Efficient Transmission Matrix Modeling and Optimization of Grating-based Biosensors

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***Abstract*—This work presents an efficient Transmission Matrix Model (TMM) for designing silicon nitride grating couplers in flow cytometry. The TMM simulates transient transmission with a four orders-of-magnitude speed increase over FDTD, enabling Bayesian Optimization that achieves a Peak-to-Baseline (P2B) transmission of 0.221.**

I. INTRODUCTION

Flow cytometry enables high-precision cell analysis but often requires bulky, cost-prohibitive setups. Integrated photonic systems aim to miniaturize this technology, improving accessibility however the poor power collection efficiency of integrated waveguides limits cell detection sensitivity. Integrated optofluidic designs with grating couplers potentially provide efficient optical coupling. However, the computational overhead of numerical modelling tools such as FDTD's is prohibitive for fast, iterative design optimization. This work introduces a TMM that accurately models light transmission in grating-based flow cytometry systems, that is then incorporated into in a Bayesian Optimization scheme to improve optical coupling and cell detection sensitivity.

II. MODELING

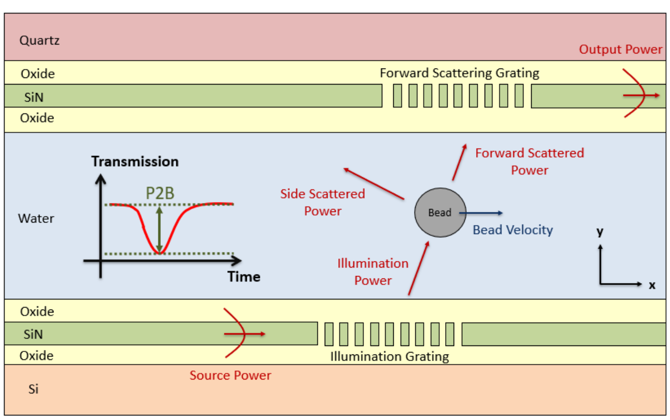

Fig. 1. Schematic of dynamic power flow in the system as a bead moves through the channel, illustrating the transient dip in power transmission used to calculate the Peak-to-Baseline (P2B) metric.

The system in Fig. 1 consists of 30 µm thick microfludic channel sandwiched between silicon nitride (Si_3N_4) waveguides with oxide cladding, similar to that described by Jooken et. all [1]. When excited with 638nm laser, an Illumination Grating (ILG) etched into the bottom Si_3N_4 scatters light across the microfluidic channel towards a Forward Scattering Grating (FSG) etched into the top Si_3N_4 waveguide. When a 3 µm radius polystyrene bead (biological cell analog) moves through the channel, it scatters the light away from the FSG, producing a transient in the FSG transmission. The goal is to maximise transient's Peak to Baseline (P2B) in Fig. 1 a metric used in other work for cell detection sensitivity [1]. Given the bead's rounded geometry, FDTD or FEM simulations might seem ideal, but the microfluidic channel's thickness makes such simulations computationally inefficient. Instead, optical power through the system can be modeled using a 2D TMM, treating the layers and components as linear, lossless dielectrics. The TMM breaks down the system into modular sub-components, each represented by a matrix that captures the coherent transmission characteristics of a plane wave spectrum propagating through through each component, see Fig. 2. The input to output power transmission can be found by coherently cascading the matrices as in Eqn. 1:

$$T_{A\to D} = |t_{A\to D}|^2 = |\mathbf{t}_{C\to D}.\mathbf{t}_{P\to C}.\mathbf{t}_P.\mathbf{t}_{B\to P}.\mathbf{t}_{A\to B}|^2 \quad (1)$$

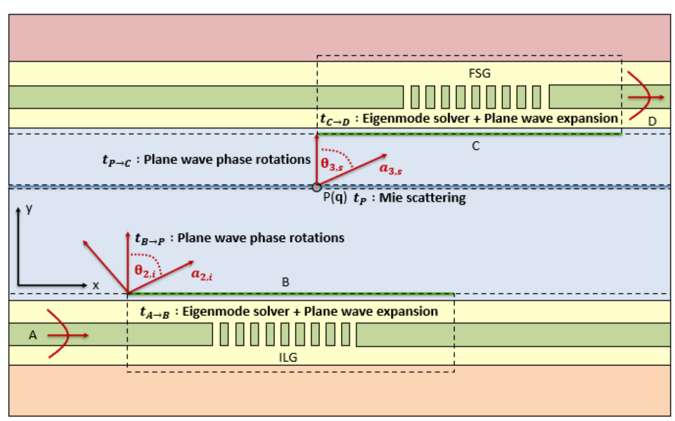

Fig. 2. TMM modularization and matrix generation methods for calculating modal coupling from A to D in the dynamic system with a bead P at a position **q** in the channel.

A. Gratings

The TMM begins with transmission matrices for the Illumination Grating (ILG) and Forward Scattering Grating (FSG), labeled $\mathbf{t}_{A\to B}$ and $\mathbf{t}_{C\to D}$, respectively. For each grating, the eigenmode expansion solver CAMFR [2] is used to calculate the fields above the grating. A Discrete Fourier Transform (DFT) then decomposes these fields into the plane wave spectrum directed toward the microfluidic channel, resulting in matrices of upward propagating plane waves. Reciprocity and coordinate transformations reverse the flow of light and orient the FSG as it appears it in Fig. 2.

B. Bead

The scattering matrix for the bead, $\mathbf{t}_P$, models the interaction of the incident plane waves with the bead. Using Mie scattering theory, the bead is treated as a 2D dielectric cylinder, and a fixed $\mathbf{t}_P$ is found that captures the angular scattering response based on the bead's refractive index and size. For a certain bead geometry, this matrix need only be generated once and may be reused for multiple TMM simulations.

C. Microfluidic Channel

The microfluidic channel is treated as a uniform dielectric medium, and two matrices, $\mathbf{t}_{B\to P}$ and $\mathbf{t}_{P\to C}$, represent the channel's transmission. These matrices propagate plane waves from the ILG to the center of the bead ($\mathbf{t}_{B\to P}$) and from the bead to the beginning FSG ($\mathbf{t}_{P\to C}$). Its elements are simple phase rotations computed for each plane wave based on its propagation angle and distance traversed through the channel. Translating the bead or FSG's position within the channel corresponds to generating a new set of $\mathbf{t}_{B\to P}$ and $\mathbf{t}_{P\to C}$ matrices, a computationally inexpensive operation.

D. Validation

The accuracy and computation of the TMM can be benchmarked against Lumerical FDTD to validate its performance. First, the matrices $\mathbf{t}_{A\to B}$ and $\mathbf{t}_{C\to D}$ were generated for gratings with a period of $\Lambda_{ILG} = \Lambda_{FSG} = 0.49\,\mu\mathrm{m}$ and 21 periods using a 2881 plane wave expansion. Using Eqn 1, power transmission through the dynamic system was iteratively calculated while sweeping the bead's x position in steps of $100\,\mathrm{nm}$ between $-5\,\mu\mathrm{m} < x_2 < 20\,\mu\mathrm{m}$ with the y position fixed at mid-channel. Figure 3 shows the results of the simulations compared to those obtained via Lumerical FDTD. The results demonstrate excellent agreement between the TMM and FDTD, demonstrating the TMM's accuracy. In the TMM, inter-component reflection is not considered, possibly accounting for the small error between the transients. Since, light propagation through the grating system is reduced to computationally inexpensive matrix generations and multiplications, it took the TMM $53\,\mathrm{s}$ to complete the 251 point sweep. By contrast, the FDTD took approximately 70 hours to compute the transient on the same computational hardware. This represents a four order-of-magnitude reduction in computation time, demonstrating the computational efficiency of the TMM.

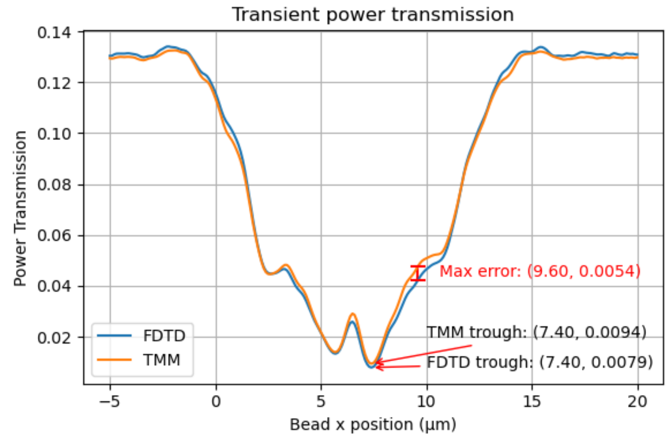

Fig. 3. Transient power transmission calculated while sweeping the bead position by both a 2881 plane wave TMM and Lumerical FDTD for gratings with $\Lambda_{ILG} = \Lambda_{FSG} = 0.49\,\mu\mathrm{m}$ and $x_{FSG} = 3.1\,\mu\mathrm{m}$.

III. Optimization

With a TMM for the efficient simulation of transients, the grating system may be optimized for maximum P2B. The grating period, number of teeth, relative position and linear apodization factor are possible grating parameterisations explored in this work. Bayesian Optimization by means of Gaussian Process was selected to efficiently search this parameter space. A $423\,\mathrm{nm}$ period (with 50% fill) grating system, with 39 periods, a relative FSG x position of $-3.959\,\mu\mathrm{m}$ and a linear apodization strength of $0.0135\,1/\mu\mathrm{m}$ was found to be the optimum configuration, yielding a power transmission P2B of 0.221. Jooken et. all [1] report an experimental maximum static power transmission (upper bound to P2B) of 0.024 from an unoptimised uniform grating system, approximately an order-of-magnitude smaller than the result in this work.

IV. Conclusion

This work presents a computationally efficient Transmission Matrix Model (TMM) for optimizing grating-based biosensors in integrated flow cytometry, achieving approximately four orders-of-magnitude faster computation than FDTD simulations. By modularizing optical transmission into matrix-based sub-components, the TMM enables rapid, iterative optimization. Bayesian Optimization identified an optimal, linearly apodized grating configuration with a Peak-to-Baseline (P2B) transmission of 0.221, an order-of-magnitude larger than the result in literature [1]. Demonstrating the TMM's potential for optimizing biosensors in silicon photonics.

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