A Summary of my PhD Thesis: *Mathematical Modelling of Hybrid Photonic Structures for Holographic Sensors*

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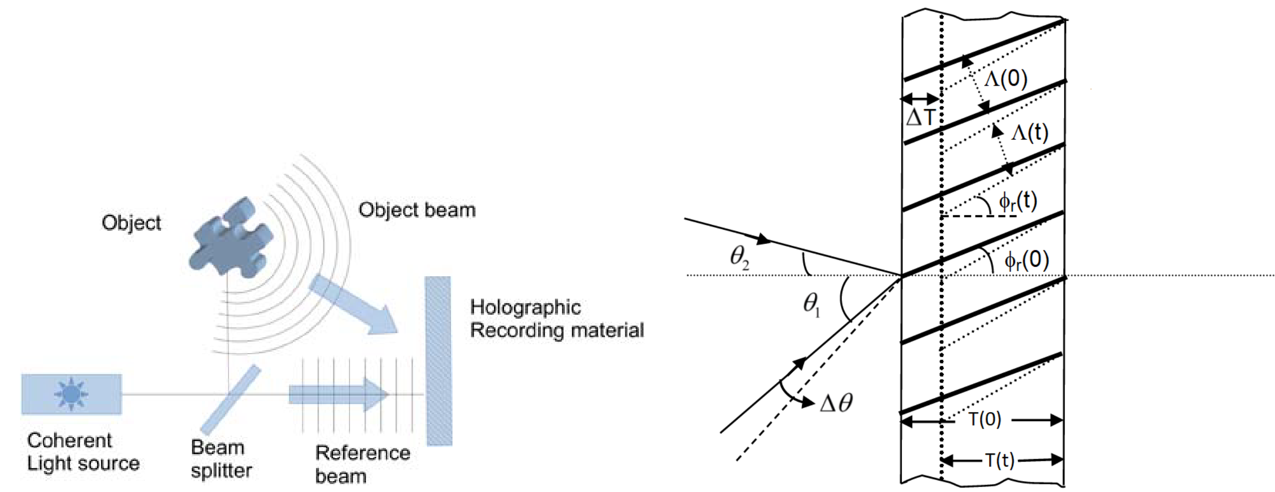
Purpose



(a) Set up (b) Geometry

Figure 1: The optical set up and geometry for a holographic grating.

Mathematical Model

In black, the previous model and in blue, the improvements I developed.

$$\frac{\partial b}{\partial t} = 0, \tag{1a}$$

$$\frac{\partial m}{\partial t} + \nabla \cdot \vec{J_m} = -\Phi(t) F(x,y,t) m, \tag{1b}$$

$$\frac{\partial p}{\partial t} + \nabla \cdot \vec{J_p} = \Phi(t) F(x,y,t) m - \Phi(t)\Gamma p^2, \tag{1c}$$

$$\frac{\partial q}{\partial t} = \Phi(t)\Gamma p^2, \tag{1d}$$

$$\frac{\partial z}{\partial t} + \nabla \cdot \vec{J_z} = 0. \tag{1e}$$

$$F(x,y,t) = k_p \left[I_0 e^{-\zeta(T-y)} \right]^a \left\{ 1 + e^{-\xi z} \cos\left[\frac{2\pi \cos\phi_r(t)}{\Lambda(t)} x - \frac{2\pi \sin\phi_r(t)}{\Lambda(t)} y \right] \right\}, \tag{2}$$

$$\vec{J_m} = -D_m \frac{\partial m}{\partial x}\vec{i} - D_m \frac{\partial m}{\partial y}\vec{j}, \tag{3a}$$

$$\vec{J_p} = -D_p \left\{ \left[\frac{\partial p}{\partial x}\vec{i} + \frac{\partial p}{\partial y}\vec{j}\right] + \epsilon_z \left[\frac{\partial (pz)}{\partial x}\vec{i} + \frac{\partial (pz)}{\partial y}\vec{j}\right] \right\}, \tag{3b}$$

$$\vec{J_z} = -D_z \left\{ \left[\frac{\partial z}{\partial x}\vec{i} + \frac{\partial z}{\partial y}\vec{j}\right] + \epsilon_z \left[\frac{\partial (pz)}{\partial x}\vec{i} + \frac{\partial (pz)}{\partial y}\vec{j}\right] + \epsilon_z \left[\frac{\partial (qz)}{\partial x}\vec{i} + \frac{\partial (qz)}{\partial y}\vec{j}\right] \right\}. \tag{3c}$$

$$0 \le x \le \hat{x}, \qquad 0 \le y \le T(t), \qquad t \ge 0. \tag{4}$$

Boundary Immobilization

$$\frac{\partial B}{\partial t} = \frac{Y}{u}\frac{du}{dt}\frac{\partial B}{\partial Y}, \tag{5a}$$

$$\frac{\partial M}{\partial t} = \frac{Y}{u}\frac{du}{dt}\frac{\partial M}{\partial Y} + \alpha_m^{(x)}\frac{\partial^2 m}{\partial x^2} + \alpha_m^{(y)}\frac{1}{u^2}\frac{\partial^2 M}{\partial Y^2} - \Phi(t)\beta F^*(x,Y,t)M, \tag{5b}$$

$$\begin{aligned}\frac{\partial P}{\partial t} = \frac{Y}{u}\frac{du}{dt}\frac{\partial P}{\partial Y} + \alpha_p^{(x)}\frac{\partial^2 P}{\partial x^2} + \alpha_p^{(y)}\frac{1}{u^2}\frac{\partial^2 P}{\partial Y^2} + \alpha_{pz}^{(x)}\frac{\partial^2 (PZ)}{\partial x^2} + \\ \alpha_{pz}^{(y)}\frac{1}{u^2}\frac{\partial^2 (PZ)}{\partial Y^2} + \Phi\beta F^*(x,Y,t)M - \Phi(t)\gamma P^2,\end{aligned} \tag{5c}$$

$$\frac{\partial Q}{\partial t} = \frac{Y}{u}\frac{du}{dt}\frac{\partial Q}{\partial Y} + \Phi(t)\gamma P^2, \tag{5d}$$

$$\begin{aligned}\frac{\partial Z}{\partial t} = \frac{Y}{u}\frac{du}{dt}\frac{\partial Z}{\partial Y} + \alpha_z^{(x)}\frac{\partial^2 Z}{\partial x^2} + \alpha_z^{(y)}\frac{1}{u^2}\frac{\partial^2 Z}{\partial Y^2} + \alpha_{pz}^{(x)}\frac{\partial^2 (PZ)}{\partial x^2} + \\ \frac{1}{u^2}\alpha_{pz}^{(y)}\frac{\partial^2 (PZ)}{\partial Y^2} + \alpha_{qz}^{(x)}\frac{\partial^2 (QZ)}{\partial x^2} + \alpha_{qz}^{(y)}\frac{1}{u^2}\frac{\partial^2 (QZ)}{\partial Y^2},\end{aligned} \tag{5e}$$

$$F^*(x,Y,t) = e^{-\alpha\zeta^* u(1-Y)}\left\{1 + e^{-\xi^* Z}\cos\left[2\pi\left(x - \frac{T_0}{\hat{x}}\tan\phi_r uY\right)\right]\right\} \tag{6}$$

Initial & Boundary Conditions

$$\begin{aligned} &M(x,Y,0) = 1, && P(x,Y,0) = 0, && Q(x,Y,0) = 0, && Z(x,Y,0) = 1, \\ &B(x,Y,0) = 1, && u(0) = 1, && u'(0) = 0. \end{aligned} \tag{7}$$

$$\frac{\partial^n M}{\partial x^n}(0,Y,t) = \frac{\partial^n M}{\partial x^n}(1,Y,t) \qquad n = \{0,1,2,...\}, \tag{8a}$$

$$\frac{\partial^n P}{\partial x^n}(0,Y,t) = \frac{\partial^n P}{\partial x^n}(1,Y,t) \qquad n = \{0,1,2,...\}, \tag{8b}$$

$$\frac{\partial^n Z}{\partial x^n}(0,Y,t) = \frac{\partial^n Z}{\partial x^n}(1,Y,t) \qquad n = \{0,1,2,...\}. \tag{8c}$$

$$\frac{\partial M}{\partial Y}(x,0,t) = \frac{\partial P}{\partial Y}(x,0,t) = \frac{\partial Q}{\partial Y}(x,0,t) = \frac{\partial Z}{\partial Y}(x,0,t) = \frac{\partial B}{\partial Y}(x,0,t) = 0, \tag{8d}$$

$$\frac{\partial M}{\partial Y}(x,1,t) = \frac{\partial P}{\partial Y}(x,1,t) = \frac{\partial Q}{\partial Y}(x,1,t) = \frac{\partial Z}{\partial Y}(x,1,t) = \frac{\partial B}{\partial Y}(x,1,t) = 0. \tag{8e}$$

Numerical Scheme

Numerical simulation can be done using the Crank-Nicolson implicit finite-difference scheme. For example Eqn. 5c would be ...

$$
\begin{aligned}
\frac{M_{i,j}^{k+1}-M_{i,j}^{k}}{\Delta t} =& \frac{Y_j}{u_k}\frac{u_k-u_{k-1}}{\Delta t}\left(\frac{M_{i,j+1}^{k+1}-M_{i,j-1}^{k+1}}{4\Delta Y}+\frac{M_{i,j+1}^{k}-M_{i,j-1}^{k}}{4\Delta Y}\right)+ \\
&\frac{\alpha_{mm}}{2}\left[\frac{M_{i-1,j}^{k+1}-2M_{i,j}^{k+1}+M_{i+1,j}^{k+1}}{\Delta x^2}+\frac{M_{i-1,j}^{k}-2M_{i,j}^{k}+M_{i+1,j}^{k}}{\Delta x^2}\right]+ \\
&\frac{\alpha_{mm}}{2u_k^2}\left[\frac{M_{i,j-1}^{k+1}-2M_{i,j}^{k+1}+M_{i,j+1}^{k+1}}{\Delta Y^2}+\frac{M_{i,j-1}^{k}-2M_{i,j}^{k}+M_{i,j+1}^{k}}{\Delta Y^2}\right]+ \\
&-\Phi^k\beta F_{i,j}^{k}\left(\frac{M_{i,j}^{k+1}+M_{i,j}^{k}}{2}\right),
\end{aligned} \tag{9a}
$$

$$
\begin{aligned}
\frac{P_{i,j}^{k+1}-P_{i,j}^{k}}{\Delta t} =& \frac{Y_j}{u_k}\frac{u_k-u_{k-1}}{\Delta t}\left(\frac{P_{i,j+1}^{k+1}-M_{i,j-1}^{k+1}}{4\Delta Y}+\frac{P_{i,j+1}^{k}-M_{i,j-1}^{k}}{4\Delta Y}\right)+ \\
&\frac{\alpha_{pp}}{2}\left[\frac{P_{i-1,j}^{k+1}-2P_{i,j}^{k+1}+P_{i+1,j}^{k+1}}{\Delta x^2}+\frac{P_{i-1,j}^{k}-2P_{i,j}^{k}+P_{i+1,j}^{k}}{\Delta x^2}\right]+ \\
&\frac{\alpha_{pp}}{2u_k^2}\left[\frac{P_{i,j-1}^{k+1}-2P_{i,j}^{k+1}+P_{i,j+1}^{k+1}}{\Delta Y^2}+\frac{P_{i,j-1}^{k}-2P_{i,j}^{k}+P_{i,j+1}^{k}}{\Delta Y^2}\right]+ \\
&\frac{\alpha_{pz}}{2}\left[\frac{Z_{i-1,j}^{k}P_{i-1,j}^{k+1}-2Z_{i,j}^{k}P_{i,j}^{k+1}+Z_{i+1,j}^{k}P_{i+1,j}^{k+1}}{\Delta x^2}+\right. \\
&\left.\frac{Z_{i-1,j}^{k}P_{i-1,j}^{k}-2Z_{i,j}^{k}P_{i,j}^{k}+Z_{i+1,j}^{k}P_{i+1,j}^{k}}{\Delta x^2}\right]+ \\
&\frac{\alpha_{pz}}{2u_k^2}\left[\frac{Z_{i,j-1}^{k}P_{i,j-1}^{k+1}-2Z_{i,j}^{k}P_{i,j}^{k+1}+Z_{i,j+1}^{k}P_{i,j+1}^{k+1}}{\Delta Y^2}+\right. \\
&\left.\frac{Z_{i,j-1}^{k}P_{i,j-1}^{k}-2Z_{i,j}^{k}P_{i,j}^{k}+Z_{i,j+1}^{k}P_{i,j+1}^{k}}{\Delta Y^2}\right]+ \\
&\Phi^k\beta F_{i,j}^{k}\left(\frac{M_{i,j}^{k+1}+M_{i,j}^{k}}{2}\right)-\Phi^k\gamma P_{i,j}^{k}\left(\frac{P_{i,j}^{k}+P_{i,j}^{k+1}}{2}\right),
\end{aligned} \tag{9b}
$$

$$
\frac{Q_{i,j}^{k+1}-Q_{i,j}^{k}}{\Delta t} = \frac{Y_j}{u_k}\frac{u_k-u_{k-1}}{\Delta t}\left(\frac{Q_{i,j+1}^{k+1}-Q_{i,j-1}^{k+1}}{4\Delta Y}+\frac{Q_{i,j+1}^{k}-Q_{i,j-1}^{k}}{4\Delta Y}\right)+\Phi^k\gamma P_{i,j}^{k}\left(\frac{P_{i,j}^{k}+P_{i,j}^{k+1}}{2}\right), \tag{9c}
$$

$$
\begin{aligned}
\frac{Z_{i,j}^{k+1}-Z_{i,j}^{k}}{\Delta t} =& \frac{Y_j}{u_k}\frac{u_k-u_{k-1}}{\Delta t}\left(\frac{Z_{i,j+1}^{k+1}-Z_{i,j-1}^{k+1}}{4\Delta Y}+\frac{Z_{i,j+1}^{k}-Z_{i,j-1}^{k}}{4\Delta Y}\right)+\\
&\frac{\alpha_{zz}}{2}\left[\frac{Z_{i-1,j}^{k+1}-2Z_{i,j}^{k+1}+Z_{i+1,j}^{k+1}}{\Delta x^2}+\frac{Z_{i-1,j}^{k}-2Z_{i,j}^{k}+Z_{i+1,j}^{k}}{\Delta x^2}\right]+\\
&\frac{\alpha_{zz}}{2u_k^2}\left[\frac{Z_{i,j-1}^{k+1}-2Z_{i,j}^{k+1}+Z_{i,j+1}^{k+1}}{\Delta Y^2}+\frac{Z_{i,j-1}^{k}-2Z_{i,j}^{k}+Z_{i,j+1}^{k}}{\Delta Y^2}\right]+\\
&\frac{\alpha_{zp}}{2}\left[\frac{P_{i-1,j}^{k}Z_{i-1,j}^{k+1}-2P_{i,j}^{k}Z_{i,j}^{k+1}+P_{i+1,j}^{k}Z_{i+1,j}^{k+1}}{\Delta x^2}\right]+\\
&\frac{\alpha_{zp}}{2}\left[\frac{P_{i-1,j}^{k}Z_{i-1,j}^{k}-2P_{i,j}^{k}Z_{i,j}^{k}+P_{i+1,j}^{k}Z_{i+1,j}^{k}}{\Delta x^2}\right]+\\
&\frac{\alpha_{zp}}{2u_k^2}\left[\frac{P_{i,j-1}^{k}Z_{i,j-1}^{k+1}-2P_{i,j}^{k}Z_{i,j}^{k+1}+P_{i,j+1}^{k}Z_{i,j+1}^{k+1}}{\Delta Y^2}\right]+\\
&\frac{\alpha_{zp}}{2u_k^2}\left[\frac{P_{i,j-1}^{k}Z_{i,j-1}^{k}-2P_{i,j}^{k}Z_{i,j}^{k}+P_{i,j+1}^{k}Z_{i,j+1}^{k}}{\Delta Y^2}\right]+\\
&\frac{\alpha_{zq}}{2}\left[\frac{Q_{i-1,j}^{k}Z_{i-1,j}^{k+1}-2Q_{i,j}^{k}Z_{i,j}^{k+1}+Q_{i+1,j}^{k}Z_{i+1,j}^{k+1}}{\Delta x^2}\right]+\\
&\frac{\alpha_{zq}}{2}\left[\frac{Q_{i-1,j}^{k}Z_{i-1,j}^{k}-2Q_{i,j}^{k}Z_{i,j}^{k}+Q_{i+1,j}^{k}Z_{i+1,j}^{k}}{\Delta x^2}\right]+\\
&\frac{\alpha_{zq}}{2u_k^2}\left[\frac{Q_{i,j-1}^{k}Z_{i,j-1}^{k+1}-2Q_{i,j}^{k}Z_{i,j}^{k+1}+Q_{i,j+1}^{k}Z_{i,j+1}^{k+1}}{\Delta Y^2}\right]+\\
&\frac{\alpha_{zq}}{2u_k^2}\left[\frac{Q_{i,j-1}^{k}Z_{i,j-1}^{k}-2Q_{i,j}^{k}Z_{i,j}^{k}+Q_{i,j+1}^{k}Z_{i,j+1}^{k}}{\Delta Y^2}\right],
\end{aligned}
\tag{9d}
$$

$$
F_{i,j}^{k}=\exp\left[-a\zeta^{*}u_k(1-Y_j)\right]\left[1+\exp\left(-\xi^{*}Z_{i,j}^{k}\right)\cos\left(2\pi x-2\pi\tan\phi_r^{k}u_kY_j\right)\right]. \tag{9e}
$$

$$
\begin{aligned}
\int_0^1\int_0^1 M\ dx\ dY \approx M_k^{*} =& \frac{\Delta x^2}{4}\left[M_{0,0}^{k}+M_{0,J}^{k}+M_{J,0}^{k}+M_{J,J}^{k}+2M_{0,1}^{k}+...+2M_{0,J-1}^{k}+\right.\\
&2M_{1,0}^{k}+...+2M_{J-1,0}^{k}+2M_{1,J}^{k}+...+2M_{J-1,J}^{k}+2M_{J,1}^{k}+...\\
&\left.+2M_{J,J-1}^{k}+4M_{2,2}^{k}+...+4M_{J-2,J-2}^{k}\right],
\end{aligned}
\tag{10a}
$$

$$
\begin{aligned}
\int_0^1\int_0^1 P\ dx\ dY \approx P_k^{*} =& \frac{\Delta x^2}{4}\left[P_{0,0}^{k}+P_{0,J}^{k}+P_{J,0}^{k}+P_{J,J}^{k}+2P_{0,1}^{k}+...+2P_{0,J-1}^{k}+\right.\\
&2P_{1,0}^{k}+...+2P_{J-1,0}^{k}+2P_{1,J}^{k}+...+2P_{J-1,J}^{k}+2P_{J,1}^{k}+...\\
&\left.+2P_{J,J-1}^{k}+4P_{2,2}^{k}+...+4P_{J-2,J-2}^{k}\right],
\end{aligned}
\tag{10b}
$$

$$
\begin{aligned}
\int_0^1\int_0^1 Q\ dx\ dY \approx Q_k^{*} =& \frac{\Delta x^2}{4}\left[Q_{0,0}^{k}+Q_{0,J}^{k}+Q_{J,0}^{k}+Q_{J,J}^{k}+2Q_{0,1}^{k}+...+2Q_{0,J-1}^{k}+\right.\\
&2Q_{1,0}^{k}+...+2Q_{J-1,0}^{k}+2Q_{1,J}^{k}+...+2Q_{J-1,J}^{k}+2Q_{J,1}^{k}+...\\
&\left.+2Q_{J,J-1}^{k}+4Q_{2,2}^{k}+...+4Q_{J-2,J-2}^{k}\right],
\end{aligned}
\tag{10c}
$$

$$u_k = \left[\frac{b_0}{\rho_b} + \frac{1}{\rho_m} + \frac{z_0}{\rho_z}\right]^{-1} \left[\frac{b_0}{\rho_b} + \frac{M_k^*}{\rho_m} + \frac{P_k^*}{\rho_p} + \frac{Q_k^*}{\rho_p} + \frac{z_0}{\rho_z}\right], \tag{10d}$$

$$\phi_r^k = \tan^{-1}\left(\frac{\tan\phi_r^0}{u_k}\right), \tag{10e}$$

$$\Lambda_k = \Lambda_0 \frac{\cos\phi_r^k}{\cos\phi_r^0}. \tag{10f}$$

Refractive Index Modulation

$$\frac{n^2-1}{n^2+2} = \phi_m \frac{n_m^2-1}{n_m^2+2} + \phi_p \frac{n_p^2-1}{n_p^2+2} + \phi_q \frac{n_q^2-1}{n_q^2+2} + \phi_z \frac{n_z^2-1}{n_z^2+2} + \phi_b \frac{n_b^2-1}{n_b^2+2}. \tag{11}$$

Solving the Lorentz-Lorenz equation will give the RI of the nanocomposite as a function of x and t. The nanocomposite RI, $n(x,t)$, can be represented by a Fourier expansion series

$$n(x,y,t) \approx \sum_{i=0} A_i(y,t)\cos\left(\frac{2\pi}{\Lambda}ix\right) + B_i(y,t)\sin\left(\frac{2\pi}{\Lambda}ix\right), \tag{12}$$

$$A_0(y,t) = \frac{1}{\Lambda}\int_0^\Lambda n(x,y,t)\ dx, \tag{13a}$$

$$A_1(y,t) = \frac{2}{\Lambda}\int_0^\Lambda n(x,y,t)\cos\left(\frac{2\pi}{\Lambda}x\right)\ dx, \tag{13b}$$

$$B_1(y,t) = \frac{2}{\Lambda}\int_0^\Lambda n(x,y,t)\sin\left(\frac{2\pi}{\Lambda}x\right)\ dx. \tag{13c}$$

RI modulation can be modelled as

$$\Delta n(y,t) = 2\sqrt{A_1^2 + B_1^2}. \tag{14}$$

Shrinkage Modelling

We can calculate the volume at time t if we have expressions for the total volume of monomer, short polymer, cross-linked polymer and nanoparticles inside the grating

$$\begin{aligned} v(t) =& \frac{1}{\rho_m}\left[\frac{1}{\hat{x}T(t)}\int_0^{T(t)}\int_0^{\hat{x}} m\ dx\ dy\right] + \frac{1}{\rho_p}\left[\frac{1}{\hat{x}T(t)}\int_0^{T(t)}\int_0^{\hat{x}} p\ dx\ dy\right] + \\ & \frac{1}{\rho_p}\left[\frac{1}{\hat{x}T(t)}\int_0^{T(t)}\int_0^{\hat{x}} q\ dx\ dy\right] + \frac{1}{\rho_z}\left[\frac{1}{\hat{x}T(t)}\int_0^{T(t)}\int_0^{\hat{x}} z\ dx\ dy\right] + \\ & \frac{1}{\rho_b}\left[\frac{1}{\hat{x}T(t)}\int_0^{T(t)}\int_0^{\hat{x}} b\ dx\ dy\right]. \end{aligned} \tag{15}$$

An important assumptions of the fringe-plane rotation model is that all loss of volume due to polymerization takes place in the thickness of the recording medium

$$u(t) = \frac{T(t)}{T_0} = \frac{v(t)}{v(0)}. \tag{16}$$

$$u(t) = \left[\frac{1}{\rho_b}\frac{b_0}{m_0} + \frac{1}{\rho_m} + \frac{1}{\rho_z}\frac{z_0}{m_0}\right]^{-1}\left[\int_0^1\int_0^1 \frac{M}{\rho_m} + \frac{P}{\rho_p} + \frac{Q}{\rho_p} + \frac{z_0/m_0 Z}{\rho_z} + \frac{b_0/m_0}{\rho_b}\ dx\ dY\right], \tag{17}$$

$$\text{Actual Shrinkage} = \frac{u(0)-u(t)}{u(0)} = 1 - u(t), \tag{18}$$

$$\phi_r(t) = \tan^{-1}\left[\frac{\tan\phi_r(0)}{u(t)}\right], \tag{19a}$$

$$\Lambda(t) = \hat{x}\cos\phi_r(t), \tag{19b}$$

$$\overline{n}(t) = \frac{1}{\hat{x}T}\int_0^T\int_0^{\hat{x}} n(x,y,t)\ dx\ dy = \int_0^1\int_0^1 n(x,Y,t)\ dx\ dY, \tag{20}$$

$$\theta_B(t) = \sin^{-1}\left(\frac{\lambda_r}{2\overline{n}(t)\Lambda(t)}\right) - \phi_r(t), \tag{21}$$

$$\text{Apparent Shrinkage} = 1 - \frac{\tan\phi_r(0)}{\tan\left[\phi_r(0)+\Delta\theta_B\right]}. \tag{22}$$

Python Script

```
import numpy as np
import pandas as pd
from math import pi, factorial
from numpy.linalg import inv

class holographic_grating:

    def __init__(
            self,
            start_exp=0,# Start of exposure
            end_exp=1e2,# End of exposure
            total_time=1e2,# Total simulation time
            lpmm=1e3,# Spatial frequency
            I0=5,# Intensity of recording beam
            slant_angle=1e-4,# Grating slant_angle
            xi=0.3,# Scattering coefficient
            n_m=1.55,# Monomer refractive index
            rhom=1.15,# Monomer density
            Dm=1.6e-7,# Monomer diffusion coefficient
            Dp=6.35e-10,# Polymer diffusion coefficient
            rhop=1.3,# Polymer density
            n_p=1.56,# Oligomer refractive index
            n_q=1.64,# Polymer refractive index
            Gamma=1,# Rate of immobilization
            wt_pc=5e-2,# Doping %
            Dz=1e-10,# Nanoparticle self-diffusion coefficient
            epsilon_pz=13,# Cross-diffusion ratio
            epsilon_qz=13,# Cross-diffusion ratio
            rhoz=1.74,# Nanoparticle mass density
            n_z=1.366,# Nanoparticle refractive index
            b0=5.05,# Ratio of binder to monomer mass
            n_b=1.5,# Binder refractive index
            rhob=1.19,# Binder mass density
            T0=50e-4,# Depth of photosensitive layer [cm]
            zeta=139,# absorption coefficient [cm**-1]
            lambda_probe=633e-7,# Wavelength of reconstruction beam
            Delta_t=1/100,# Numerical scheme time step
            Delta_x=1/20,# Numerical scheme spatial step
            output_time_step=1# Seconds
        ):

        self.total_time = total_time
        self.end_exp = end_exp
        self.lpmm = lpmm
        self.T0 = T0
        self.I0 = I0
        self.slant_angle = slant_angle
        self.T0 = T0
        self.zeta = zeta
        self.xi = xi
        self.Dm = Dm
        self.n_m = n_m
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```
        self.rhom = rhom
        self.Dp = Dp
        self.rhop = rhop
        self.n_p = n_p
        self.n_q = n_q
        self.Gamma = Gamma
        self.Dz = Dz
        self.epsilon_pz = epsilon_pz
        self.epsilon_qz = epsilon_qz
        self.wt_pc = wt_pc
        self.rhoz = rhoz
        self.n_z = n_z
        self.b0 = b0
        self.n_b = n_b
        self.rhob = rhob
        self.lambda_probe = lambda_probe
        self.Delta_x = Delta_x
        self.Delta_Y = Delta_x
        self.Delta_t = Delta_t
        self.output_time_step = output_time_step

    def trapezoidal_rule_integration(array):
        array=array.reshape(Nx,Nx).T
        return self.Delta_x*self.Delta_x/4*(array[0,0] + array[Nx-1,0] + array[0,Nx-1] + array[Nx-1,Nx-1] + np.sum(2*array[0,1:(Nx-1)]) + np.sum(2*array[1:(Nx-1),0]) + np.sum(2*array[Nx-1,1:(Nx-1)]) + np.sum(2*array[1:(Nx-1),Nx-1]) + np.sum(4*array[1:(Nx-1),1:(Nx-1)]))

    def simpsons_rule_1D(arr1D):
        intpts=list(range(1,len(arr1D)-1))
        times_4=[i for i in intpts if i%2!=0]
        times_2=[i for i in intpts if i%2==0]
        return self.Delta_x/3*(arr1D[0] + 4*sum(arr1D[times_4]) + 2*sum(arr1D[times_2]) + arr1D[len(arr1D)-1])

    def slanted_grating_simulation_v22(self):

        # 1.2 --- Define parameters
        Nx=int(1/self.Delta_x) + 1# Number of spatial points
        Ny=int(1/self.Delta_Y) + 1# Number of spatial points
        if Nx%2==0:
          return "Number of x mesh points must be an odd number."
        if Ny%2==0:
           return "Number of y mesh points must be an odd number."

        x=np.linspace(0,1,Nx)# Non-dimensional grating distance
        n_iterations = int(self.total_time/self.Delta_t)+1# Total number of iterations
        r=self.Delta_t/self.Delta_x/self.Delta_x# Ratio of finite time step to squared finite spatial step
        m0=1# Initial mass of monomer
        t0=1 #  Reference time [s]
        Lambda0=1/10/self.lpmm # Grating period [cm]
        Lambda1=Lambda0
        j_end_exp = self.end_exp/self.Delta_t # Iteration of exposure end
        z0 = self.wt_pc/(1 - self.wt_pc)*(m0 + self.b0)# Initial nanoparticle to monomer

        # 1.3 --- Matrix initial conditions
        u1=1
        du_dt=0
        m1 = np.ones(Nx*Nx)# m at j=0
        p1 = np.zeros(Nx*Nx)# p at j=0
        q1 = np.zeros(Nx*Nx)# q at j=0
        z1 = np.ones(Nx*Nx)# z at j=0
        b1 = self.b0*np.ones(Nx*Nx)# b at j=0

        Volume0=m0/self.rhom + self.b0/self.rhob + self.z0/self.rhoz

        phi_m0=m0/self.rhom/Volume0
        phi_z0=self.z0/self.rhoz/Volume0
        phi_b0=self.b0/self.rhob/Volume0

        Lorentz_Lorenz_RHS = phi_m0*(self.n_m*self.n_m - 1)/(self.n_m*self.n_m + 2) + phi_b0*(self.n_b*self.n_b - 1)/(self.n_b*self.n_b + 2) + phi_z0*(self.n_z*self.n_z - 1)/(self.n_z*self.n_z + 2)

```

```
        Initial_RI = np.sqrt((2*Lorentz_Lorenz_RHS + 1)/(1 - Lorentz_Lorenz_RHS))

        n1=Initial_RI*np.ones(Nx*Nx)

        if self.slant_angle==0:
            slant_angle=1e-05
        phi_0=np.arcsin(np.sin(slant_angle/180*pi)/Initial_RI)
        phi_1=phi_0
        theta_B0=np.arcsin(self.lambda_probe/2/Initial_RI/Lambda0) - phi_0
        y_hat0=Lambda0/np.sin(phi_0)
        y_hat1=y_hat0
        x_hat=Lambda0/np.cos(phi_0)

        # 1.5 --- Nondimensionalized parameters
        alpha_m_x=self.Dm*t0/x_hat/x_hat
        alpha_m_y=self.Dm*t0/self.T0/self.T0
        alpha_p_x=self.Dp*t0/x_hat/x_hat
        alpha_p_y=self.Dp*t0/self.T0/self.T0
        alpha_z_x=self.Dz*t0/x_hat/x_hat
        alpha_z_y=self.Dz*t0/self.T0/self.T0
        F0=0.1*self.I0**0.3
        beta=F0*t0
        gamma = self.Gamma*m0*t0
        zeta_star = self.zeta*self.T0
        xi_star=self.xi*self.z0
        interior_points = list(range(1,Nx-1))
        times_4 = [interior_points[i] for i in range(len(interior_points)) if interior_points[i]%2 != 0]
        times_2 = [interior_points[i] for i in range(len(interior_points)) if interior_points[i]%2 == 0]
        Y=np.arange(0,1+self.Delta_x, self.Delta_x)
        time=np.arange(1,self.total_time+self.output_time_step, self.output_time_step)
        Y1=[]
        x1=[]
        for i in range(Nx):
            for j in list(Y):
                Y1.append(j)
            for j in x:
                x1.append(j)
        Y1=np.sort(Y1)
        indexDF=pd.DataFrame({'x':x1, 'y':Y1})

        spatial_profile_DF=pd.DataFrame({"x": x1, 'Y': Y1, "monomer": m1, "short_polymer": p1, "immobile_polymer": q1, 'nanoparticles': z1, 'binder':b1, 'refractive_index': n1, "time": np.zeros(len(n1)), 'N0':np.zeros(len(n1))+Initial_RI, 'Delta_n':np.zeros(len(n1)), 'd2':np.zeros(len(n1))})

        optical_properties_DF=pd.DataFrame({'Y': Y, "time": np.zeros(len(Y)), 'N0':np.zeros(len(Y))+Initial_RI,'Delta_n':np.zeros(len(Y)),'nu':np.zeros(len(Y)),'d2':np.zeros(len(Y))})

        shrinkage_DF=pd.DataFrame({'time':[0], 'actual_shrinkage':[0],'phi_t':[phi_0],'theta_B':[theta_B0],'apparent_shrinkage':[0]})

        # 1.6 --- Calculate each time step via implicit finite difference method
        for j in range(1,n_iterations):

            if j <= j_end_exp:
                Phi=1
            else:
                Phi = 0# Phi=1 if illumination is on, 0 otherwise

            f = np.zeros(Nx*Nx).reshape(Nx,Nx)
            for i in range(Nx):
                matrix_z1=z1.reshape(Nx,Nx)
                z1_i=matrix_z1[:,i]
                f[:,i] = np.exp(-0.3*zeta_star*u1*(1-Y[i]))*(1 + np.exp(-xi_star*z1_i)*np.cos(2*pi*x - 2*pi*self.T0/y_hat1*u1*Y[i]))

            f = f.reshape(Nx*Nx,)

            MM2 = (2 + Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
            MM1 = (2 - Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
            PP2 = (2 + self.Delta_t*gamma*p1)*np.identity(Nx*Nx)
            PP1 = (2 - self.Delta_t*gamma*p1)*np.identity(Nx*Nx)
```

```
        PM2 = (+Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
        PM1 = (+Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
        QQ2 = 2*np.identity(Nx*Nx)
        QQ1 = 2*np.identity(Nx*Nx)
        QP2 = (+Phi*gamma*self.Delta_t*p1)*np.identity(Nx*Nx)
        QP1 = (+Phi*gamma*self.Delta_t*p1)*np.identity(Nx*Nx)
        ZZ2 = 2*np.identity(Nx*Nx)
        ZZ1 = 2*np.identity(Nx*Nx)
        BB2 = 2*np.identity(Nx*Nx)
        BB1 = 2*np.identity(Nx*Nx)

        for i in range(Nx*Nx):

            if i in list(indexDF.loc[indexDF.x==0,].index):
                i_minus_1 = i+Nx-2
            else:
                i_minus_1 = i-1

            if i in list(indexDF.loc[indexDF.x==1,].index):
                i_plus_1 = i-Nx+2
            else:
                i_plus_1 = i+1

            if i in list(indexDF.loc[indexDF.y==0,].index):
                j_minus_1 = i+Nx
            else:
                j_minus_1 = i-Nx

            if i in list(indexDF.loc[indexDF.y==1,].index):
                j_plus_1 = i-Nx
            else:
                j_plus_1 = i+Nx

            MM2[i, i_minus_1] = MM2[i, i_minus_1] - r*alpha_m_x
            MM2[i, j_minus_1] = MM2[i, j_minus_1] - r*alpha_m_y/u1/u1
            MM2[i, i] = MM2[i, i] + 2*r*alpha_m_x
            MM2[i, i] = MM2[i, i] + 2*r*alpha_m_y/u1/u1
            MM2[i, i_plus_1] = MM2[i, i_plus_1] - r*alpha_m_x
            MM2[i, j_plus_1] = MM2[i, j_plus_1] - r*alpha_m_y/u1/u1

            MM1[i, i_minus_1] = MM1[i, i_minus_1] + r*alpha_m_x
            MM1[i, j_minus_1] = MM1[i, j_minus_1] + r*alpha_m_y/u1/u1
            MM1[i, i] = MM1[i, i] - 2*r*alpha_m_x
            MM1[i, i] = MM1[i, i] - 2*r*alpha_m_y/u1/u1
            MM1[i, i_plus_1] = MM1[i, i_plus_1] + r*alpha_m_x
            MM1[i, j_plus_1] = MM1[i, j_plus_1] + r*alpha_m_y/u1/u1

            PP2[i, i_minus_1] = PP2[i, i_minus_1] - r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i_minus_1])
            PP2[i, j_minus_1] = PP2[i, j_minus_1] - r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[j_minus_1])
            PP2[i, i] = PP2[i, i] + 2*r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i])
            PP2[i, i] = PP2[i, i] + 2*r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[i])
            PP2[i, i_plus_1] = PP2[i, i_plus_1] - r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i_plus_1])
            PP2[i, j_plus_1] = PP2[i, j_plus_1] - r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[j_plus_1])

            PP1[i, i_minus_1] = PP1[i, i_minus_1] + r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i_minus_1])
            PP1[i, j_minus_1] = PP1[i, j_minus_1] + r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[j_minus_1])
            PP1[i, i] = PP1[i, i] - 2*r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i])
            PP1[i, i] = PP1[i, i] - 2*r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[i])
            PP1[i, i_plus_1] = PP1[i, i_plus_1] + r*alpha_p_x*(1 + self.epsilon_pz*self.z0*z1[i_plus_1])
            PP1[i, j_plus_1] = PP1[i, j_plus_1] + r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*self.z0*z1[j_plus_1])

            ZZ2[i, i_minus_1] = ZZ2[i, i_minus_1] - r*alpha_z_x*(1 + self.epsilon_qz*q1[i_minus_1] + self.epsilon_pz*p1[i_minus_1])
            ZZ2[i, j_minus_1] = ZZ2[i, j_minus_1] - r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[j_minus_1] + self.epsilon_pz*p1[j_minus_1])
            ZZ2[i, i] = ZZ2[i, i] + 2*r*alpha_z_x*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz
```

```
*p1[i])
                ZZ2[i, i] = ZZ2[i, i] + 2*r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz*p1[i])
                ZZ2[i, i_plus_1] = ZZ2[i, i_plus_1] - r*alpha_z_x*(1 + self.epsilon_qz*q1[i_plus_1] + self.epsilon_pz*p1[i_plus_1])
                ZZ2[i, j_plus_1] = ZZ2[i, j_plus_1] - r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[j_plus_1] + self.epsilon_pz*p1[j_plus_1])

                ZZ1[i, i_minus_1] = ZZ1[i, i_minus_1] + r*alpha_z_x*(1 + self.epsilon_qz*q1[i_minus_1] + self.epsilon_pz*p1[i_minus_1])
                ZZ1[i, j_minus_1] = ZZ1[i, j_minus_1] + r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[j_minus_1] + self.epsilon_pz*p1[j_minus_1])
                ZZ1[i, i] = ZZ1[i, i] - 2*r*alpha_z_x*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz*p1[i])
                ZZ1[i, i] = ZZ1[i, i] - 2*r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz*p1[i])
                ZZ1[i, i_plus_1] = ZZ1[i, i_plus_1] + r*alpha_z_x*(1 + self.epsilon_qz*q1[i_plus_1] + self.epsilon_pz*p1[i_plus_1])
                ZZ1[i, j_plus_1] = ZZ1[i, j_plus_1] + r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[j_plus_1] + self.epsilon_pz*p1[j_plus_1])

                MM2[i, j_minus_1] = MM2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                MM1[i, j_minus_1] = MM1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                MM2[i, j_plus_1] = MM2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                MM1[i, j_plus_1] = MM1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt

                PP2[i, j_minus_1] = PP2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                PP1[i, j_minus_1] = PP1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                PP2[i, j_plus_1] = PP2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                PP1[i, j_plus_1] = PP1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt

                QQ2[i, j_minus_1] = QQ2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                QQ1[i, j_minus_1] = QQ1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                QQ2[i, j_plus_1] = QQ2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                QQ1[i, j_plus_1] = QQ1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt

                ZZ2[i, j_minus_1] = ZZ2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                ZZ1[i, j_minus_1] = ZZ1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                ZZ2[i, j_plus_1] = ZZ2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                ZZ1[i, j_plus_1] = ZZ1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt

                BB2[i, j_minus_1] = BB2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                BB1[i, j_minus_1] = BB1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                BB2[i, j_plus_1] = BB2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
                BB1[i, j_plus_1] = BB1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt

            m2 = np.matmul(inv(MM2), np.matmul(MM1,m1))

            p2 = np.matmul(inv(PP2), np.matmul(PP1,p1) + np.matmul(PM2,m2) + np.matmul(PM1,m1))

            q2 = np.matmul(inv(QQ2), np.matmul(QQ1, q1) + np.matmul(QP2,p2) + np.matmul(QP1,p1))

            if z0==0:
                z2 = z1
            else:
                z2 = np.matmul(inv(ZZ2), np.matmul(ZZ1,z1))

            b2 = np.matmul(inv(BB2), np.matmul(BB1,b1))

            Vb = b2/self.rhob # cm**3
            Vm = m2*m0/self.rhom # cm**3
            Vp = p2*m0/self.rhop # cm**3
            Vq = q2*m0/self.rhop # cm**3
            Vz = z2*self.z0/self.rhoz # cm**3
            Vtotal=Vb+Vm+Vp+Vq+Vz # cm**3
            phi_m = Vm/Vtotal
            phi_b = Vb/Vtotal
            phi_p = Vp/Vtotal
            phi_q = Vq/Vtotal
            phi_z = Vz/Vtotal

            Lorentz_Lorenz_RHS = phi_m*(self.n_m*self.n_m - 1)/(self.n_m*self.n_m + 2) + phi_b*(self.n_b*self.n_b - 1)/(self.n_b*self.n_b + 2) + phi_p*(self.n_p*self.n_p - 1)/(self.n_p*self.n_p + 2) + phi_q*(self.n_q*self.n_q - 1)/(self.n_q*self.n_q + 2) + phi_z*(self.n_z*self.n_z -
```

```
1)/(self.n_z*self.n_z + 2)

        n2=np.sqrt((2*Lorentz_Lorenz_RHS + 1)/(1 - Lorentz_Lorenz_RHS))
        n2=n2.reshape(Nx,Nx).T

        inside_ri=simpsons_rule_1D(n2[int((Nx-1)/2)])

        N0=[(self.Delta_x/3*(n2[0,i] + np.sum(2*n2[times_2,i]) + np.sum(4*n2[times_4,i]) + n2[(Nx-1),i])) for i in range(Nx)]

        n2_cos=np.zeros(n2.shape)
        for i in range(Nx):
            n2_cos[:,i] = n2[:,i]*np.cos(2*pi*x)

        n2_sin=np.zeros(n2.shape)
        for i in range(Nx):
            n2_sin[:,i] = n2[:,i]*np.sin(2*pi*x)

        N1_a=np.array([2*self.Delta_x/3*(n2_cos[0,i] + np.sum(2*n2_cos[times_2,i]) + np.sum(4*n2_cos[times_4,i]) + n2_cos[(Nx-1),i]) for i in range(Nx)])

        N1_b=np.array([2*self.Delta_x/3*(n2_sin[0,i] + np.sum(2*n2_sin[times_2,i]) + np.sum(4*n2_sin[times_4,i]) + n2_sin[(Nx-1),i]) for i in range(Nx)])

        n_tilde=np.ones((Nx,Nx))
        for i in range(Nx):
            n_tilde[:,i]=N0[i]*n_tilde[:,i] + N1_a[i]*np.cos(2*pi*x) + N1_b[i]*np.sin(2*pi*x)

        sq_diff=(n2 - n_tilde)**2

        d2=[(self.Delta_x/3*(sq_diff[0,i] + np.sum(2*sq_diff[times_2,i]) + np.sum(4*sq_diff[times_4,i]) + sq_diff[(Nx-1),i])) for i in range(Nx)]

        n2=n2.T.reshape(Nx*Nx,)

        Volume1=(trapezoidal_rule_integration(m2)/self.rhom + trapezoidal_rule_integration(p2)/self.rhop + trapezoidal_rule_integration(q2)/self.rhop + trapezoidal_rule_integration(z2)*self.z0/self.rhoz + trapezoidal_rule_integration(b2)/self.rhob)

        u1 = Volume1/Volume0

        phi_1=np.arctan(np.tan(phi_0)/u1)

        Lambda1=np.cos(phi_1)/np.cos(phi_0)*Lambda0

        y_hat1=Lambda1/np.sin(phi_1)

        theta_B=np.arcsin(self.lambda_probe/2/inside_ri/Lambda1)-phi_1

        Delta_theta_B=theta_B0-theta_B,

        Delta_n=np.sqrt(N1_a*N1_a+N1_b*N1_b)

        nu=pi*Delta_n*self.T0*u1/self.lambda_probe/np.cos(theta_B)

        m1 = m2
        p1 = p2
        q1 = q2
        z1 = z2
        b1 = b2
        n1 = n2

        if self.Delta_t*j in time:

            spatial_profile_DF=pd.concat([spatial_profile_DF, pd.DataFrame({"x": x1,
                                      'Y': Y1,"monomer": m1,"short_polymer": p1,"immobile_polymer": q1,'nanoparticles': z1,'binder':b1,'refractive_index': n1,"time":j*self.Delta_t*np.ones(len(n1))})]).reset_index(drop=True)

            optical_properties_DF=pd.concat([optical_properties_DF,pd.DataFrame({'time':j*self.Delta_t,'Y':Y,'N0':N0,'Delta_n':Delta_n,'d2':d2, 'nu':nu})]).reset_index(drop=True)

            shrinkage_DF=pd.concat([shrinkage_DF,pd.DataFrame({'time':[self.Delta_t*j], 'actual_shrinkage':[1-u1],'phi_t':[phi_1], 'theta_B':[theta_B], 'apparent_shrinkage':[1 - np.
```

```
    tan(phi_0)/np.tan(phi_0 + Delta_theta_B)][0]})]).reset_index(drop=True)


        #Moharam_Young=lambda_probe*lambda_probe/Mean_RI/Delta_n/Lambda1/Lambda1/np.cos(phi_1)

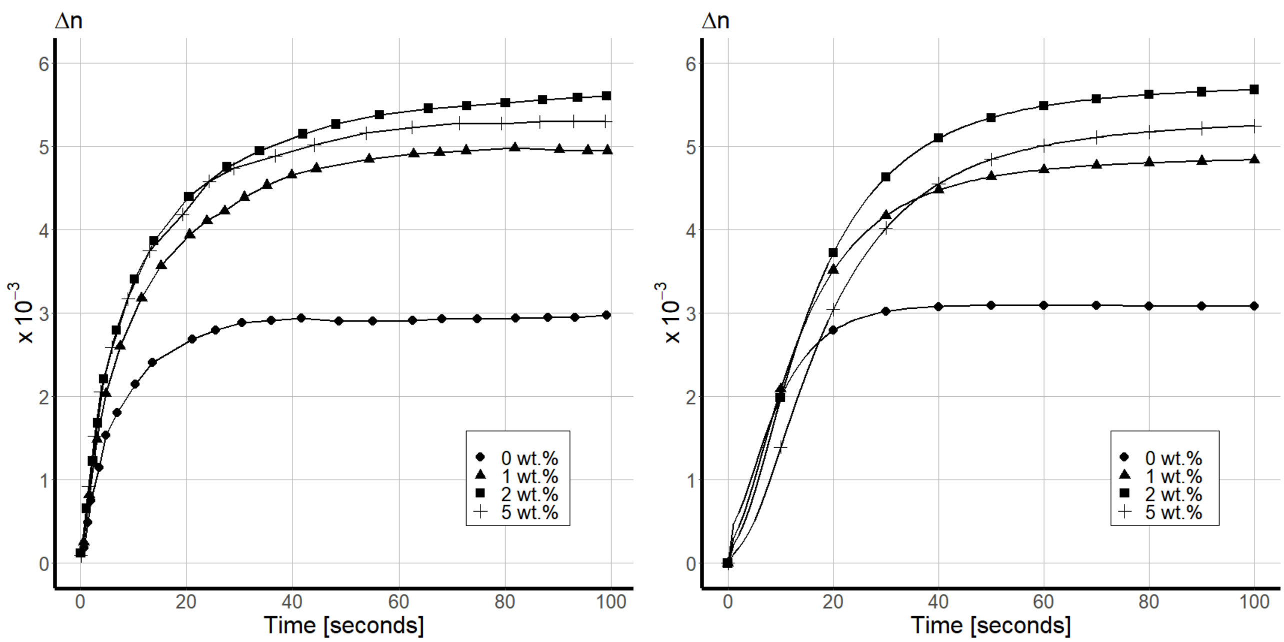
        Klein_Cook=2*pi*self.lambda_probe*self.T0*u1/inside_ri/Lambda1/Lambda1/np.cos(phi_1)

        if Klein_Cook < 10:
            self.Geometry='Planar'
            J0=optical_properties_DF.nu/2
            J1=J0
            for l in range(1,101):
                J1 = J1 + ((-1)**l)/factorial(l)/factorial(l+1)*(J0**(2*l + 1))
            eta=J1*J1
        else:
            self.Geometry='Volume'
            eta=np.sin(np.sqrt(optical_properties_DF.nu*optical_properties_DF.nu))**2

        optical_properties_DF['eta']=eta

        return spatial_profile_DF, optical_properties_DF, shrinkage_DF
```

Results

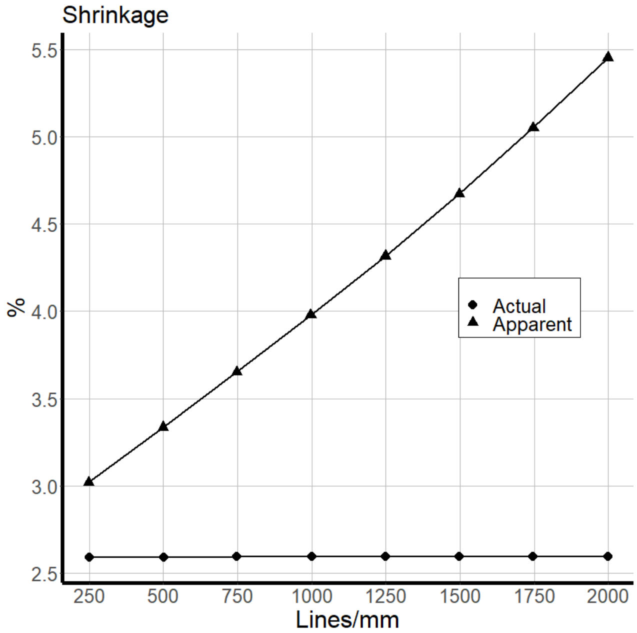


(a) Observed[1]

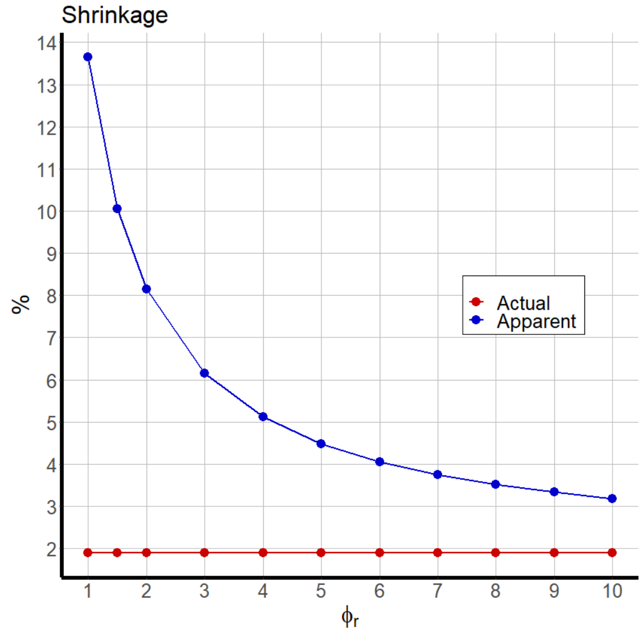
(b) Predicted; $\epsilon_z = 13$; $\xi = 1.6$

Figure 2: Time evolution of Δn of an unslanted holographic grating recorded in AA/PVA photopolymer with increased doping of BEA nanozeolites.

[1] Cody, D et al. (2014), *Effect of zeolite nanoparticles on the optical properties of diacetone acrylamide-based photopolymer*, Optical Materials 37, 181-187



(a) ... spatial frequencies ranging from 250 - 2000 lines/mm



(b) ... slant angles up to 10°

Figure 3: The predicted actual and apparent shrinkage for ...