minimum-length displacement vector between the two axes as $\boldsymbol{\delta}$. The error is then the projection of $\boldsymbol{\delta}$ onto the stage's translation axis $\boldsymbol{m}$.

Define the mean beam direction vector $\overline{\boldsymbol{k}} = (\hat{\mathbf{k}}_0^{(a)} + \hat{\mathbf{k}}_0^{(b)})/2$. For target with plane normal $\hat{\mathbf{z}}$, the objective is

$$\min_{\psi} 1 - \overline{\boldsymbol{k}}^\top \hat{\mathbf{z}}(\psi) \tag{3.25}$$

where $\hat{\mathbf{z}}(\psi) = \boldsymbol{R}_{\hat{\mathbf{w}}}\hat{\mathbf{z}}_0$ is the initial normal vector rotated about $\hat{\mathbf{w}}$ by an angle ψ.

Two points $\boldsymbol{P}_1, \boldsymbol{P}_2$ on plane Π_a with corresponding image points $\boldsymbol{p}_1, \boldsymbol{p}_2 \in \mathbb{P}^2$ create the line $\boldsymbol{\ell} = \boldsymbol{p}_1 \times \boldsymbol{p}_2$. We write the Euclidean intersection of the $\boldsymbol{w}$ axis with plane Π_a as $\boldsymbol{P}_i = \boldsymbol{P}_{w'} + \gamma_{\Pi_b}\hat{\mathbf{w}}$ where Π_b: kernel$(\boldsymbol{P}_1, \boldsymbol{P}_2, \boldsymbol{P}_3)$ s.t. $\measuredangle(\Pi_a, \Pi_b) = \pi/4$. Goal: Adjust compact stage position such that $\boldsymbol{P}_i$ lies on $\boldsymbol{\ell}$. This is true when $\boldsymbol{p}_i^\top \boldsymbol{\ell} = 0$ in the image frame.

$$\hat{\mathbf{z}}' = \frac{(\boldsymbol{P}_2 - \boldsymbol{P}_1) \times (\boldsymbol{P}_3 - \boldsymbol{P}_1)}{\|(\boldsymbol{P}_2 - \boldsymbol{P}_1) \times (\boldsymbol{P}_3 - \boldsymbol{P}_1)\|} \tag{3.26}$$

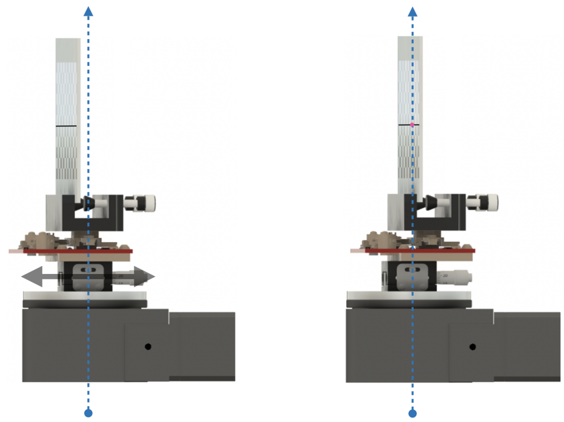


Figure 3.4: Sample motion assembly without sample mount

$$\boldsymbol{p}_i = \tau \boldsymbol{M}\Big((\boldsymbol{\alpha}^\intercal \hat{\mathbf{z}}')\delta + \hat{\mathbf{w}}(\boldsymbol{P}_1 - \boldsymbol{P}_{w'})^\intercal \hat{\mathbf{z}}' + \frac{1}{\tau}\boldsymbol{P}_{w'}\Big) \tag{3.27}$$

where $\boldsymbol{M}$ is the camera projection matrix, and $\tau = (\boldsymbol{w}^\intercal \hat{\mathbf{z}}')^{-1}$

$$\boldsymbol{\ell} = \boldsymbol{M}\Big((\boldsymbol{\alpha} \times \boldsymbol{P}_2 + \boldsymbol{P}_1 \times \boldsymbol{\alpha})\delta + \boldsymbol{P}_1 \times \boldsymbol{P}_2\Big) \tag{3.28}$$

The signed error is

$$\epsilon = \boldsymbol{p}_i^\intercal \boldsymbol{\ell} \tag{3.29}$$

3.6 Aligning Sample Motion Assembly and Illumination Beams

The objectives for beam alignment are to orient the two laser beams such that 1) their intersection point is located on the RT-3 and RT-5 rotation axes, 2) their mean direction is perpendicular to the rotation axis, and 3) they are normal to the calibration target's surface. We will consider the upper and lower stages' axes collinear, and alignment will be discussed with respect to the azimuthal axis of the lower stage assembly.

Beams equianglular with respect to RT-3 and RT-5 axes The mean direction is perpendicular to the rotation axis when both beams' projections onto the azimuthal axis are equal and opposite:

$$0 = \hat{\mathbf{k}}_a^\intercal \boldsymbol{h} + \hat{\mathbf{k}}_b^\intercal \boldsymbol{h}. \tag{3.30}$$

Define both collimators' positions $\boldsymbol{c}_a, \boldsymbol{c}_b$, and assume both beams intersect at point $\boldsymbol{p}$ on the azimuthal axis. The ideal intersection point $\boldsymbol{p}^*$ is located at the intersection of the collimators' horizontal plane of symmetry and the azimutahl axis. $\boldsymbol{p}$ is offset from the ideal intersection point by displacement vector $\boldsymbol{\delta} = \boldsymbol{p}^* - \boldsymbol{p} = d \cdot \boldsymbol{h}$. Equation 3.30 can be rewritten in terms of these variables to solve for the displacement distance d along $\hat{\mathbf{h}}$:

$$\begin{aligned} 0 &= (\boldsymbol{p} + \boldsymbol{\delta} - \boldsymbol{c_a})^\top \boldsymbol{h} + (\boldsymbol{p} + \boldsymbol{\delta} - \boldsymbol{c_b})^\top \boldsymbol{h} \\ 2\boldsymbol{\delta}^\top \boldsymbol{h} &= (\boldsymbol{c_a} - \boldsymbol{p})^\top \boldsymbol{h} + (\boldsymbol{c_b} - \boldsymbol{p})^\top \boldsymbol{h} \\ 2\boldsymbol{\delta}^\top \boldsymbol{h} &= (\boldsymbol{c_a} - \boldsymbol{p} + \boldsymbol{c_b} - \boldsymbol{p})^\top \boldsymbol{h} \\ d \cdot \boldsymbol{h}^\top \boldsymbol{h} &= \tfrac{1}{2}(\boldsymbol{c_a} - \boldsymbol{p} + \boldsymbol{c_b} - \boldsymbol{p})^\top \boldsymbol{h} \\ d &= \tfrac{1}{2}\big[(\boldsymbol{c_a} - \boldsymbol{p}) + (\boldsymbol{c_b} - \boldsymbol{p})\big]^\top \boldsymbol{h} \end{aligned} \tag{3.31}$$

The displacement vectors $\boldsymbol{c_a} - \boldsymbol{p}$ and $\boldsymbol{c_b} - \boldsymbol{p}$ are unknown since the collimator positions are unknown. However, the normalized beam directions $\hat{\mathbf{k}}_a, \hat{\mathbf{k}}_b$ are parallel to these displacement vectors, so we use a scalar coefficient s to achieve the correct scale. We determine s using the CAD model based on the nominal design geometry, and the final beam intersection displacement expression is

$$d = -\frac{s}{2}(\hat{\mathbf{k}}_a + \hat{\mathbf{k}}_b)^\top \boldsymbol{h}. \tag{3.32}$$

The alignment procedure is as follows. Since the beams' orientations have been adjusted since their initial estimation, we begin by updating their estimates. We use a method similar to that detailed in section 3.2, but we make measurements at a single azimuthal position $\theta = 0$. With updated $\hat{\mathbf{k}}_a$ and $\hat{\mathbf{k}}_b$, we compute the required intersection point displacement via Equation 3.32. The displacement is projected into the image frame, and the beams are commanded to the corresponding pixel backprojected to the calibration target. This process is repeated iteratively until the displacement distance is below a threshold due to inaccuracies introduced by the rough estimate of the scale factor s and other noise sources.

3.7 Aligning Calibration Target with Illumination Beams

This alignment step determines the "home" position of the sample assembly's rotation stage which corresponds to sample illumination along its normal vector. The home position maximizes the inner product of the target's normal vector and the mean illumination beam vector $\overline{\boldsymbol{k}} = (\hat{\mathbf{k}}_a + \hat{\mathbf{k}}_b)/2$.

3.8 Note: Poporsal:Acquisition Camera Calibration

The projection matrix can be estimated via PnP in theory. However, we found it challenging in practice due to 3D points at infinity providing no depth information, and the geometry of a camera focused at

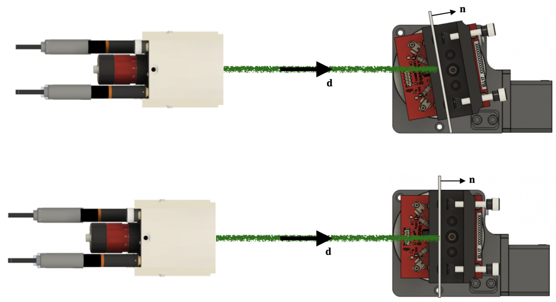


Figure 3.5: Top: Target and beam misaligned due to non-zero angle between the beam and the target normal; Bottom: $\boldsymbol{d}$ aligned with normal vector $\boldsymbol{n}$. Note: Update by replacing d with kbar.

infinity producing unstable estimates due to an effective coupling of the intrinsic parameters. Note: Add reasons they fail. Since the acquisition camera maps points from the plane at infinity to the image plane, the homography for these planes is the projection matrix. However, there is an effective coupling of intrinsic parameters that complicates decomposing the projection matrix into a product of intrinsic and extrinsic matrices.

A camera focused at infinity maps rays along its optical axis to its principal point; all directions measured relative to the optical axis are mapped to image points relative to the principal point. Translating the principal point is similar to rotating the camera externally under the small angle approximation $\tan(\phi) \approx \phi$. Therefore, these two parameters are effectively coupled for a non-WFOV camera. Note: Insert figure showing reprojection error loss vs. pp and rotation. To avoid this issue, we estimate the focal length using a simple geometric relationship describing pinhole cameras focused at infinity followed principal point estimation via inspection. Once the intrinsics are known, we estimate the rotation matrix and the lens distortion coefficients simultaneously.

3.8.1 Intrinsics

Rays entering the camera at an angle ϕ with respect to the optical axis are mapped to a point $f_{px}\tan(\phi)$ pixels from the principal point. This relation can be used to estimate the focal length given a set of rays with known directions and their corresponding image pixel coordinates. Since beam directions are known for all azimuth angles from lower stage calibration Note: Insert reference, we acquire images of beams rotated azimuthally, we compute the ray angle with respect to the optical axis and the pixel spacing. If we plot the pixel spacing vs. the tangent of the local ray angle, the line of best fit has a slope equal to the equivalent pinhole's focal length. We estimate the principal point by shining a collimated source into the lens oriented so it is approximately parallel to the lens' optical axis. The location of its

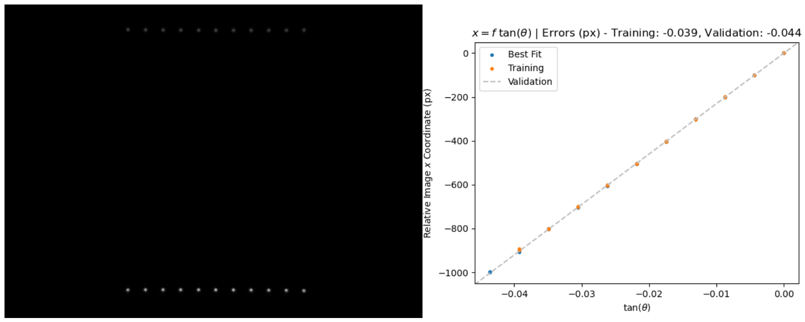


Figure 3.6: Left: Composite of 11 images of both illuminators spanning an azimuth range 3.5°. Right: The acquisition camera's focal length is the constant of proportionality of image point displacement and the tangent of the internal ray angle with respect to the optical axis.

image is assumed to be the principal point.

3.8.2 Extrinsics & Lens Distortion

Note: Newton-Raphson method via pytorch-minimize.

3.8.3 Validation

The calibration model is validated on the physical acquisition system by learning a model on training data and then evaluating performance via a validation dataset. First, a checkerboard calibration target is placed at two different locations, and its poses are determined using a calibrated camera. A laser is attached to a rotation stage, and an image of the beam spot on the target is acquired at each position. The 3D beam-plane intersection point is then calculated using beam spot centroiding to find the pixel coordinates which are backprojected to the camera's frame using the camera matrix. The rotation stage axis $\mathbf{h}$ is determined by placing a target face-up on the stage and estimating the target's normal with the camera.

Validation Results Figure 3.1d shows the training and validation estimation errors of 3D points. Angles less than 90° correspond to the target illuminated from the front with 0° corresponding to Figure 3.1c. Those to the right correspond to a back-illuminated target with 180° being anti-normal. The training and validation errors have similar trends with reduced validation error, suggesting the data was not over-fit. There is no error benchmark rooted in a performance metric. However, since centroiding and the homography computed during calibration both have sub-pixel accuracy and this is ultimately an interpolation task, the targeted prediction accuracy is sub-pixel. Considering the minimum validation error is 1.5 pixels with a mean error of 2.8 pixels, the targeted accuracy seems achievable if the issue of worsening error with angle of incidence is alleviated and the beam direction estimates are improved.

3.9 Note: Poporsal:Illuminator Assembly Calibration

The goal for calibrating the illuminator assembly is estimating its rotation axis and the 3D orientation of the illumination beams as a function of the azimuth angle θ. We do so by computing the 3D intersection of each illumination beam with a series of N planes whose poses we know. This process is repeated for all $\theta \in \Theta$ for a total of $2N|\Theta|$ points. From this point set, we can estimate illumination directions for both beams as a function of θ and the azimuth stage pose up to a rotational ambiguity about its rotation axis.

Note: Poporsal:Azimuth Stage Rotation Axis Each beam is associated with a set of $N|\Theta|$ points. Define a set of difference vectors $\{\tilde{\boldsymbol{k}}_\theta\},\ |\{\tilde{\boldsymbol{k}}_\theta\}| = L$ as the differences between all N permute 2 points along a ray. We define a ray as a beam located at any particular $\theta \in \Theta$. Each $\tilde{\boldsymbol{k}}_\theta$ makes an angle $\pi/2 - \alpha$ with the rotation axis. However, the ${}_LP_2$ 2nd order difference vectors are perpendicular to the azimuth rotation axis $\hat{\mathbf{h}}$, and we estimate $\hat{\mathbf{h}}$ as their null space.

Note: Poporsal:Beam Direction Vector Once we know the azimuth rotation axis, we can use it to estimate both illuminators' beam directions. For each $\theta \in \Theta$, we compute the centroid $\overline{\boldsymbol{p}}_\theta = \frac{1}{N}\sum p_n$. We subtract the centroid from the point set so it is zero mean, and we rotate it about $\hat{\mathbf{h}}$ by $-\theta$ so all points are aligned with $\theta = 0$. The beam direction $\boldsymbol{k}_0$ is simply the point set's principal component. For any arbitrary azimuthal angle θ, we can compute the beam direction $\boldsymbol{k}_0 = \boldsymbol{R}_{\hat{\mathbf{h}}}\boldsymbol{k}_0$ where $\boldsymbol{R}_{\hat{\mathbf{h}}}$ is a 3×3 rotation matrix with azimuthal axis $\hat{\mathbf{h}}$.

3.9.1 Note: Poporsal:Stage Position & Beam Direction as a Function of θ

Assume a collimated beam fixed to a rotation stage with location $\boldsymbol{r}$ and rotation axis $\hat{\mathbf{h}}$. If the stage is rotated 360 degrees, the pencil of rays created by the rotated beam will form a paraboloid with axis $\hat{\mathbf{h}}$ and small radius ρ equal to the distance of closest encounter of the beam with the paraboloid axis. The locus of these points of closest encounter constitute the beam's ray envelope. The isoline of the ray envelope is

$$\boldsymbol{c}(\theta) = \boldsymbol{r} + \delta\hat{\mathbf{h}} + r(\theta)\boldsymbol{\rho}_0, \tag{3.33}$$

where δ is the height of the circle above the stage, $\boldsymbol{\rho}$ is a 2×1 vector. $r(\theta)$ is a 3×2 matrix consisting of a rotation of two basis vectors $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$ through an angle of θ about the rotation axis $\hat{\mathbf{h}}$ with each basis

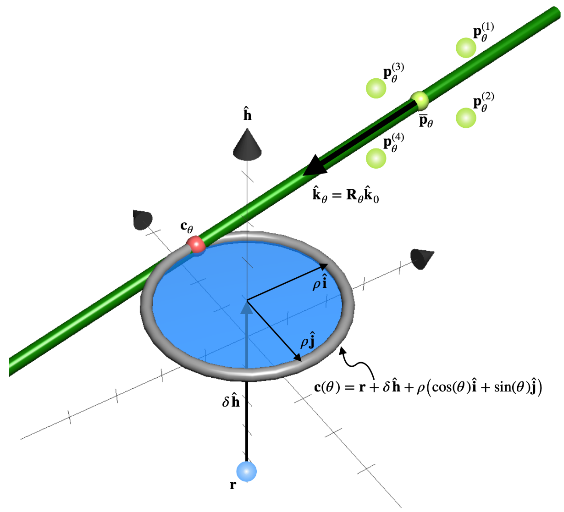


Figure 3.7: Ray envelope defined as the locus of points of closest encounter between the illumination beam and its rotation axis

vector being perpendicular to $\hat{\mathbf{h}}$

$$r(\theta) = \boldsymbol{R}(\hat{\mathbf{h}}, \theta)\begin{bmatrix}\hat{\mathbf{i}} & \hat{\mathbf{j}}\end{bmatrix}, \quad \boldsymbol{R}(\hat{\mathbf{h}}, \theta) \in \mathbb{R}^{3\times 3}. \tag{3.34}$$

If M points $\boldsymbol{p}_\theta^{(1)}, \boldsymbol{p}_\theta^{(2)}, ..., \boldsymbol{p}_\theta^{(M)}$ are measured along the ray at a given rotation stage position $\theta \in \Theta$, then the beam with direction $\hat{\mathbf{k}}_\theta$ passes through their centroid $\overline{\boldsymbol{p}}_\theta$ with its pencil defined

$$\boldsymbol{l}_\theta(s) = \overline{\boldsymbol{p}}_\theta + s\hat{\mathbf{k}}_\theta \tag{3.35}$$

3.9.2 Note: Poporsal:Azimuth Stage Location

Given the problem formulation, the objective is to find the circular conic section with perimeter $\boldsymbol{c}(\theta)$ by choosing $\boldsymbol{r}$ such that the circle's radius ρ is minimized. We achieve this by computing the minimum distance of each beam from the axis of rotation and minimizing the variance across all angles:

$$\min_{\boldsymbol{r}} \sum_{\theta\in\Theta} (\rho_\theta - \overline{\rho})^2 \tag{3.36}$$

where

$$\rho_\theta = \hat{\mathbf{n}}_\theta^\intercal(\overline{\boldsymbol{p}}_\theta - \boldsymbol{r}), \quad \hat{\mathbf{n}}_\theta = \frac{\hat{\mathbf{k}}_\theta \times \hat{\mathbf{h}}}{||\hat{\mathbf{k}}_\theta \times \hat{\mathbf{h}}||}, \quad \overline{\rho} = \frac{1}{|\Theta|}\sum \rho_\theta \tag{3.37}$$

We minimize the objective by computing its partial derivative with respect to $\boldsymbol{r}$. Firstly we define

$$\overline{\boldsymbol{n}}_{\overline{\boldsymbol{p}}} = \frac{1}{|\Theta|}\sum \hat{\mathbf{n}}_\theta^\intercal \overline{\boldsymbol{p}}_\theta, \quad \overline{\boldsymbol{n}} = \frac{1}{|\Theta|}\sum_\theta \hat{\mathbf{n}}_\theta, \tag{3.38}$$

and compute the partial derivative with respect to $\boldsymbol{r}$:

$$\frac{\partial g_2(\boldsymbol{r})}{\partial \boldsymbol{r}} = \sum_{\theta} (\rho_\theta - \overline{\rho})(\overline{\boldsymbol{n}} - \hat{\mathbf{n}}_\theta) \tag{3.39}$$

$$= \sum_{\theta} \Big[- (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta + \overline{\boldsymbol{n}}_{\overline{p}}\hat{\mathbf{n}}_\theta + (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\overline{\boldsymbol{n}} - \overline{\boldsymbol{n}}_{\overline{p}}\overline{\boldsymbol{n}} \Big] + \sum_{\theta} \Big[(\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta - (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\hat{\mathbf{n}}_\theta - (\hat{\mathbf{n}}_\theta^\top \boldsymbol{r})\overline{\boldsymbol{n}} + (\overline{\boldsymbol{n}}^\top \boldsymbol{r})\overline{\boldsymbol{n}} \Big] \tag{3.40}$$

We define

$$\boldsymbol{N}_\theta = \sum_{\theta} \hat{\mathbf{n}}_\theta \hat{\mathbf{n}}_\theta^\top, \quad \overline{\boldsymbol{N}}_\theta = \sum_{\theta} \hat{\mathbf{n}}_\theta \overline{\boldsymbol{n}}^\top, \quad \overline{\boldsymbol{N}} = \sum_{\theta} \overline{\boldsymbol{n}}\overline{\boldsymbol{n}}^\top, \tag{3.41}$$

set the partial derivative equal to zero, and rearrange it to the form $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$:

$$\big(\boldsymbol{N}_\theta - 2\overline{\boldsymbol{N}}_\theta + \overline{\boldsymbol{N}}\big)\boldsymbol{r} = \sum_{\theta} (\hat{\mathbf{n}}_\theta^\top \overline{\boldsymbol{p}}_\theta)\hat{\mathbf{n}}_\theta - |\Theta|\overline{\boldsymbol{n}}_{\overline{p}}\overline{\boldsymbol{n}} \tag{3.42}$$

We solve equation 3.42 with the equality constraint $\hat{\mathbf{h}}^\top (\boldsymbol{r} - \boldsymbol{t}_2) = 0$. The resulting RT-5 location $\boldsymbol{r}$ is similar to the estimate in the first method with a displacement vector norm of only 0.001 mm, and the mean distance $\overline{\rho} = 0.42$mm (as expected).

3.9.3 Note: Poporsal:Ray Envelope Center

Given $\boldsymbol{r}$ and $\{\rho_\theta\}_\Theta$, a point $\boldsymbol{c}_\theta$ is defined on each ray such that its distance from the RT-5 axis is equal to ρ_θ.

$$\boldsymbol{c}_\theta = \overline{\boldsymbol{p}}_\theta + t_\theta \hat{\mathbf{k}}_\theta \tag{3.43}$$

where

$$t_\theta = \frac{\boldsymbol{m}_\theta^\top B(\boldsymbol{r} - \overline{\boldsymbol{p}}_\theta)}{\boldsymbol{m}_\theta^\top B \hat{\mathbf{k}}_\theta}, \quad \boldsymbol{m}_\theta = \hat{\mathbf{n}}_\theta \times \hat{\mathbf{k}}_\theta \tag{3.44}$$

Given the set $\{\boldsymbol{c}_\theta\}_\Theta$, we solve the following minimization problem to find the optimal center of the circular ray envelope $\boldsymbol{r} + \delta\hat{\mathbf{h}}$ whose radius is $\overline{\rho}_\theta$ and minimizes the sum of the squared distances of points from the circle:

$$\begin{aligned} &\min_{\delta} g_3(\boldsymbol{r}, \delta, \boldsymbol{c}_\theta) \\ &\min_{\delta} \sum_{\theta\in\Theta} \big(\|\boldsymbol{c}_\theta - \boldsymbol{r} - \delta\hat{\mathbf{h}}\|^2 - \overline{\rho}^2\big)^2 . \end{aligned} \tag{3.45}$$

The partial derivative with respect to δ is

$$\frac{\partial g_3(\boldsymbol{r}, \delta, \boldsymbol{c}_\theta)}{\partial \delta} = 4|\Theta|\delta^3 + 3B\delta^2 + 2C\delta + D = 0 \tag{3.46}$$

where

$$B = 4\hat{\mathbf{h}}^\intercal \sum (\boldsymbol{r} - \boldsymbol{c}_\theta), \quad C = 2\sum \left[2(\boldsymbol{r} - \boldsymbol{c}_\theta)^\intercal \hat{\mathbf{h}}\hat{\mathbf{h}}^\intercal (\boldsymbol{r} - \boldsymbol{c}_\theta) + \|\boldsymbol{c}_\theta\|^2 - 2\boldsymbol{c}_\theta^\intercal \boldsymbol{r} + \|\boldsymbol{r}\|^2\right], \tag{3.47}$$

$$D = 4\hat{\mathbf{h}}^\intercal \sum (\boldsymbol{r} - \boldsymbol{c}_\theta)(\|\boldsymbol{c}_\theta\|^2 - 2\boldsymbol{c}_\theta^\intercal \boldsymbol{r} + \|\boldsymbol{r}\|^2). \tag{3.48}$$

The partial derivative is a third degree polynomial whose roots minimize the objective function $g_3(\boldsymbol{r}, \delta, \boldsymbol{c}_\theta)$.

3.9.4 Note: Poporsal:Ray Envelope Isoline

We find its radius and orientation defined by the vector $\boldsymbol{\rho}_0$ such that $\boldsymbol{c}(0) = \boldsymbol{r} + \delta\hat{\mathbf{h}} + \boldsymbol{\rho}_0$ is the point on the ray envelope corresponding to azimuthal position $0°$. Given $\boldsymbol{r}$ and δ, and a set of points $\{\boldsymbol{c}_\theta\}$ defined by the intersections of rays with the ray envelope plane, we can solve for the least-squares optimal $\boldsymbol{\rho}_0$ using Equation 3.33:

$$\min_{\boldsymbol{\rho}_0} \sum_\theta \|\boldsymbol{R}_\theta \boldsymbol{\rho}_0 - (\boldsymbol{c} - \boldsymbol{r} - \delta\hat{\mathbf{h}})\|. \tag{3.49}$$

3.10 Acquisition Camera Calibration

The projection matrix can be estimated using PnP in theory. However, we found it challenging in practice due to 3-D points at infinity providing no depth information, resulting in unstable estimation. Since the acquisition camera maps points from the plane at infinity to the image plane, the homography relating these planes is the projection matrix. However, there is an effective coupling of intrinsic and extrinsic parameters that complicates decomposing the projection matrix into a product of intrinsic and extrinsic matrices.

A camera focused at infinity maps rays parallel to its optical axis to its principal point; all directions measured relative to the optical axis are mapped to image points relative to the principal point. If p is the distance of a pixel from the principal point of a camera with focal length f, then $p = f\tan(\phi)$ for an incoming ray at angle θ with respect to the optical axis. Under the small angle approximation, $p \approx f\phi$ which means the pixel distance change proportionally to the incoming ray angle. Therefore, shifting the principal point is analogous to rotating the camera externally for small angles, and these two parameters are effectively coupled for a non-WFOV camera. This numerical coupling results in a reprojection error loss topology that is not strictly convex as shown in Figure 3.8(c). Therefore, we estimate the intrinsics by computing the focal length as the ambiguity's constant of proportionality and choosing a principal point. Once the intrinsics are known, we estimate the rotation matrix and the lens distortion coefficients simultaneously.

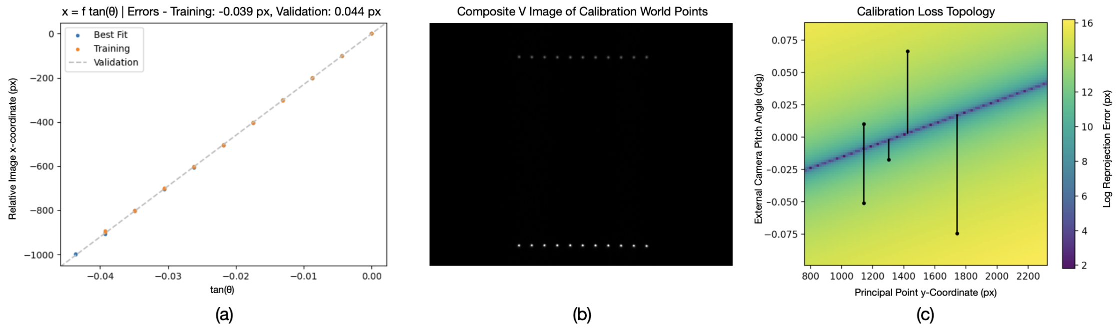


Figure 3.8: (a) The acquisition camera's focal length is the constant of proportionality of image point displacement and the tangent of the internal ray angle with respect to the optical axis; (b) Composite of 11 images of both illuminators spanning an azimuth range 3.5°; (c) Reprojection error as a function of principal point shifts along the y-axis and external pitch rotation is not strictly convex, showing the numerical ambiguity of principal point shifting and camera rotation. This ambiguity holds for the x-axis and panning as well.

Since the focal length is the constant of proportionality for beam angle and image pixel displacement and the beam directions are known for all azimuth angles from illuminator assembly calibration, we can compute the focal length. We acquire images of the two illumination beams rotated azimuthally and compute ray angles with respect to the optical axis. If we plot the pixel spacing vs. the tangent of the local ray angle, the line of best fit has a slope equal to the equivalent pinhole camera's focal length (Figure 3.8(a,b). We separately estimate the principal point by shining a collimated source into the lens oriented so it is approximately parallel to the lens' optical axis. The location of its image is assumed to be the principal point. Finally, we estimate the camera's rotation matrix and lens distortion coefficients numerically as the parameters that minimize the reprojection error given the previously determined focal length and principal point.

3.11 Note: Proposal:Acquisition Light Efficiency

Given a linearly polarized illumination laser beam, an acquisition sensor offset by a scattering angle θ, and a scattering sample inside a glass cell, the goal is to determine 1) the optimal sample orientation and 2) the optimal angle of polarization to maximize light transmitted from the illuminator to the acquisition sensor. All theory below assumes scattering particles are small compared with the wavelength and are detailed in [8].

Note: Proposal:Fresnel Formulae

Consider a plane wave with amplitude A incident on a surface. The electric and magnetic field vectors can be decomposed into two components parallel and perpendicular to the surface plane. The incident electric field is

$$E^{(i)} = \begin{bmatrix} -A_{||} \cos\theta_i e^{-i\tau_i} \\ A_{\perp} e^{-i\tau_i} \\ A_{||} \sin\theta_i e^{-i\tau_i} \end{bmatrix} \tag{3.50}$$

where E_x, E_z are in the plane, E_y is along the plane normal, and the complex exponential argument is defined

$$\tau_i = \omega\left(t - \tfrac{\mathbf{r}^{\intercal}\mathbf{s}^{(\mathrm{i})}}{v}\right) = \omega\left(t - \tfrac{x\sin\theta_i + z\cos\theta_i}{v}\right). \tag{3.51}$$

The magnetic field vector H is written similarly through the relation $H = \sqrt{\epsilon}\mathbf{s} \times \mathbf{E}$. where $\mathbf{s}$ is the light's velocity vector. If T and R denote the transmitted and reflected amplitudes, then the transmitted field is

$$E^{(t)} = \begin{bmatrix} -T_{||} \cos\theta_t e^{-i\tau_t} \\ T_{\perp} e^{-i\tau_t} \\ T_{||} \sin\theta_t e^{-i\tau_t} \end{bmatrix}, \tag{3.52}$$

and the reflected field is

$$E^{(r)} = \begin{bmatrix} -R_{||} \cos\theta_r e^{-i\tau_r} \\ R_{\perp} e^{-i\tau_r} \\ R_{||} \sin\theta_r e^{-i\tau_r} \end{bmatrix}. \tag{3.53}$$

The tangential components of the electric and magnetic fields must be continuous across the boundary, resulting in four boundary conditions:

$$E_x^{(i)} + E_x^{(r)} = E_x^{(t)} \quad E_y^{(i)} + E_y^{(r)} = E_y^{(t)} \tag{3.54}$$

$$H_x^{(i)} + H_x^{(r)} = H_x^{(t)} \quad H_y^{(i)} + H_y^{(r)} = H_y^{(t)}. \tag{3.55}$$

These boundary conditions can be solved for an expression of the transmitted and reflected amplitudes components by using the Maxwell relation $n = \sqrt{\epsilon}$

$$T_{||} = \frac{2n_1\cos\theta_i}{n_2\cos\theta_i + n_1\cos\theta_t}A_{||} \quad T_{\perp} = \frac{2n_1\cos\theta_i}{n_1\cos\theta_i + n_2\cos\theta_t}A_{\perp} \tag{3.56}$$

$$R_{||} = \frac{n_2\cos\theta_i - n_1\cos\theta_t}{n_2\cos\theta_i + n_1\cos\theta_t}A_{||} \quad R_{\perp} = \frac{n_1\cos\theta_i - n_2\cos\theta_t}{n_1\cos\theta_i + n_2\cos\theta_t}A_{\perp}. \tag{3.57}$$

Note: Poporsal:Effects of Polarization on Fresnel Formulae

The light intensity is

$$S = \frac{c}{4\pi}\sqrt{\epsilon}E^2 = \frac{cn}{4\pi}E^2 \tag{3.58}$$

The resulting energy incident on a surface with unit area A is

$$J^{(i)} = S^{(i)}\cos\theta_i = \frac{cn_1}{4\pi}|A|^2\cos\theta_i \tag{3.59}$$

with reflected and transmitted energies

$$J^{(r)} = \frac{cn_1}{4\pi}|R|^2\cos\theta_i \quad \textit{and} \quad J^{(t)} = \frac{cn_2}{4\pi}|T|^2\cos\theta_t. \tag{3.60}$$

The reflectivity and transmissivity are

$$\mathcal{R} = \frac{J^{(r)}}{J^{(i)}} = \frac{|R|^2}{|A|^2} \quad \textit{and} \quad \mathcal{T} = \frac{J^{(t)}}{J^{(i)}} = \frac{|T|^2}{|A|^2} \tag{3.61}$$

which satisfy the law of conservation of energy by summing to 1

$$\mathcal{R} + \mathcal{T} = 1. \tag{3.62}$$

The reflectivity and transmissivity are functions of polarization with respect to the parallel and perpendicular directions. If the incident electric field $\mathbf{E}$ makes an angle α_i with respect to the plane, the parallel and perpendicular area components are

$$A_{||} = A\cos\alpha_i \quad \textit{and} \quad A_{\perp} = A\sin\alpha_i \tag{3.63}$$

The parallel energy component of the incident light is

$$\begin{aligned} J_{||}^{(i)} &= \frac{cn_1}{4\pi}|A_{||}|^2\cos\theta_i \\ &= \frac{cn_1}{4\pi}|A|^2\cos^2\alpha_i\cos\theta_i \\ &= J^{(i)}\cos^2\alpha_i \end{aligned} \tag{3.64}$$

with that of the perpendicular component following similarly:

$$J_{\perp}^{(i)} = J^{(i)}\sin^2\alpha_i. \tag{3.65}$$

The reflectivity in terms of polarized light is

$$\begin{aligned} \mathcal{R} = \frac{J^{(r)}}{J^{(i)}} &= \frac{J_{||}^{(r)} + J_{\perp}^{(r)}}{J^{(i)}} \\ &= \frac{J_{||}^{(r)}}{J_{||}^{(i)}}\cos^2\alpha_i + \frac{J_{\perp}^{(r)}}{J_{\perp}^{(i)}}\sin^2\alpha_i \\ &= \mathcal{R}_{||}\cos^2\alpha_i + \mathcal{R}_{\perp}\sin^2\alpha_i, \end{aligned} \tag{3.66}$$

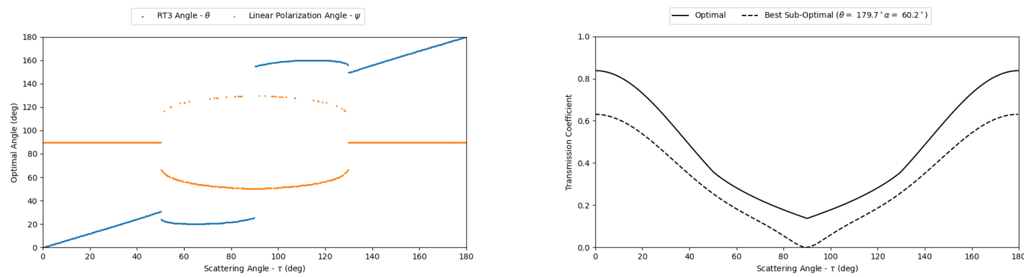


Figure 3.9: Left: Optimal sample rotation stage position and linear polarization angle as a function of azimuthal illumination angle. The linear polarization angle schedule contains discontinuities in the range $(-50°, 50°)$ due to rounding errors; Right: Comparison of light transmitted towards camera when choosing the optimal sample orientation versus a static sample shows an approximate 15% increase on average.

and the transmissivity is

$$\mathcal{T} = \mathcal{T}_{||} \cos^2 \alpha_i + \mathcal{T}_{\perp} \sin^2 \alpha_i. \tag{3.67}$$

Reflectivity and transmissivity must satisfy conservation of energy respectively:

$$\mathcal{R}_{||} + \mathcal{T}_{||} = 1, \qquad \mathcal{R}_{\perp} + \mathcal{T}_{\perp} = 1. \tag{3.68}$$

When light is incident normal to the surface, $\alpha_i = 0$ for all E-field orientations, meaning there is no distinction between the parallel and perpendicular components, and the reflectivity and transmissivity are written

$$\mathcal{R} = \left(\frac{n-1}{n+1}\right)^2, \qquad \mathcal{T} = \frac{4n}{(n+1)^2} \tag{3.69}$$

where $n = n_2/n_1$.

These relations were used to find the optimal sample assembly rotation angle and the angle of polarization for every acquisition scattering angle. The result is a lookup table plotted as a chart in Figure 4.2.

3.12 Note: Proposal:Expected Results

We have identified imaging configurations that produce high-contrast speckle images with well-resolved speckle grains through HDR acquisition and proper camera specifications. Examples of images we have acquired to date are shown in Figure 3.10. These speckle images are high-contrast which is indicative of a suitable beamwidth (5mm) for the sample's scattering cross-section, and the speckle grains are well-resolved, meaning the camera's angular resolution is sufficient.

A preliminary result that indicates we are on the right track is computing and plotting 2D speckle correlation and showing that this correlation increases with decreasing sample optical density as suggested

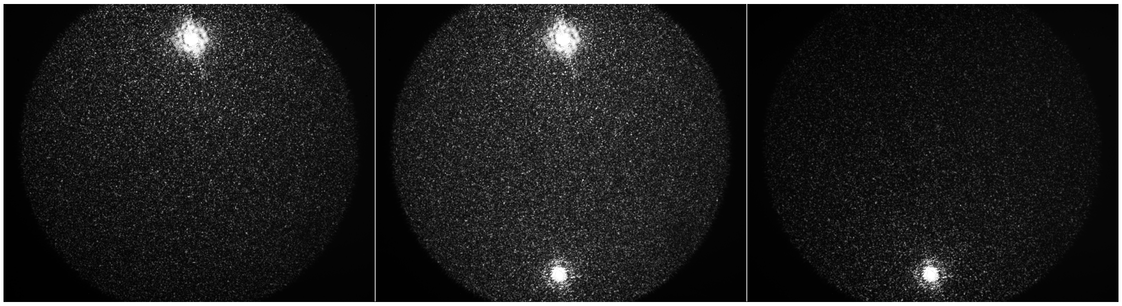


Figure 3.10: Speckle images of 10μm monodisperse SiO_2 beads acquired using scatterometer setup. Left: Top illuminator activated; Center: Both illuminators activated; Right: Bottom illuminator activated

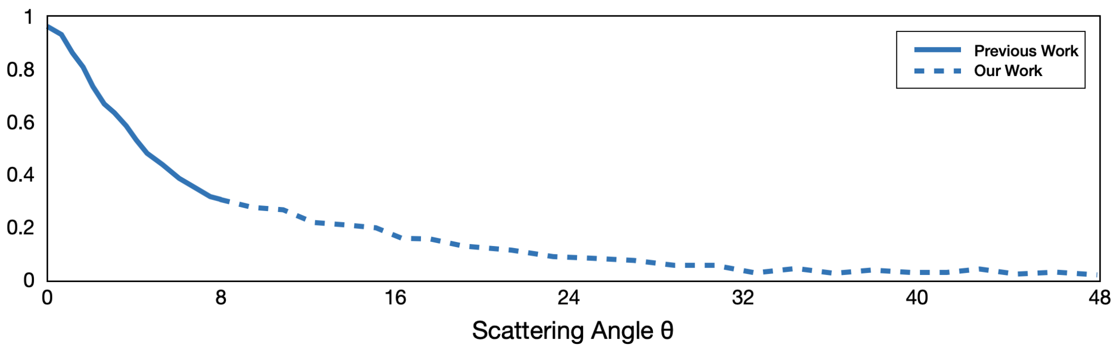


Figure 3.11: An expected result is acquiring the scattering phase function for a larger range of scattering angles than the literature.

by Equation 1.9. Next, we plan to acquire phase functions of materials similar those acquired in [1] over a larger range of scattering angles. Figure 3.11 shows our planned extension of the scattering angle range. If our phase functions agree with [1], it will help validate our acquisition configuration and correlation scripts.

Chapter 4

Acquisition

In this chapter, we delve into the scatterometer design as well as the calibration and alignment process.

4.1 Scattering Samples

4.2 Acquisition

4.3 Maximizing Light Scattered Towards Camera

4.4 Illumination Polarization

The Verdi output beam is linearly polarized and passed through single-mode (SM) fibers prior to illuminating scattering samples with the resulting beam having an unknown polarization state due to use of non-polarization-maintaining fibers. This raises several questions 1) What is the beam's polarization state?; 2) Is it constant?; and 3) What is the optimal polarization state of the output beam to maximize light transmission into the sample?

Literature suggests the output beam will have an elliptical polarization state (1) that is variable/unstable (2) due to variable birefringence induced in SM fibers caused by variable internal stresses and temperature fluctuations.

The output polarization state's stability was characterized by placing a power meter photodiode with a static LPF to measure the power of a collimator on the dual collimator stand attached to the RT-5 rail. The measured power for 10 sweeps of the RT-5 through a range of 280 degrees is shown in Figure 4.1. There is a clear relationship between the measured power through an LPF and the RT-5 stage position which suggests the polarization state does not remain constant across illumination angles. The ellipticity

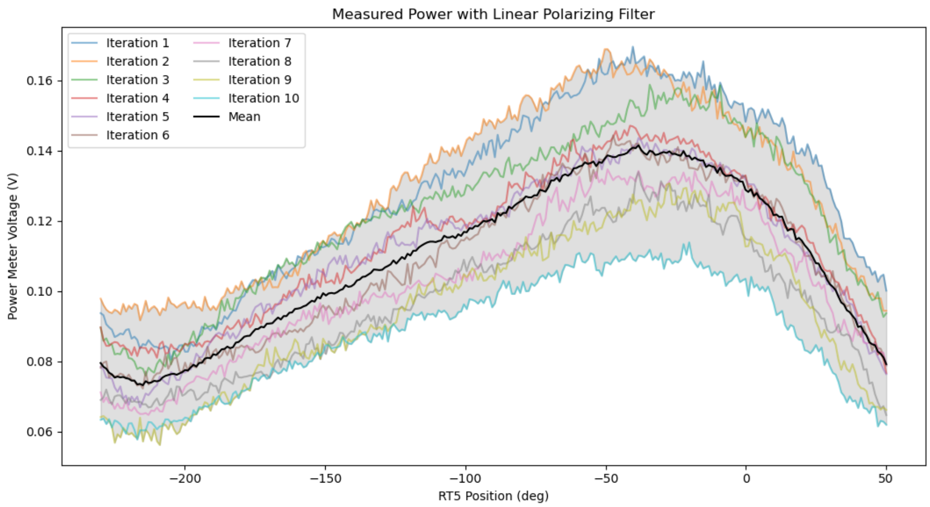


Figure 4.1

was not investigated due to requiring a circular polarizing filter (CPF). Fluctuations in measured power across sweeps was due to insertion losses caused by motion of unstable FC/PC fiber connectors on the RT-5 rail. Fixing those connectors to the rail saw significant reductions in fluctuations.

4.4.1 Optimizing Illumination & Sample Orientation to Maximize Light Transmission

Given a linearly polarized illumination laser beam, an acquisition sensor offset by some scattering angle, and a scattering sample inside a glass cell, the goal is to determine 1) the optimal sample orientation and 2) the optimal angle of polarization to maximize light transmitted from the illuminator to the acquisition sensor.

Fresnel Formulae

The contents in this section are paraphrased from [8]. Consider a plane wave with amplitude A incident on a surface. The electric and magnetic field vectors can be decomposed into two components parallel and perpendicular to the surface plane. The incident electric field is

$$E^{(i)} = \begin{bmatrix} -A_{||} \cos\theta_i e^{-i\tau_i} \\ A_{\perp} e^{-i\tau_i} \\ A_{||} \sin\theta_i e^{-i\tau_i} \end{bmatrix} \tag{4.1}$$

where E_x, E_z are in the plane, and E_y is along the plane normal. The complex exponential argument is defined

$$\tau_i = \omega\left(t - \tfrac{\mathbf{r}^\intercal \mathbf{s}^{(i)}}{v}\right) = \omega\left(t - \tfrac{x \sin\theta_i + z\cos\theta_i}{v}\right) \tag{4.2}$$

The magnetic field vector H is written similarly through the relation $H = \sqrt{\epsilon}\mathbf{s} \times \mathbf{E}$. where $\mathbf{s}$ is the light's velocity vector. If T and R denote the transmitted and reflected amplitudes, then the transmitted field is

$$E^{(t)} = \begin{bmatrix} -T_{||}\cos\theta_t e^{-i\tau_t} \\ T_{\perp} e^{-i\tau_t} \\ T_{||}\sin\theta_t e^{-i\tau_t} \end{bmatrix}, \tag{4.3}$$

and the reflected field is

$$E^{(r)} = \begin{bmatrix} -R_{||}\cos\theta_r e^{-i\tau_r} \\ R_{\perp} e^{-i\tau_r} \\ R_{||}\sin\theta_r e^{-i\tau_r} \end{bmatrix}. \tag{4.4}$$

The tangential components of the electric and magnetic fields must be continuous across the boundary, resulting in four boundary conditions:

$$E_x^{(i)} + E_x^{(r)} = E_x^{(t)} \quad E_y^{(i)} + E_y^{(r)} = E_y^{(t)} \tag{4.5}$$

$$H_x^{(i)} + H_x^{(r)} = H_x^{(t)} \quad H_y^{(i)} + H_y^{(r)} = H_y^{(t)} \tag{4.6}$$

These boundary conditions can be solved for an expression of the transmitted and reflected amplitudes components by using the Maxwell relation $n = \sqrt{\epsilon}$

$$T_{||} = \frac{2n_1\cos\theta_i}{n_2\cos\theta_i + n_1\cos\theta_t}A_{||} \quad T_{\perp} = \frac{2n_1\cos\theta_i}{n_1\cos\theta_i + n_2\cos\theta_t}A_{\perp} \tag{4.7}$$

$$R_{||} = \frac{n_2\cos\theta_i - n_1\cos\theta_t}{n_2\cos\theta_i + n_1\cos\theta_t}A_{||} \quad R_{\perp} = \frac{n_1\cos\theta_i - n_2\cos\theta_t}{n_1\cos\theta_i + n_2\cos\theta_t}A_{\perp} \tag{4.8}$$

Effects of Polarization on Fresnel Formulae

The light intensity is

$$S = \frac{c}{4\pi}\sqrt{\epsilon}E^2 = \frac{cn}{4\pi}E^2 \tag{4.9}$$

The resulting energy incident on a surface with unit area A is

$$J^{(i)} = S^{(i)} \cos\theta_i = \frac{cn_1}{4\pi}|A|^2 \cos\theta_i \tag{4.10}$$

with reflected and transmitted energies

$$J^{(r)} = \frac{cn_1}{4\pi}|R|^2 \cos\theta_i \quad and \quad J^{(t)} = \frac{cn_2}{4\pi}|T|^2 \cos\theta_t. \tag{4.11}$$

The reflectivity and transmissivity are

$$\mathcal{R} = \frac{J^{(r)}}{J^{(i)}} = \frac{|R|^2}{|A|^2} \quad and \quad \mathcal{T} = \frac{J^{(t)}}{J^{(i)}} = \frac{|T|^2}{|A|^2} \tag{4.12}$$

which satisfy the law of conservation of energy by summing to 1

$$\mathcal{R} + \mathcal{T} = 1. \tag{4.13}$$

The reflectivity and transmissivity are functions of polarization with respect to the parallel and perpendicular directions. If the incident electric field **E** makes an angle α_i with respect to the plane, the parallel and perpendicular area components are

$$A_{||} = A\cos\alpha_i \quad and \quad A_{\perp} = A\sin\alpha_i \tag{4.14}$$

The parallel energy component of the incident light is

$$\begin{aligned} J^{(i)}_{||} &= \frac{cn_1}{4\pi}|A_{||}|^2 \cos\theta_i \\ &= \frac{cn_1}{4\pi}|A|^2 \cos^2\alpha_i \cos\theta_i \\ &= J^{(i)} \cos^2\alpha_i \end{aligned} \tag{4.15}$$

with that of the perpendicular component following similarly:

$$J^{(i)}_{\perp} = J^{(i)} \sin^2\alpha_i. \tag{4.16}$$

The reflectivity in terms of polarized light is

$$\begin{aligned}\mathcal{R} = \frac{J^{(r)}}{J^{(i)}} &= \frac{J_{||}^{(r)} + J_{\perp}^{(r)}}{J^{(i)}} \\ &= \frac{J_{||}^{(r)}}{J_{||}^{(i)}} \cos^2 \alpha_i + \frac{J_{\perp}^{(r)}}{J_{\perp}^{(i)}} \sin^2 \alpha_i \\ &= \mathcal{R}_{||} \cos^2 \alpha_i + \mathcal{R}_{\perp} \sin^2 \alpha_i, \end{aligned} \tag{4.17}$$

and the transmissivity is

$$\mathcal{T} = \mathcal{T}_{||} \cos^2 \alpha_i + \mathcal{T}_{\perp} \sin^2 \alpha_i. \tag{4.18}$$

Reflectivity and transmissivity must satisfy conservation of energy respectively:

$$\mathcal{R}_{||} + \mathcal{T}_{||} = 1, \qquad \mathcal{R}_{\perp} + \mathcal{T}_{\perp} = 1. \tag{4.19}$$

When light is incident normal to the surface, $\alpha_i = 0$ for all E-field orientations, meaning there is no distinction between the parallel and perpendicular components, and the reflectivity and transmissivity are written

$$\mathcal{R} = \left(\frac{n-1}{n+1}\right)^2, \qquad \mathcal{T} = \frac{4n}{(n+1)^2} \tag{4.20}$$

where $n = n_2/n_1$.

Fresnel Relations as Mueller Matrices

Transmission

Scattering This section summarizes the results in [7]. Assuming light with wavevector k is scattered from a small sphere with radius a with scattering amplitude coefficient $a_1 \in \mathbb{C}$, the scattered field at distance r from the scatterer, the Mueller matrix is

$$\mathbf{M}_s = \frac{9|a_1|^2}{4k^2r^2} \begin{bmatrix} \frac{1}{2}(1+\cos^2\theta) & \frac{1}{2}(\cos^2\theta - 1) & 0 & 0 \\ \frac{1}{2}(\cos^2\theta - 1) & \frac{1}{2}(1+\cos^2\theta) & 0 & 0 \\ 0 & 0 & \cos\theta & 0 \\ 0 & 0 & 0 & \cos\theta \end{bmatrix} \tag{4.21}$$

where the scattering coefficient is defined

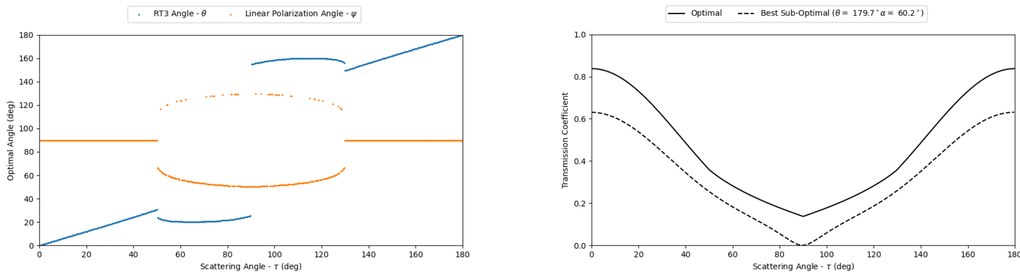


Figure 4.2

$$a_1 = -\frac{i2x^3}{e}\frac{m^2-1}{m^2+2} - \frac{i2x^5}{5}\frac{(m^2-2)(m^2-1)}{(m^2+2)^2} \tag{4.22}$$

with scale factor and relative refractive index

$$x = ka = \frac{2\pi Na}{\lambda}, \qquad m = \frac{N_1}{N} = \frac{k_1}{k} \tag{4.23}$$

where N and N_1 are the medium's and particle's refractive indices respectively. The scattering Mueller matrix is defined within the scattering plane containing the incoming and outgoing directions as well as the scattering particle.

Simulation Results

Unpolarized Beam

Linearly Polarized Beam

4.4.2 Simulation

4.4.3 Depolarizer Spatial Characterization

One option is to depolarize the illumination beams via Thorlabs DPP25-A liquid crystal polymer depolarizer. This optic is a series of linear polarizing strips each oriented in 45-degree increments. The incident beam is passed through these strips, and the output beam is a combination of linear polarization states with different angles of polarization. Since strips are distributed spatially, the output beam's polarization state is a function of the incident beam size.

The affect of beam size on output polarization state was characterized by measuring the spatial distribution of polarization state using a camera. The Verdi output beam was coupled into a 2-meter

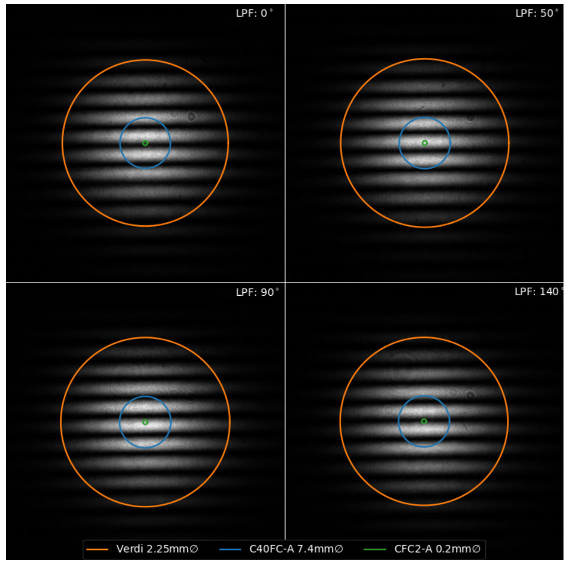


Figure 4.3

single-mode fiber whose output was collimated using Thorlabs C40FC-A. That beam was passed through the depolarizer mounted on Thorlabs CRM1PT followed by a linear polarizing filter mounted on Thorlabs CRM1T. The beam was then passed through an ND=2.0 filter prior to measurement by the camera. The camera was Grasshopper3 GS3-PGE-91S6M with a Leica Summicron-A 50mm 1:2 lens focused at its shortest working distance (1:6.6 magnification). Acquisition consisted of rotating the LPF in 10-degree increments over a range of 170 degrees and acquiring a 16-bit image for each LPF orientation.

The intensity profiles of the depolarized beam for four LPF orientations is shown in Figure 4.3. Each profile is a Gaussian-enveloped sinusoid whose phase changes with the LPF orientation. Each image is overlaid with $1/e^2$ beam diameters for two collimators' output beams and the Verdi output beam. The C40FC-A and Verdi beam profiles are large enough to cover at least a full period of the depolarizer's structure, while the CFC2-A beam does not. Therefore, the depolarizer would not be effective if used with the CFC2-A collimator.

Chapter 5

Appendices

5.1 Calibration Target Design

A contiguous calibration target was chosen initially for beam direction estimation. However, the variable albedo due to ink created structured noise. This caused estimates of beams partially overlapping black regions to become biased towards the white regions. As a result, a window was added to the target allowing all centroiding estimates to occur on a surface of constant albedo. See Figure 5.1.

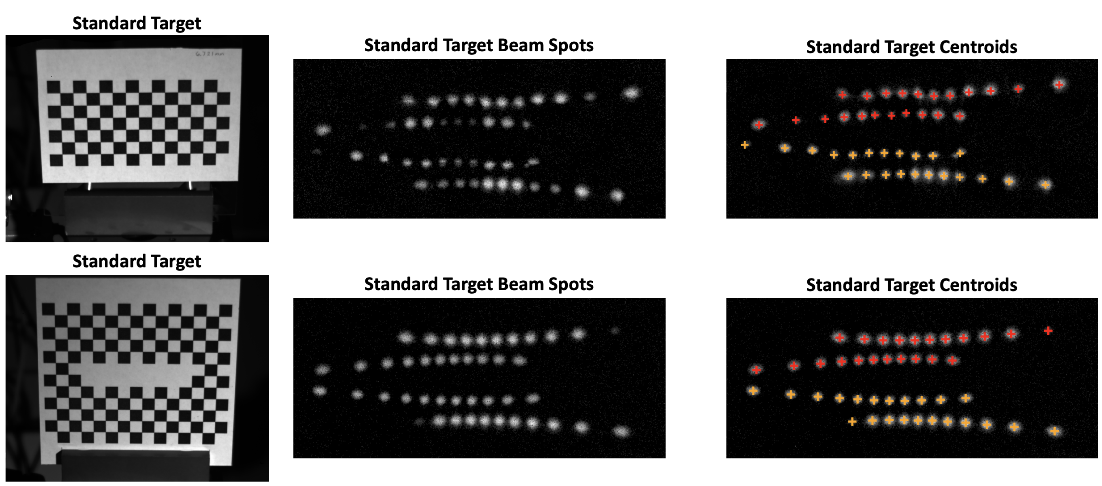


Figure 5.1: Top row: Original target used for calibration caused irregular beam spot shapes which produced noisy centroids. Bottom row: Windowed target used now to avoid albedo issues when imaging beam spots.

5.2 Sample Preparation

Equipment Required

- Microscope slides (two per sample)
- Dropper or syringe with capacity greater than or equal to the target sample volume
- Ethanol
- Isopropyl alcohol
- Non-abrasive working surface to prevent scratching slides

Part No.	Vendor	Qty.	Description
30392080	Ohaus	1	Dry Block Tube Heater
30400154	Ohaus	1	Module Block 20mm 8 Wells
30400193	Ohaus	1	Module Block 50, 15, 1.5mL
FA10006M	Gilson	1	P1000L 100-1000uL pipette
AB0576	Thermo Fisher	1	25uL gene frame
AB0577	Thermo Fisher	1	65uL gene frame
AB0578	Thermo Fisher	1	125uL gene frame
GEMINI-20-BLK	American Weigh Scales	1	Milligram scale + boat
F167014	Gilson	1	D1000 tip reload pack
4916345	Scientific Labwares	1	oval lab spoon
CHWB 1020B	Eisco	1	Water squeeze bottle
CHWB 1030	Eisco	1	IPA squeeze bottle
CHWB 1037	Eisco	1	Ethanol squeeze bottle
A20090-50.0	RPI	1	Agarose, 50 G
???	Swift	1	Microscope
EC 1.3MP	Swift	1	Microscope camera
W5-4	Fisher Chemical	1	4L HPLC Water
904341-2G	Millipore Sigma	1	Silica monodisperse 3um spheres
34155	Kimtech	1	Kimwipes
MPR-50504	Med Pride	1	Nitrile gloves
55105	SPL Life Sciences	1	5mL centrifuge snap tubes
50215	SPL Life Sciences	1	15mL centrifuge snap tubes
???		1	Microfiber towel

1. Clean all labware with IPA and dry with Kimtech wipes. Clean slides with IPA and dry with optical cleaning cloth.

2. Pour 5 mL HPLC water in a 15 mL tube using a squeeze bottle.

3. Set the tube heater to 95°C and place the 15 mL tube in a heating block.

4. Once the heater has reach the set point, place a clean 5 mL tube in a heating block. Let both tubes remain in the block for 5 minutes.

5. Cut _ mm off the end of a clean pipette tip so its opening is 2 mm in diameter.
6. Transfer heated HPLC water from the 15 mL tube to the 5 mL tube.
7. Measure _ mg agarose powder in a clean weighting boat and add it to the 5 mL tube. Place it in a heating block for 10 minutes, using bottoms-up agitation every 2 minutes.
8. While waiting, measure _ mg silica beads in the weigh boat and set aside.
9. Attach a gene frame to a microscope slide.
10. Once the water has been heated for 10 minutes, place the slide on a heating block. Then add the silica beads to the agarose solution and let the suspension heat for 5 minutes, using bottoms-up agitation every minute.
11. Using a 1 mL pipette, cycle the liquid within the 5 mL tube several times.
12. Ensure the pipette's volume is set to 96% of the gene frame's volume.

    Note: The following sequence should occur quickly. Otherwise the suspension will cool and begin gelling, reducing the sample quality:
13. Using heat-resistant gloves, remove the heated slide and place it on a microfiber towel.
14. Intake the desired volume of the suspension and aliquot it while moving the pipette tip across the area of the gene frame. This will minimize the height of the liquid and will prevent overflow when placing the slide cover on the gene frame.
15. Using another microscope slides, attach the slide cover from one side to another, lengthwise along the gene frame.
16. Press the slide flat against the slide cover and leave it in place to ensure the cover is parallel with the surface of the sample slide.
17. Weigh-out the amount using a scooper and clean weigh boat
18. Combine microspheres with _ mL ethanol in a centrifuge tube
    - Micro sphere volume: $14.137 \mu m^3 = 1.4137 \times 10^{-11} cm^3$
    - Micro spheres per gram: $3.1 \times 10^{11} \frac{sphere}{g} = \frac{1\ cm^3}{2.196\ g} \left(\frac{10^4\ \mu m}{1\ cm}\right)^3 \frac{1}{(\frac{4}{3}\pi 1.5^3)\ \mu m^3}$
    - Ethanol Volume: $\frac{3.1\times10^{11}\ spheres}{1\ g} \cdot \frac{1.4137\times10^{-11} cm^3}{1\ sphere} \cdot \frac{1\ mL}{1\ cm^3} \cdot 125 \cdot x\ grams$

19. Measure-out 0.1 g of agarose powder and place in second tube
20. Fill second tube with 10 mL HPCL water
21. Fill 10 tubes with HPCL water
22. Insert all 12 tubes in heating block
23. Set the mixer to _ degrees Celsius and begin heating the tubes.
24. After _ minutes, start mixing the tubes at _ RPM for _ minutes.
25. Once done, pour the water tubes into a TBD container and place the slides in the water.
26. Pour the microsphere-Ethanol mixture into the agarose mixture and resume mixing and heating for _ minutes (depending on time required to heat-up slides).
27. Remove slides, dry them, attach gene frames, and place on non-abrasive surface. The next few steps should be completed quickly to avoid the slides cooling too much.
28. When mixing is complete, remove tube and agitate 20 times using the bottoms-up method
29. Place the mixture back in the mixer and use a pipette to transfer liquid to the center of the gene frame. The amount transferred should match the volume of the gene frame.
30. Sandwich the sample using the top face of another microscope slide (not the side that was facing down on the table). While sandwiching, touch the slides as far away from the gene frame as possible, and on the edges.
31. Place on the rotator at _ RPM for _ minutes (need to calculate cooling rate). The liquid and slides should now be at a uniform temperature.
32. Inspect the sample using a microscope objective to determine the uniformity. Need to develop procedure for this. Maybe 8 locations (3 along top, 3 along bottom, two intermediate positions along sample center line). Then compute variance of number of particles visible across images? Use that as a benchmark.
33. Clean pipette internals, glassware using IPA

5.3 Ziegler-Nichols Tuning Method

The Ziegler-Nichols tuning method is a PID tuning heuristic based on two principal characteristics affecting process controllability [38]:

1. The ultimate gain K_u is the proportional gain above which oscillations will increase to a maximum amplitude, and below which oscillations will decay to zero response.

2. The period of oscillation T_u is the period in minutes of constant-amplitude oscillations corresponding to a P controller with gain K_u.

It defines the necessary proportional (K_p), integral (K_i), and derivative (K_d) gains for control stability given the ultimate gain and period of oscillation.

Table 5.1: Ziegler-Nichols method

Control Type	K_p	T_i	T_d	K_i	K_d
P	0.5 K_u	-	-	-	-
PI	0.45 K_u	0.83 T_u	-	0.54 K_u/T_u	-
PD	0.3 K_u	-	0.125 T_u	-	0.10 K_uT_u
classic PID	0.6 K_u	0.5 T_u	0.125 T_u	1.2 K_u/T_u	0.075 K_uT_u
Pessen Integral Rule	0.7 K_u	0.4 T_u	0.15 T_u	1.75 K_u/T_u	0.105 K_uT_u
some overshoot	0.33 K_u	0.50 T_u	0.33 T_u	0.66 K_u/T_u	0.11 K_uT_u
no overshoot	0.20 K_u	0.50 T_u	0.33 T_u	0.40 K_u/T_u	0.066 K_uT_u

Note: Alternative is Tyreus-Luyben method [20] For example, assume the error is directly proportional to the actuation distance of a translation stage. If the initial

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