

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

Jack Lyons, PhD

Purpose

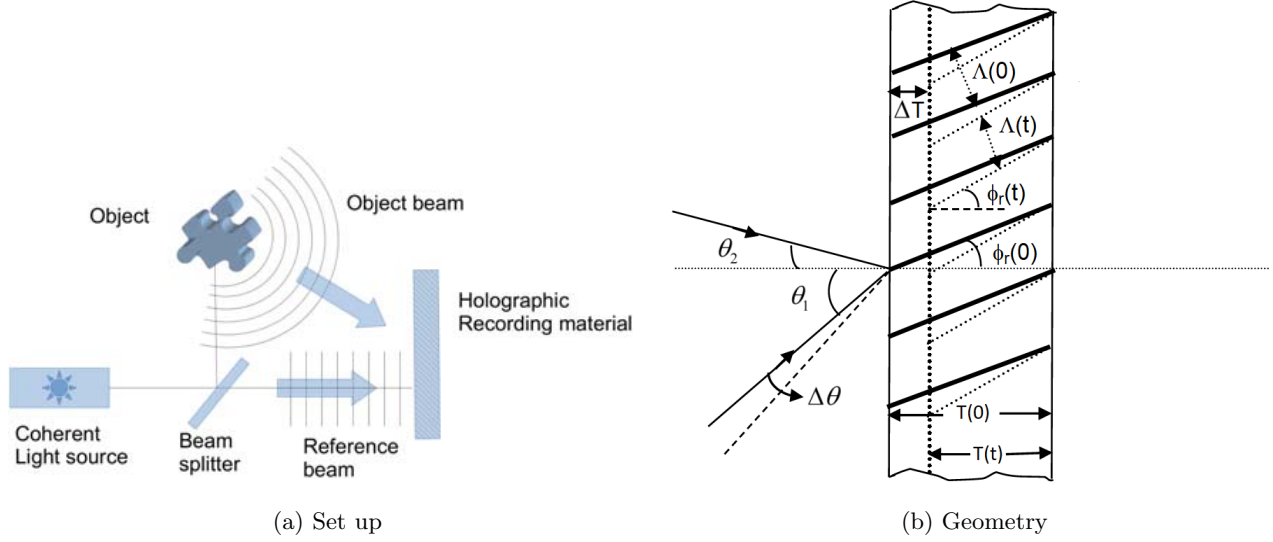


Figure 1: The optical set up and geometry for a holographic grating.

Mathematical Model

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

$$\frac{\partial b}{\partial t} = 0, \quad (1a)$$

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

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

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

$$\frac{\partial z}{\partial t} + \nabla \cdot \vec{J}_z = 0. \quad (1e)$$

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

$$\vec{J}_m = -D_m \frac{\partial m}{\partial x} \vec{i} - D_m \frac{\partial m}{\partial y} \vec{j}, \quad (3a)$$

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

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

$$0 \leq x \leq \hat{x}, \quad 0 \leq y \leq T(t), \quad t \geq 0. \quad (4)$$

Boundary Immobilization

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

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

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

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

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

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

Initial & Boundary Conditions

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

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

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

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

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

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

Numerical Scheme

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

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

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

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

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

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

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

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

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

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

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

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

Refractive Index Modulation

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

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

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

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

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

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

RI modulation can be modelled as

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

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

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

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

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

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

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

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

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

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

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

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

Python Script

```

1 from warnings import filterwarnings
2 filterwarnings("ignore")
3 import numpy as np
4 import pandas as pd
5 from math import pi, factorial
6 from numpy.linalg import inv
7 from time import time as gettime
8
9 class holographic_grating:
10
11     def __init__(
12         self,
13         start_exp=0, # Start of exposure
14         end_exp=1e2, # End of exposure
15         total_time=1e2, # Total simulation time
16         lpmm=1e3, # Spatial frequency
17         I0=5, # Intensity of recording beam
18         slant_angle=1e-4, # Grating slant_angle
19         xi=0.3, # Scattering coefficient
20         n_m=1.55, # Monomer refractive index
21         rhom=1.15, # Monomer density
22         Dm=1.6e-7, # Monomer diffusion coefficient
23         Dp=6.35e-10, # Polymer diffusion coefficient
24         rhop=1.3, # Polymer density
25         n_p=1.56, # Oligomer refractive index
26         n_q=1.64, # Polymer refractive index
27         Gamma=1, # Rate of immobilization
28         wt_pc=5e-2, # Doping %
29         Dz=1e-10, # Nanoparticle self-diffusion coefficient
30         epsilon_pz=13, # Cross-diffusion ratio
31         epsilon_qz=13, # Cross-diffusion ratio
32         rhoz=1.74, # Nanoparticle mass density
33         n_z=1.366, # Nanoparticle refractive index
34         b0=5.05, # Ratio of binder to monomer mass
35         n_b=1.5, # Binder refractive index
36         rhob=1.19, # Binder mass density
37         T0=50e-4, # Depth of photosensitive layer [cm]
38         zeta=139, # absorption coefficient [cm**-1]
39         lambda_probe=633e-7, # Wavelength of reconstruction beam
40         Delta_t=1/100, # Numerical scheme time step
41         Delta_x=1/20, # Numerical scheme spatial step
42         output_time_step=1 # Seconds
43     ):
44
45         self.total_time = total_time
46         self.end_exp = end_exp
47         self.lpmm = lpmm
48         self.T0 = T0
49         self.I0 = I0
50         if slant_angle == 0:
51             self.slant_angle = 1e-5
52         else:

```

```

53         self.slant_angle = slant_angle
54         self.T0 = T0
55         self.zeta = zeta
56         self.xi = xi
57         self.Dm = Dm
58         self.n_m = n_m
59         self.rhom = rhom
60         self.Dp = Dp
61         self.rhop = rhop
62         self.n_p = n_p
63         self.n_q = n_q
64         self.Gamma = Gamma
65         self.Dz = Dz
66         self.epsilon_pz = epsilon_pz
67         self.epsilon_qz = epsilon_qz
68         self.wt_pc = wt_pc
69         self.rhoz = rhoz
70         self.n_z = n_z
71         self.b0 = b0
72         self.n_b = n_b
73         self.rhob = rhob
74         self.lambda_probe = lambda_probe
75         self.Delta_x = Delta_x
76         self.Nx = int(1/Delta_x) + 1
77         self.Delta_Y = Delta_x
78         self.Delta_t = Delta_t
79         self.output_time_step = output_time_step
80
81
82     def slanted_grating_simulation_v22(self):
83
84         start_computation = gettime()
85         # 1.2 --- Define parameters
86         Nx=int(1/self.Delta_x) + 1# Number of spatial points
87         Ny=int(1/self.Delta_Y) + 1# Number of spatial points
88         if Nx%2==0:
89             return "Number of x mesh points must be an odd number."
90         if Ny%2==0:
91             return "Number of y mesh points must be an odd number."
92
93         x=np.linspace(0,1,Nx)# Non-dimensional grating distance
94         n_iterations = int(self.total_time/self.Delta_t)+1# Total number of iterations
95         r=self.Delta_t/self.Delta_x/self.Delta_x# Ratio of finite time step to squared finite
96         spatial step
97         m0=1# Initial mass of monomer
98         t0=1 # Reference time [s]
99         Lambda0=1/10/self.lpm # Grating period [cm]
100         Lambda1=Lambda0
101         j_end_exp = self.end_exp/self.Delta_t # Iteration of exposure end
102         z0 = self.wt_pc/(1 - self.wt_pc)*(m0 + self.b0)# Initial nanoparticle to monomer
103
104         # 1.3 --- Matrix initial conditions
105         u1=1
106         du_dt=0
107         m1 = np.ones(Nx*Nx)# m at j=0
108         p1 = np.zeros(Nx*Nx)# p at j=0
109         q1 = np.zeros(Nx*Nx)# q at j=0
110         z1 = np.ones(Nx*Nx)# z at j=0
111         b1 = self.b0*np.ones(Nx*Nx)# b at j=0
112
113         Volume0=m0/self.rhom + self.b0/self.rhob + z0/self.rhoz
114
115         phi_m0=m0/self.rhom/Volume0
116         phi_z0=z0/self.rhoz/Volume0
117         phi_b0=self.b0/self.rhob/Volume0
118
119         Lorentz_Lorenz_RHS = phi_m0*(self.n_m*self.n_m - 1)/(self.n_m*self.n_m + 2) + phi_b0*(self
120         .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
121         + 2)
122
123         Initial_RI = np.sqrt((2*Lorentz_Lorenz_RHS + 1)/(1 - Lorentz_Lorenz_RHS))
124
125         inside_ri = Initial_RI

```

```

124     n1=Initial_RI*np.ones(Nx*Nx)
125
126     phi_0=np.arcsin(np.sin(self.slant_angle/180*pi)/Initial_RI)
127     phi_1=phi_0
128     theta_B0=np.arcsin(self.lambda_probe/2/Initial_RI/Lambda0) - phi_0
129     y_hat0=Lambda0/np.sin(phi_0)
130     y_hat1=y_hat0
131     x_hat=Lambda0/np.cos(phi_0)
132
133     # 1.5 --- Nondimensionalized parameters
134     alpha_m_x=self.Dm*t0/x_hat/x_hat
135     alpha_m_y=self.Dm*t0/self.T0/self.T0
136     alpha_p_x=self.Dp*t0/x_hat/x_hat
137     alpha_p_y=self.Dp*t0/self.T0/self.T0
138     alpha_z_x=self.Dz*t0/x_hat/x_hat
139     alpha_z_y=self.Dz*t0/self.T0/self.T0
140     F0=0.1*self.I0**0.3
141     beta=F0*t0
142     gamma = self.Gamma*m0*t0
143     zeta_star = self.zeta*self.T0
144     xi_star=self.xi*z0
145     interior_points = list(range(1,Nx-1))
146     times_4 = [interior_points[i] for i in range(len(interior_points)) if interior_points[i]%2
147 != 0]
148     times_2 = [interior_points[i] for i in range(len(interior_points)) if interior_points[i]%2
149 == 0]
150     Y=np.arange(0,1+self.Delta_x, self.Delta_x)
151     time=np.arange(1,self.total_time+self.output_time_step, self.output_time_step)
152     Y1=[]
153     x1=[]
154     for i in range(Nx):
155         for j in list(Y):
156             Y1.append(j)
157             for j in x:
158                 x1.append(j)
159     Y1=np.sort(Y1)
160     indexDF=pd.DataFrame({'x':x1, 'y':Y1})
161
162     spatial_profile_DF=pd.DataFrame({'x': x1, 'Y': Y1, "monomer": m1, "short_polymer": p1, "
163 immobile_polymer": q1, 'nanoparticles': z1, 'binder':b1, 'refractive_index': n1, "time": np.
164 zeros(len(n1)), 'N0':np.zeros(len(n1))+Initial_RI, 'Delta_n':np.zeros(len(n1)), 'd2':np.zeros(
165 len(n1))})
166
167     optical_properties_DF=pd.DataFrame({'Y': Y, "time": np.zeros(len(Y)), 'N0':np.zeros(len(Y))
168 +Initial_RI, 'Delta_n':np.zeros(len(Y)), 'nu':np.zeros(len(Y)), 'd2':np.zeros(len(Y))})
169
170     shrinkage_DF=pd.DataFrame({'time': [0], 'actual_shrinkage': [0], 'phi_t': [phi_0], 'theta_B': [
171 theta_B0], 'apparent_shrinkage': [0]})
172
173     def trapezoidal_rule_integration(array):
174
175         array=array.reshape(Nx,Nx).T
176
177         return Delta_x*Delta_x/4*(array[0,0] + array[Nx-1,0] + array[0,Nx-1] + array[Nx-1,Nx
178 -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)
179 ] + np.sum(2*array[1:(Nx-1),Nx-1]) + np.sum(4*array[1:(Nx-1),1:(Nx-1)]))
180
181     def simpsons_rule_1D(arr1D):
182
183         intpts=list(range(1,len(arr1D)-1))
184         times_4=[i for i in intpts if i%2!=0]
185         times_2=[i for i in intpts if i%2==0]
186
187         return Delta_x/3*(arr1D[0] + 4*sum(arr1D[times_4]) + 2*sum(arr1D[times_2]) + arr1D[len
188 (arr1D)-1])
189
190     # 1.6 --- Calculate each time step via implicit finite difference method
191     for j in range(1,n_iterations):
192
193         if j <= j_end_exp:
194             Phi=1
195         else:

```



```

188         Phi = 0# Phi=1 if illumination is on, 0 otherwise
189
190         f = np.zeros(Nx*Nx).reshape(Nx,Nx)
191         for i in range(Nx):
192             matrix_z1=z1.reshape(Nx,Nx)
193             z1_i=matrix_z1[:,i]
194             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]))
195
196         f = f.reshape(Nx*Nx,)
197
198         MM2 = (2 + Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
199         MM1 = (2 - Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
200         PP2 = (2 + self.Delta_t*gamma*p1)*np.identity(Nx*Nx)
201         PP1 = (2 - self.Delta_t*gamma*p1)*np.identity(Nx*Nx)
202         PM2 = (+Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
203         PM1 = (+Phi*self.Delta_t*beta*f)*np.identity(Nx*Nx)
204         QQ2 = 2*np.identity(Nx*Nx)
205         QQ1 = 2*np.identity(Nx*Nx)
206         QP2 = (+Phi*gamma*self.Delta_t*p1)*np.identity(Nx*Nx)
207         QP1 = (+Phi*gamma*self.Delta_t*p1)*np.identity(Nx*Nx)
208         ZZ2 = 2*np.identity(Nx*Nx)
209         ZZ1 = 2*np.identity(Nx*Nx)
210         BB2 = 2*np.identity(Nx*Nx)
211         BB1 = 2*np.identity(Nx*Nx)
212
213         for i in range(Nx*Nx):
214
215             if i in list(indexDF.loc[indexDF.x==0,].index):
216                 i_minus_1 = i+Nx-2
217             else:
218                 i_minus_1 = i-1
219
220             if i in list(indexDF.loc[indexDF.x==1,].index):
221                 i_plus_1 = i-Nx+2
222             else:
223                 i_plus_1 = i+1
224
225             if i in list(indexDF.loc[indexDF.y==0,].index):
226                 j_minus_1 = i+Nx
227             else:
228                 j_minus_1 = i-Nx
229
230             if i in list(indexDF.loc[indexDF.y==1,].index):
231                 j_plus_1 = i-Nx
232             else:
233                 j_plus_1 = i+Nx
234
235             MM2[i, i_minus_1] = MM2[i, i_minus_1] - r*alpha_m_x
236             MM2[i, j_minus_1] = MM2[i, j_minus_1] - r*alpha_m_y/u1/u1
237             MM2[i, i] = MM2[i, i] + 2*r*alpha_m_x
238             MM2[i, i] = MM2[i, i] + 2*r*alpha_m_y/u1/u1
239             MM2[i, i_plus_1] = MM2[i, i_plus_1] - r*alpha_m_x
240             MM2[i, j_plus_1] = MM2[i, j_plus_1] - r*alpha_m_y/u1/u1
241
242             MM1[i, i_minus_1] = MM1[i, i_minus_1] + r*alpha_m_x
243             MM1[i, j_minus_1] = MM1[i, j_minus_1] + r*alpha_m_y/u1/u1
244             MM1[i, i] = MM1[i, i] - 2*r*alpha_m_x
245             MM1[i, i] = MM1[i, i] - 2*r*alpha_m_y/u1/u1
246             MM1[i, i_plus_1] = MM1[i, i_plus_1] + r*alpha_m_x
247             MM1[i, j_plus_1] = MM1[i, j_plus_1] + r*alpha_m_y/u1/u1
248
249             PP2[i, i_minus_1] = PP2[i, i_minus_1] - r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[
i_minus_1])
250             PP2[i, j_minus_1] = PP2[i, j_minus_1] - r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*
z1[j_minus_1])
251             PP2[i, i] = PP2[i, i] + 2*r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[i])
252             PP2[i, i] = PP2[i, i] + 2*r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*z1[i])
253             PP2[i, i_plus_1] = PP2[i, i_plus_1] - r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[
i_plus_1])
254             PP2[i, j_plus_1] = PP2[i, j_plus_1] - r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*
z1[j_plus_1])
255
256             PP1[i, i_minus_1] = PP1[i, i_minus_1] + r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[

```

```

i_minus_1])
257     PP1[i, j_minus_1] = PP1[i, j_minus_1] + r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*
z1[j_minus_1])
258     PP1[i, i] = PP1[i, i] - 2*r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[i])
259     PP1[i, i] = PP1[i, i] - 2*r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*z1[i])
260     PP1[i, i_plus_1] = PP1[i, i_plus_1] + r*alpha_p_x*(1 + self.epsilon_pz*z0*z1[
i_plus_1])
261     PP1[i, j_plus_1] = PP1[i, j_plus_1] + r*alpha_p_y/u1/u1*(1 + self.epsilon_pz*z0*z1
[j_plus_1])
262
263     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])
264     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])
265     ZZ2[i, i] = ZZ2[i, i] + 2*r*alpha_z_x*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz
*p1[i])
266     ZZ2[i, i] = ZZ2[i, i] + 2*r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[i] + self.
epsilon_pz*p1[i])
267     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])
268     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])
269
270     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])
271     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])
272     ZZ1[i, i] = ZZ1[i, i] - 2*r*alpha_z_x*(1 + self.epsilon_qz*q1[i] + self.epsilon_pz
*p1[i])
273     ZZ1[i, i] = ZZ1[i, i] - 2*r*alpha_z_y/u1/u1*(1 + self.epsilon_qz*q1[i] + self.
epsilon_pz*p1[i])
274     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])
275     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])
276
277     MM2[i, j_minus_1] = MM2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
278     MM1[i, j_minus_1] = MM1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
279     MM2[i, j_plus_1] = MM2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
280     MM1[i, j_plus_1] = MM1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
281
282     PP2[i, j_minus_1] = PP2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
283     PP1[i, j_minus_1] = PP1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
284     PP2[i, j_plus_1] = PP2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
285     PP1[i, j_plus_1] = PP1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
286
287     QQ2[i, j_minus_1] = QQ2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
288     QQ1[i, j_minus_1] = QQ1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
289     QQ2[i, j_plus_1] = QQ2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
290     QQ1[i, j_plus_1] = QQ1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
291
292     ZZ2[i, j_minus_1] = ZZ2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
293     ZZ1[i, j_minus_1] = ZZ1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
294     ZZ2[i, j_plus_1] = ZZ2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
295     ZZ1[i, j_plus_1] = ZZ1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
296
297     BB2[i, j_minus_1] = BB2[i, j_minus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
298     BB1[i, j_minus_1] = BB1[i, j_minus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
299     BB2[i, j_plus_1] = BB2[i, j_plus_1] - Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
300     BB1[i, j_plus_1] = BB1[i, j_plus_1] + Y1[i]/u1*self.Delta_t/2/self.Delta_x*du_dt
301
302     m2 = np.matmul(inv(MM2), np.matmul(MM1,m1))
303
304     p2 = np.matmul(inv(PP2), np.matmul(PP1,p1) + np.matmul(PM2,m2) + np.matmul(PM1,m1))
305
306     q2 = np.matmul(inv(QQ2), np.matmul(QQ1, q1) + np.matmul(QP2,p2) + np.matmul(QP1,p1))
307
308     if z0==0:
309         z2 = z1
310     else:
311         z2 = np.matmul(inv(ZZ2), np.matmul(ZZ1,z1))
312
313     b2 = np.matmul(inv(BB2), np.matmul(BB1,b1))
314

```

```

315     Vb = b2/self.rhob # cm**3
316     Vm = m2*m0/self.rhom # cm**3
317     Vp = p2*m0/self.rhop # cm**3
318     Vq = q2*m0/self.rhop # cm**3
319     Vz = z2*z0/self.rhoz # cm**3
320     Vtotal=Vb+Vm+Vp+Vq+Vz # cm**3
321     phi_m = Vm/Vtotal
322     phi_b = Vb/Vtotal
323     phi_p = Vp/Vtotal
324     phi_q = Vq/Vtotal
325     phi_z = Vz/Vtotal
326
327     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)
328
329     n2=np.sqrt((2*Lorentz_Lorenz_RHS + 1)/(1 - Lorentz_Lorenz_RHS))
330     n2=n2.reshape(Nx,Nx).T
331
332     inside_ri = simpsons_rule_1D(n2[int((Nx-1)/2)])
333
334     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)]
335
336     n2_cos=np.zeros(n2.shape)
337     for i in range(Nx):
338         n2_cos[:,i] = n2[:,i]*np.cos(2*pi*x)
339
340     n2_sin=np.zeros(n2.shape)
341     for i in range(Nx):
342         n2_sin[:,i] = n2[:,i]*np.sin(2*pi*x)
343
344     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)])
345
346     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)])
347
348     n_tilde=np.ones((Nx,Nx))
349     for i in range(Nx):
350         n_tilde[:,i]=N0[i]*n_tilde[:,i] + N1_a[i]*np.cos(2*pi*x) + N1_b[i]*np.sin(2*pi*x)
351
352     sq_diff=(n2 - n_tilde)**2
353
354     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)]
355
356     n2=n2.T.reshape(Nx*Nx,)
357
358     Volume1=(trapezoidal_rule_integration(m2)/self.rhom + trapezoidal_rule_integration(p2)
/self.rhop + trapezoidal_rule_integration(q2)/self.rhop + trapezoidal_rule_integration(z2)*z0/
self.rhoz + trapezoidal_rule_integration(b2)/self.rhob)
359
360     u1 = Volume1/Volume0
361
362     phi_1=np.arctan(np.tan(phi_0)/u1)
363
364     Lambda1=np.cos(phi_1)/np.cos(phi_0)*Lambda0
365
366     y_hat1=Lambda1/np.sin(phi_1)
367
368     theta_B=np.arcsin(self.lambda_probe/2/inside_ri/Lambda1)-phi_1
369
370     Delta_theta_B=theta_B0-theta_B,
371
372     Delta_n=np.sqrt(N1_a*N1_a+N1_b*N1_b)
373
374     nu=pi*Delta_n*self.T0*u1/self.lambda_probe/np.cos(theta_B)
375
376     m1 = m2
377     p1 = p2
378     q1 = q2
379     z1 = z2

```

```

380         b1 = b2
381         n1 = n2
382
383         if self.Delta_t*j in time:
384
385             spatial_profile_DF=pd.concat([spatial_profile_DF, pd.DataFrame({'x': x1,
386                                     'Y': Y1,"monomer": m1,"short_polymer": p1,"
387                                     immobile_polymer": q1,'nanoparticles': z1,'binder':b1,'refractive_index': n1,"time":j*self.
388                                     Delta_t*np.ones(len(n1))})]).reset_index(drop=True)
389
390             optical_properties_DF=pd.concat([optical_properties_DF,pd.DataFrame({'time':j*self
391                                     .Delta_t, 'Y':Y, 'N0':N0, 'Delta_n':Delta_n, 'd2':d2, 'nu':nu})]).reset_index(drop=True)
392
393             shrinkage_DF=pd.concat([shrinkage_DF,pd.DataFrame({'time':[self.Delta_t*j], '
394                                     actual_shrinkage':[1-u1], 'phi_t':[phi_1], 'theta_B':[theta_B], 'apparent_shrinkage':[1 - np.
395                                     tan(phi_0)/np.tan(phi_0 + Delta_theta_B)][0]})]).reset_index(drop=True)
396
397             #Moharam_Young=lambda_probe*lambda_probe/Mean_RI/Delta_n/Lambda1/Lambda1/np.cos(phi_1)
398
399             Klein_Cook=2*pi*self.lambda_probe*self.T0*u1/inside_ri/Lambda1/Lambda1/np.cos(phi_1)
400
401             if Klein_Cook < 10:
402                 self.Geometry='Planar'
403                 J0=optical_properties_DF.nu/2
404                 J1=J0
405                 for l in range(1,101):
406                     J1 = J1 + ((-1)**l)/factorial(l)/factorial(l+1)*(J0**(2*l + 1))
407                 eta=J1*J1
408             else:
409                 self.Geometry='Volume'
410                 eta=np.sin(np.sqrt(optical_properties_DF.nu*optical_properties_DF.nu))*2
411
412             optical_properties_DF['eta']=eta
413
414             end_computation = gettime()
415
416             computation_duration = end_computation-start_computation
417
418             return spatial_profile_DF, optical_properties_DF, shrinkage_DF, computation_duration
419
420 if __name__ == "__main__":
421
422     a = holographic_grating(total_time=0)
423     df1, df2, df3, t0 = a.slanted_grating_simulation_v22()
424     assert len(df3) == 1
425     assert len(df2) == a.Nx
426     assert len(df1) == a.Nx*a.Nx
427     del a, df1, df2, df3, t0
428     print("All tests passed.")

```

Results

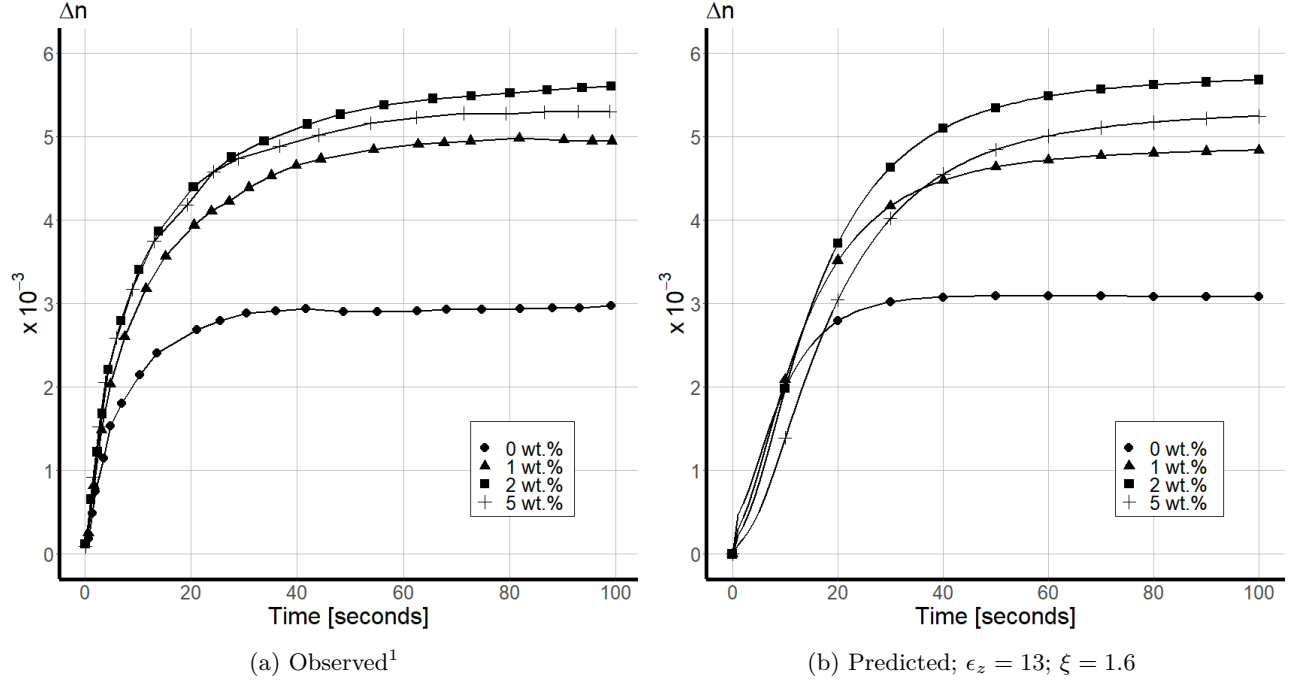


Figure 2: Time evolution of Δn of an unslanted holographic grating recorded in AA/PVA photopolymer with increased doping of BEA nanozeolites.

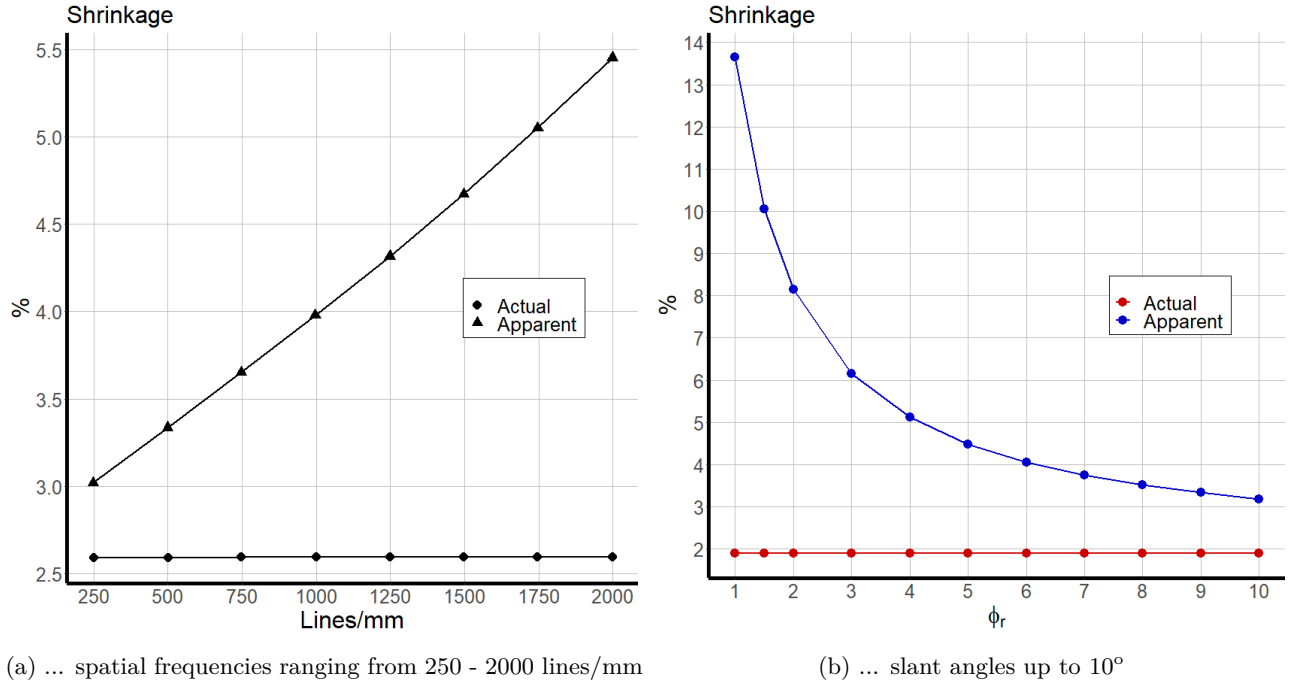


Figure 3: The predicted actual and apparent shrinkage for ...

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