Design, modeling, and experimental realization of tunable Fabry-Perot nanocavities for broadband and narrow-band applications

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DESIGN, MODELING, AND EXPERIMENTAL REALIZATION OF TUNABLE FABRY-PEROT NANOCAVITIES FOR BROADBAND AND NARROW-BAND APPLICATIONS

Kirtankumar Pravin Dixit

A DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in The Department of Physics & Astronomy to The Graduate School of The University of Alabama in Huntsville

May 2024

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Abstract

DESIGN, MODELING, AND EXPERIMENTAL REALIZATION OF TUNABLE FABRY-PEROT NANOCAVITIES FOR BROADBAND AND NARROW-BAND APPLICATIONS

Kirtankumar Pravin Dixit

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy

Physics & Astronomy
The University of Alabama in Huntsville
May 2024

Efficient control of light absorption at the nanoscale has become a popular area of research, leveraging metal, semiconductor, and dielectric thin film technologies to engineer multilayer structures that modulate light through interference. A Fabry-Perot nanocavity can be configured with a dielectric or semiconductor layer sandwiched between two metal layers to exploit interference. This necessarily involves multiple optical paths through a spacer medium. The ensemble structures can be configured for anti-reflection, high-reflection, and dichroism. This dissertation is structured around four main objectives, each aimed at demonstrating the advanced capabilities of these nanocavities in manipulating light. The goals specifically focus on showcasing enhanced narrowband color reflection, dynamically tunable narrowband color absorption, ultra-broadband absorption spanning the visible to near-infrared spectrum, and a comprehensive sensitivity analysis of the dynamically tunable system based on variations in structural parameters. The initial objective was the modeling and experimental realization of a dynamically tunable Fabry-Perot nanocavity, incor-
porating a metal-oxide-semiconductor (MOS) structure to achieve real-time control of absorption wavelengths in the visible spectrum. This involves using n-type-doped semiconductors like indium antimonide and indium arsenide within an MOS configuration, enabling substantial optical property tuning by electrically controlling the induced carrier accumulation. The second (and easier to experimentally realize) objective entails modeling and building reflective color filters and broadband absorbers for the near-infrared range based on an asymmetric Fabry-Perot nanocavity design. This setup revealed enhanced spectral and angular sensitivity, functioning as an RGB color reflector. The third objective explores the use of an asymmetric Fabry-Perot nanocavity as an ultra-broadband absorber for visible to near-infrared wavelengths, achieving over 80% absorption at incidence angles up to 60 degrees. The final objective quantifies the impact of fabrication inaccuracies on the optical performance of Fabry-Perot nanocavities using Monte Carlo simulations to assess the effect of variations in optical and structural parameters. This research contributes to advancements in the new fields of electrically tunable color filters, solid-state color reflectors, biosensors, photovoltaics, and high-speed electro-optical modulators. The lithography-free fabrication process presented enhances the cost-effectiveness of these devices, which can lead to applications being found in any field employing active or passive optical elements.
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Chapter 1. General Introduction

1.1 Lithography-free Nanoscale Optical Devices

Recent advancements in nanofabrication have inspired nanoscale geometries with high resolutions useful in the development of nanoscale optical devices. However, challenges in scalability and repeatability limit their widespread applications. Lithography-free nanostructures (LFNS) offer a promising solution to address these limitations and scale up the designs of such devices. LFNS-based optical devices are nano-sized architectures that do not require conventional lithographic techniques; they typically involve complex patterns at the nanoscale. In LFNS, alternative methods, such as self-assembly (spontaneous organization of materials into structured patterns) or deposition (controlled placement of material layers onto a substrate), are employed to fabricate nanostructures, without relying on traditional lithography [1, 2, 3]. This approach offers simplicity and cost-effectiveness in the production of nanoscale features. The absence of lithography simplifies the fabrication process, making it accessible for various applications that require intricate nanostructured designs. The application of LFNS in optical device fabrication, especially at the nanophotonics scale holds great promise for advancing optical technologies. These structures enable precise control over light-matter interactions at the nanoscale. In nanophotonic applications, LFNS
play a pivotal role in optimal light absorption, reflection, and manipulation, making them essential in the development of advanced sensors, imaging devices, and photonic circuits. In nanophotonics, LFNS encompass plasmonic and dielectric nanostructures. Plasmonic LFNS leverage metallic materials in order to exploit surface plasmon resonances, facilitating enhanced light-matter interactions for applications like surface-enhanced spectroscopy and sensing. On the other hand, dielectric LFNS utilize non-metallic materials like semiconductors or dielectrics, manipulating light at the nanoscale in applications like optical waveguiding and metasurfaces. Although LFNS offer a relatively straightforward alternative for the development of nanoscale optical devices, the selection of appropriate materials for the target application remains crucial.

This research uses one of the well-known lithography-free methodologies metal-insulator-metal (MIM) nanostructures, called Fabry-Perot nanocavities (FPN) to realize narrowband perfect absorbers, narrowband reflective color filters, and broadband near-perfect absorbers for the visible and near-infrared (NIR) regions. The investigation extends to both static and dynamic tunability in these nanocavities. A schematic diagram of an FPN cavity is presented in fig. 1.1(A).

The FPN operates on the principle of optical interference within a confined space. Light entering the cavity undergoes multiple reflections between the two metal layers, which act as mirrors (fig. 1.1(B)). The insulator layer between the metals has a specific thickness that determines the cavity’s optical path length. Constructive interference occurs when the reflected waves are in phase, reinforce-
ing each other to enhance specific wavelengths of light, leading to high reflection. Conversely, destructive interference happens when the reflected waves are out of phase, canceling each other out and thereby enabling the device to act as an absorber across a range of wavelengths. The Fabry-Perot nanocavity is crucial for the design of devices that need to regulate interactions between light and materials. Such devices include filters, which selectively allow certain wavelengths of light to pass, sensors that detect light, and photovoltaic cells for solar energy conversion. Chapter 2 of the dissertation provides details of the scientific principles involved, particularly how constructive and destructive interference of light within the nanocavity facilitates the precise engineering of these devices.

For a better explanation of MIM architecture-based nanostructures and other commonly utilized LFNS, the following section provides a comprehensive overview of LFNS development, covering design and material considerations, while also exploring promising optical and electro-optical applications.
1.2 Comprehensive Review of Relevant Literature

This section provides a comprehensive review of the existing research landscape, focusing on the innovative use of LFNS and a diverse array of materials designed to absorb and reflect light. Such studies are pivotal for a wide range of applications, including photonic devices, sensors, and energy harvesting systems.

1.2.1 Pathways and Materials for LFNS

The study of light confinement in architectures significantly smaller than the wavelength of the electro-magnetic (EM) waves being modulated has been a key focus in the field of metamaterial-based perfect absorbers. In sub-wavelength ranges, metals exhibit strong light-matter interaction across a broad spectral range [1]. This interaction is due to the coordinated oscillation of free conduction electrons, known as localized surface plasmon resonances (LSPR), or inter-band transitions. However, the fabrication of plasmonic nanostructures requires complex and large-scale hardware, such as lithography. As a result, the LFNS technology has gained attention [2, 3]. Among the scalable LFNS, planar multilayer designs are common, mainly utilizing the absorption of Fabry-Perot (FP) resonance modes [2]. Particularly, MIM, MIM-insulator (MIMI), and periodic (MI)$_N$ cavity configurations are often classified as cavity absorbers.

Figure 1.2 illustrates the optimal material selections for constructing LFNS to be used as narrow and broadband optical absorbers [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. Across the ultraviolet (UV) and visible spec-
tra, a diverse range of semiconductors and metals are candidates for achieving this objective. To extend this functionality to longer wavelengths, such as the near-infrared (NIR), lossy metals like titanium (Ti), chromium (Cr), nickel (Ni), tungsten (W), and bismuth (Bi) may be employed [3]. Additionally, doped metal oxides, like aluminum-doped zinc oxide (AZO) [4], gallium-doped zinc oxide (GZO) [5], indium-doped tin oxide (ITO) [6], indium-doped cadmium oxide (ICO) [7, 8], and cerium-doped indium oxide (CIO) [9] are possible candidates. They all exhibit a nonlinear change in refractive index (a requirement of Epsilon-Near-Zero or ENZ materials or structures) in the NIR to mid-IR (MIR) range. These are reasonable choices for Lithography-free metamaterial absorbers (LFMAs). Metal nitrides, including titanium nitride (TiN), zinc nitride (ZrN), hafnium nitride (HfN), and indium nitride (InN), exhibit a plasmonic response in the infrared (IR) range [10, 11, 12], and a tunable plasma frequency in the MIR range.

**Figure 1.2:** Candidate absorptive materials for the implementation of LFNS across various segments of the optical spectrum.
1.2.2 Applications

Materials suitable for creating LFNS for optical applications can be broadly divided into two groups: i) metallic and ii) non-metallic. Their applications are determined by their operational wavelength regions: i) covering the sun blackbody radiation spectrum (Sun-BBRS), commonly known as the solar spectrum, spanning UV - visible - NIR - MIR ranges, and ii) within the Earth blackbody radiation spectrum (earth-BBRS), encompassing NIR - MIR - Far infrared (FIR).

1.2.2.1 Sun-BBRS

**Metallic LFNS**: Planar metallic LFNS exhibit spectrally selective characteristics, allowing for either narrowband or broadband light absorption. Commonly used in color filtering applications [13], narrowband planar LFNS excel in generating additive red-green-blue (RGB) colors in transmissive mode through a simple MIM cavity design. Alternatively, architectures with multiple MIM cavities arranged sequentially or in layers demonstrate high-efficiency RGB color generation in reflection mode [14, 15, 16]. These planar LFNS (transmissive or reflective) also exhibit dynamically tunable color production by adjusting the central layer’s (spacer’s) effective refractive index or thickness in MIM cavities. Phase change materials (PCMs), such as germanium-antimony-tellurium (GST) [17, 18], vanadium dioxide (VO$_2$) [19], antimony tri-sulfide (Sb$_2$S$_3$) [20], or antimony (Sb) [21], serve as spacers for obtaining thermally tunable colors through effective refractive index modulation. Furthermore, for nanoscale thickness tun-
ing of the spacer, the use of humidity-sensitive polymers and hydrogels facilitates the fabrication of dynamic MIM color filters [22, 23, 24]. Beyond filtering applications, narrowband LFNS show promise in colorimetric sensing platforms, including bio-sensing and gas-sensing, where external stimuli induce shifts in the LFNS absorption wavelength [25, 26]. However, in sensing applications, a high surface area is desirable to maximize light interaction with the surrounding environment. Consequently, nanostructures like dewetted (resulting from the breakup of a thin film into separated structures or droplets) or oblique-angle-deposited plasmonic units (depositing plasmonic material onto a substrate at an angle other than the normal) offer heightened sensitivities [27, 28].

On the other hand, LFNS capable of broad absorption efficiently utilize a significant portion of the solar spectrum, making them highly desirable for applications like photoconversion, photodetection, and photoelectrochemical water splitting (PEC-WS). In metallic LFNS, photoconversion functionality relies on exciting and extracting energetic hot electrons [29]. However, the efficiency decreases for planar structures and large particle sizes, where absorption stems from non-resonant inter-band transitions rather than localized surface plasmon resonances (LSPRs) [30]. Despite efforts to identify alternative, high-performance, and cost-effective plasmonic elements like Al [31, 32, 33], conductive oxides [11, 34, 35], transition metal nitrides/carbides (e.g. titanium nitride (TiN)) [36, 37], and doped semiconductors [38, 39, 40], the efficiency of hot electron designs remains modest.
Similar efficiency challenges arise in hot electron-based photodetection and PEC-WS applications [41]. An alternative strategy involves employing metallic LFNS in application platforms where metals do not act as the photoactive layer, such as thermal photovoltaic (TPV). In TPV, a broadband LFNS absorbs photons, converting them into heat, and reradiates the heat using a selective emitter with a spectral emission peak overlapping the photovoltaic (PV) bandgap. Theoretically, a solar TPV, with an optimally designed absorber and emitter, can achieve efficiencies surpassing the Shockley-Queisser limit (a theoretical efficiency limit for converting sunlight into electricity using a single-junction semiconductor solar cell, indicating the maximum efficiency possible under ideal conditions.) [42]. A narrowband emitter can be achieved using a multilayer dielectric-based one-dimensional Photonic Crystal (1DPC) design, rendering the overall system a lithography-free architecture [43].

Non-metallic NFLS: Analogous to their metallic counterparts, non-metallic LFNS find application in the sun-BBRS, specifically in photoconversion processes, with semiconductors serving as primary building blocks [44]. In most semiconductors, the carrier diffusion length is considerably shorter than the light penetration depth, thereby limiting efficiency due to bulk carrier recombination. Nevertheless, sub-wavelength semiconductor-based LFNS offer optically thick, electrically thin platforms well-suited for various photoconversion applications, including photovoltaics (PV), photodetection, and photoelectrochemical water splitting (PEC-WS) [43]. Established planar metal - semiconductor (MS) and metal - dielectric - semiconductor (MDS) cavity designs have demonstrated
near-unity optical absorption in deep subwavelength semiconductor thicknesses for specific applications [45, 46, 47, 48, 49, 50, 51, 52]. In addition to the optical response, the electrical characteristics of these semiconductors play a crucial role in determining performance outcomes.

Ideally, achieving ultrathin dimensions for a crystalline semiconductor film is a challenging task. Crystalline thin films [52, 53], and the chemical vapor deposition (CVD) growth of 2D semiconductors offer the promise of high-quality thin films. In the context of PEC-WS, two specific criteria are required in engineered LFNS design: i) optimizing surface area and ii) ensuring the long-term structural integrity or stability of the photoelectrode [44]. While planar LFNS have been employed as components of photoanodes and photocathodes in PEC-WS [53, 54], nanostructured designs featuring an enhanced water-semiconductor interface can enhance activity. To achieve a high surface area and good crystallinity, template-assisted etching of the crystalline semiconductor host appears to be a promising approach [4].

1.2.2.2 Earth-BBRS

Metallic LFNS: In most metals, the excitation of LSPR and interband transitions occur within the UV-visible range. However, lossy metals in (MI)_N and metal-1DPC configurations can exhibit resonant light absorption in the NIR to MIR range [15, 55, 56, 57]. These planar absorbers have the potential to function as selective or broadband thermal emitters, offering applications in radiative cooling and thermal camouflage [58, 59, 60, 61]. The integration of these LFNS
with PCMs provides dynamically tunable IR emitters and absorbers [62, 63, 64]. Such a design could lead to passive radiative thermostats by adjusting visible and IR absorption or emission [65].

**Non-metallic LFNS:** Highly doped semiconductors, doped metal oxides, metal nitrides/carbides, and two-dimensional materials like graphene and black phosphorus (BP) serve as alternative plasmonic materials within the MIR and far-IR (FIR) spectral ranges [13]. Heavily doped semiconductors such as germanium (Ge), silicon (Si), and III-V compounds are compelling alternatives to metals in the field of IR plasmonics [12]. The plasma frequency of these materials can be chemically, optically, or electrically tuned across a broad spectrum. The development of semiconductor-based hyperbolic metamaterials, consisting of doped-undoped pairs, holds the potential for achieving narrowband directional IR emission [66, 67], and perhaps contribute to ultrafast and low-power all-optical switching [68].

Two-dimensional materials characterized by unique electrical and optical properties represent a class within IR plasmonics. Graphene, the most recognized member of this group, exhibits the ability to sustain guided plasmonic modes in the IR. The spectral position of these modes can be effectively manipulated by adjusting the chemical potential ($\mu$) [69, 70, 71]. LFNS-based graphene monolayers have been achieved, resulting in the excitation of Tamm plasmons (a type of surface plasmon polaritons that occur at the interface between metal and dielectric materials) in 1DPC structures [72, 73, 74]. The incorporation of a distributed Bragg reflector (DBR) within a cavity design has shown the capacity
to couple light efficiently into the graphene monolayer[109]. Employing a similar
design approach, LFNS can be achieved through a monolayer of BP [75]. Because
of their high carrier mobility, LFNS composed of these two-dimensional materi-
als, coupled with narrow bandgap semiconductors, exhibit promising applications
in the design of IR photodetectors [76, 77]. In contrast to graphene, the BP
monolayer exhibits pronounced in-plane anisotropy, offering a basis for designing
polarization-selective absorbers [78]. Opposed to common narrow bandgap semi-
conductors, BP possesses a tunable bandgap ranging from 2 eV (in monolayer) to
0.3 eV (in bulk). Recent investigations [79] indicate that a vertical electric field
can change the bandgap of BP, providing tunability (from 3.7 to 7.7 µm) in its
photoluminescence and, consequently, absorption peak spectral response.

1.3 Metal-Insulator-Metal Architecture Based Light Absorbers

The distinctive characteristics of metal-insulator-metal (MIM) structures
make them promising candidates for enhancing the efficiency of devices reliant
on light-matter interactions within the nanoscale regime. In the nanoscale, where
dimensions are on the order of a billionth of a meter, conventional materials
exhibit non-classical optical behavior due to phenomena like plasmon resonance
and the creation of surface plasmon polaritons [1, 9, 45, 52, 53].

In a typical MIM structure, two metallic layers such as gold (Au), sil-
ver (Ag), aluminum (Al), titanium (Ti), or chromium (Cr) sandwich an insula-
tor such as titanium dioxide (TiO$_2$), silicon dioxide (SiO$_2$), or aluminum oxide
(Al$_2$O$_3$), forming a nanoscale cavity also known as Fabry-Perot nanocavity (FPN)
This arrangement exploits the plasmonic properties of the metals and the optical characteristics of the insulator to achieve efficient light absorption. The metallic layers support surface plasmon resonances, which interact strongly with incident light of the right wavelength. The insulating layer plays a crucial role by mediating the interaction between the metal layers, which helps confine and enhance the electromagnetic fields within the cavity, leading to increased absorption. This resonant behavior can be tuned by adjusting the dimensions and materials of the MIM structure, allowing for customization for specific applications. The combination of metal and insulator layers enables MIM structures to capture and utilize light more effectively than their traditional counterparts such as single-layer thin-film-based absorbers or planar metallic structure-based absorbers. Advancement in the field of MIM light absorbers has led to additional exploration of metal-semiconductor-metal (MSM) structures as well [44, 45, 46, 47, 48].

Improvements are inevitable in the efficiency of nanoscale devices, such as spectrally selective absorption/transmission filters, optoelectronics devices, light emitting devices, and narrow-band photodetectors. These devices allow precise control over light-matter interactions not possible before. MIM structures, with their tailored resonant behavior and customizable features, offer a pathway for enhancing the performance of electro-optical devices, paving the way toward advancements in all nanoscale optical technologies.
1.4 Dissertation Outline

The dissertation is organized as follows:

- Chapter 1 provides the objectives and rationale of the dissertation, offering a broad perspective on LFNS and potential applications in Optics and Nanophotonics.

- Chapter 2 explores the scientific foundation of the dissertation, with special emphasis on the operational principles of the Fabry-Perot nanocavity as a lithography-free nanostructure.

- Chapter 3 provides concise insights into the latest advancements in Nanophotonics employing Fabry-Perot nanocavities. The chapter also presents comprehensive details about the modeling and simulation methods used in this research.

- Chapter 4 is concerned with the nanoscale modeling and experimental realization of dynamically tunable planar narrowband perfect absorbers for color filtering.

- Chapter 5 explores the modeling and experimental investigation into narrowband color reflectors.

- Chapter 6 explains the modeling aspects of visible and near-infrared broadband absorbers.
• Chapter 7 provides sensitivity analysis, focusing on the impact of optical parameters and physical dimensions on the performance metrics of narrow-band perfect absorbers.

• Chapter 8 concludes this dissertation, summarizing the work and outlining potential paths for future research.
Chapter 2. Scientific Foundation

2.1 Preface

The operational principles of the Fabry-Perot interferometer are discussed, emphasizing design at the nanoscale. The chapter also provides a physical optics model of the Fabry-Perot nanocavity, explaining the interaction between light and matter within this nanoscale structure. The possibility of both static and dynamic tuning of these Fabry-Perot nanocavities is introduced.

2.2 The Fabry-Perot Interferometer

The Fabry-Perot interferometer is named after Charles Fabry and Alfred Perot who developed it in the late 19th century. It is a pivotal optical instrument for applications in spectral analysis and optical filtering [80]. It consists of two parallel, highly reflective mirrors separated by a certain distance, creating an optical cavity through which light is transmitted, reflected, and interfered with itself. The interference within the Fabry-Perot interferometer yields distinct spectral patterns that find applications throughout science and engineering [81, 82, 83, 84]. These include spectroscopy, where precise spectral control is essential, and optical filtering, where the interference selectively transmits or blocks specific wavelengths of light [81, 82]. The Fabry-Perot interferometer is also used
in telecommunications for wavelength filtering and detecting minute changes in optical signals [83, 84].

Figure 2.1: Schematic diagram of Fabry–Perot interferometer.

The Fabry-Perot design also represented an enhancement over preceding interferometric instruments by leveraging multiple reflections to amplify interference phenomena. In subsequent years, the Fabry-Perot interferometer has undergone a process of evolution, marked by significant progress in mirror coatings, manufacturing methods, and an expanding range of practical applications [85, 86, 87, 88].

The operation of the Fabry-Perot interferometer is based on the principle of multiple-beam interference. Light enters the interferometer and undergoes numerous successive reflections between the two highly reflective mirrors. These multiple reflected beams interact, either constructively or destructively, contingent upon the optical path difference (OPD) they accumulate. A critical resonance condition occurs when the OPD is an integer multiple of the incident light’s
wavelength (\(\lambda\)). Under these circumstances, constructive interference occurs, resulting in heightened transmission at specific wavelengths. This fundamental process is the basis of the Fabry-Perot interferometer’s functionality and its utility in optical applications.

Recent years have produced significant advancements in Fabry-Perot interferometry, leading to creative applications in a range of scientific and technological fields such as laser stabilization, enabling the precise control of laser frequencies [89, 90]. Obviously, the utility extends to precision spectroscopy, in the study of atomic and molecular transitions [91, 92]. In telecommunications, Fabry-Perot interferometers facilitate wavelength filtering and signal enhancement [93, 94]. In astronomy, they are used in analyzing stellar spectra and detecting exoplanets [95, 96]. Fabry-Perot interferometers can be highly sensitive sensors, effectively measuring physical parameters including pressure and strain [97, 98]. They play an important role in countless scientific and technical fields.

The integration of Fabry-Perot interferometry into the field of nanophotonics represents a significant breakthrough. Fabry-Perot nanocavities [99, 100, 101, 102, 103], typically on a nanoscale, have assumed a pivotal role in nanophotonics for several reasons. Firstly, their size allows the confinement and manipulation of light over subwavelength dimensions, which significantly modifies optical effects [2, 3]. This has led to enhanced light-matter interactions, finding applications in quantum optics, photonic crystals, and integrated photonics [2, 3, 45, 46, 47, 48, 49]. Fabry-Perot nanocavities are used in the confinement and manipulation of quantum emitters, including quantum dots and single-photon
sources. Applications are found in quantum information processing, and quantum cryptography [104, 105]. These nanocavities are also highly sensitive sensors, capable of detecting minute changes in refractive index, rendering them ideal for applications in biochemical sensing and environmental monitoring [106, 107]. The integration of Fabry-Perot interferometry and nanophotonics has led to the development of miniaturized, ultra-sensitive optical devices, pushing the boundaries of photonic technologies into areas requiring precise control of light-matter interactions. This progress is transforming fields like quantum optics, biosensing, and communication.

2.3 The Fabry-Perot Nanocavity

Fabry-Perot nanocavities are small optical resonators. These structures can be used to amplify light-matter interactions on the nanoscale. In the field of nanophotonics, they have become useful tools for manipulating light in tight spaces.

A Fabry-Perot nanocavity consists of two parallel, highly reflective metal layers with a dielectric layer in between. The nanocavity is characterized by its thickness (d), the refractive indices of the materials involved, and the incident wavelength (λ) of light. These nanocavities excel in confining light within much smaller dimensions than the light’s wavelength. They can also enhance the interaction between light and matter, making them useful in applications requiring strong light-matter coupling. They are used in single-photon sources, which are essential for quantum technologies, quantum key distribution, and quantum com-
puting. In photonic crystal devices, they provide manipulation of light at the nanoscale. In integrated photonics, Fabry-Perot nanocavities play a vital role in compact photonic circuits and devices used in optical communication and signal processing.

2.4 Working Principle of the Fabry-Perot Nanocavity

The Fabry-Perot nanocavity (FPN), akin to its macroscopic precursor, operates on the principle of multiple-beam interference within an optical cavity. The physical optics model for analyzing FPN’s optical response begins with light as an electromagnetic (EM) wave. Describing the interaction between this EM wave and the FPN involves reflection coefficients, interference and resonance, optical resonant modes and free spectral range, and quality factor and mode selectivity.

These topics collectively determine the physical optics model for any FPN. This model serves then as a framework for characterizing the optical behavior of the cavities, to include measured parameters such as reflectance, and transmittance, which determine the allowed modes (resonances).

Light interactions within the nanocavity are described using classical wave optics and Maxwell’s equations. Which aids in designing cavities for multiple applications in nanophotonics. When light is directed into the nanocavity, it undergoes reflection and transmission, depending on the properties of the constituent layers and the angle of incidence. A detailed explanation of the pertinent pa-
arameters required to describe the interaction between electromagnetic waves and Fabry-Perot nanocavities is provided below.

2.4.1 Reflection Coefficients

At each interface between the layers in an FPN (e.g., between the dielectric layer and the metal layer), reflection coefficients \( r_1 \) and \( r_2 \) describe how much of the incident light is reflected. These coefficients are derived from the Fresnel equations, which take into account the refractive indices of the materials involved. The reflection coefficients for light-polarized parallel (TM polarization or P-polarization) and perpendicular (TE polarization or S-polarization) to the plane of incidence is usually different. To gain a better understanding of the optics, the reflection and transmission of electromagnetic radiation at a thin dielectric layer between two semi-infinite media is considered.

Referring to Figure 2.2, assume that the incident plane is the x-z plane and apply Maxwell’s equations in free space to obtain

1) \( \nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \),
2) \( \nabla \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = 0 \),
3) \( \nabla \cdot \vec{D} = 0 \),
4) \( \nabla \cdot \vec{B} = 0 \),

where \( \vec{E} \) is the electric field, \( \vec{H} \) is the magnetic field, \( \vec{D} \) is the electric flux density or displacement (\( \vec{D} = \varepsilon_0 \vec{E} \)), and \( \vec{B} \) is the magnetic flux density (\( \vec{B} = \mu_0 \vec{H} \)). Taking the curl of \( \vec{E} \) and \( \vec{B} \) gives
Figure 2.2: A thin homogenous layer of dielectric or semiconductor material with a refractive index of $n_2$ sandwiched between two semi-infinite media with refractive indices of $n_1$ and $n_3$. Here the directions of the Electric (E) and Magnetic fields (H) are shown for TE and TM polarization.

\[
\nabla \times \vec{E} = \begin{vmatrix}
i & j & k \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
0 & \vec{E}(z,t) & 0 \\
\end{vmatrix} = -\frac{\partial \vec{E}(x,t)}{\partial z} \hat{i} \Rightarrow \frac{\partial \vec{E}}{\partial z} = \frac{\partial \vec{B}}{\partial t},
\]

\[
\nabla \times \vec{B} = \begin{vmatrix}
i & j & k \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
\vec{B}(z,t) & 0 & \vec{B}(z,t) \\
\end{vmatrix} = \frac{\partial \vec{B}(x,t)}{\partial z} \hat{j} \Rightarrow \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t} = \frac{\partial \vec{B}}{\partial z},
\]
\[ \frac{\partial^2 \vec{E}}{\partial z^2} = \frac{\partial}{\partial z} \left( \frac{\partial \vec{B}}{\partial t} \right) = \frac{\partial}{\partial t} \left( \frac{\partial \vec{B}}{\partial z} \right) = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2}, \]

results in
\[ \frac{\partial^2 \vec{E}}{\partial z^2} - \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0, \]

which is the wave equation for the free-space electric field. Similarly, the wave equation for the corresponding magnetic field is
\[ \frac{\partial^2 \vec{H}}{\partial z^2} - \epsilon_0 \mu_0 \frac{\partial^2 \vec{H}}{\partial t^2} = 0. \]

The standard solution of the electromagnetic wave equation is then:
\[
\begin{cases}
\vec{E}(z, t) = \vec{E}(z) e^{j\omega t} \\
\vec{H}(z, t) = \vec{H}(z) e^{j\omega t}
\end{cases}
\]

Referring to Figure 2.2, the electric field vector \( \vec{E}(z) \) can be written as
\[
E(z) = \begin{cases}
A e^{-jk_{1z}z} + B e^{jk_{1z}z} & z < 0 \\
C e^{-jk_{2z}z} + D e^{jk_{2z}z} & 0 < z < d \\
F e^{jk_{3z}(z-d)} & z > d,
\end{cases}
\]

where
\[ k_{iz} = \frac{2\pi n_i \cos \theta_i}{\lambda} \quad (i = 1, 2, 3). \]

The terms \( k_{1z}, k_{2z}, \) and \( k_{3z} \) are the \( z \) components of the wavevectors, and \( \theta_i \) is the angle of the light ray in medium \( i \) measured from the \( z \)-axis. \( A \) is the (purely real in this case) amplitude of the incident light, \( B \) is the (complex) amplitude of the reflected light, and \( F \) is the (complex) amplitude of the transmitted wave. The optical reflectance is \( R = |r|^2 \), where \( r \) (the reflection coefficient) is the ratio of the amplitude of the reflected light to the amplitude of the incident light, \( r = \frac{B}{A} \) [108].
For lossy media, such as semiconductors, wavevectors are complex $(k_{iz} = k'_{iz} - jk''_{iz})$. Thus,

$$
E(z) = \begin{cases} 
A e^{-j(k'_{iz} - jk''_{iz})z} + B e^{j(k'_{iz} - jk''_{iz})z} & z < 0 \\
C e^{-j(k'_{iz} - jk''_{iz})z} + D e^{j(k'_{iz} - jk''_{iz})z} & 0 < z < d \\
F e^{j(k'_{iz} - jk''_{iz})(z-d)} & z > d,
\end{cases}
$$

$$
E(z) = \begin{cases} 
A e^{-(k''_{iz})z} A e^{-j(k'_{iz})z} + B e^{(k'_iz)z} B e^{j(k'_iz)z} & z < 0 \\
C e^{-(k''_{iz})z} C e^{-j(k'_{iz})z} + D e^{(k'_iz)z} D e^{j(k'_iz)z} & 0 < z < d \\
F e^{(k''_{iz})(z-d)} F e^{j(k'_iz)(z-d)} & z > d.
\end{cases}
$$

The imaginary part of the wavevector, $k''_{iz}$, in a lossy medium, is proportional to the imaginary part of the refractive index, extinction coefficient ($\kappa$), of that medium. The coefficient $\kappa$ is also related to the absorption coefficient, $a$, as in Beer’s law

$$
I = I_0 e^{-ad},
$$

$$
a = \frac{4\pi\kappa}{\lambda},
$$

where $d$ is the thickness of the absorbing medium, $I_0$ is the intensity of the incident light and $I$ is the intensity of the light emerging from the medium. Thus, materials with high imaginary refractive indices are lossier and absorb more light. It is through the imaginary part of the index of refraction, $\kappa$ (and thus $k''_{iz}$ as well) that losses are incorporated into the models and simulations presented later.

The magnetic field vector $\vec{H}(z)$ can be expressed as

$$
\vec{H}(z, t) = \vec{H}(z)e^{j\omega t} \Rightarrow \frac{\partial \vec{H}}{\partial t} = j\omega \vec{H}(z)e^{j\omega t} \Rightarrow \frac{\partial^2 \vec{H}}{\partial t^2} = j\omega \vec{H}(z, t),
$$
\[ \nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \Rightarrow \mu_0 \frac{\partial \vec{H}}{\partial t} = -\nabla \times \vec{E} \Rightarrow \mu_0 j \omega \vec{H} = -\nabla \times \vec{E} \]
\[ \Rightarrow \vec{H}(z) = \frac{j}{\omega \mu_0} \nabla \times \vec{E} \Rightarrow \vec{H}(z) = \frac{j}{\omega \mu_0} \frac{\partial \vec{E}}{\partial z}, \]

The boundary conditions require the tangential components of the electric fields and the normal component of the magnetic fields, \( \vec{E}_y, \vec{E}_x, \vec{H}_y, \) and \( \vec{H}_x \) to be continuous at the interfaces \( z = 0 \) and \( z = d \). Using these conditions, it is possible to obtain \( B, C, D \), and \( F \) in terms of \( A \). Then, the reflection coefficient of the layered structure is given by \( r = B/A \) and the transmission coefficient is \( t = F/A \).

For the case of TE polarization in particular, boundary conditions require that \( \vec{E}_y \) and \( \vec{H}_x \) be continuous at the interfaces \( z = 0 \) and \( z = d \), which means \( \vec{E}_{1y} = \vec{E}_{2y} = \vec{E}_{3y} \) and \( \vec{H}_{1x} = \vec{H}_{2x} = \vec{H}_{3x} \). This leads to

\[
\begin{align*}
A + B &= C + D \\
k_{1z}(A - B) &= k_{2z}(C - D) \\
Ce^{-jk_{2z}d} + De^{jk_{2z}d} &= F \\
k_{2z}(Ce^{-jk_{2z}d} + De^{jk_{2z}d}) &= k_{3z}F.
\end{align*}
\]

These equations can be used to solve for \( B, C, D, \) and \( F \) in terms of \( A \) (which is presumably known). After a few steps involving algebraic manipulation...
only, the result is

\[
B = A \frac{(k_{1z} - k_{2z})(k_{2z} + k_{3z}) + (k_{1z} + k_{2z})(k_{2z} - k_{3z})e^{-2jk_{2z}d}}{(k_{1z} + k_{2z})(k_{2z} + k_{3z}) + (k_{1z} - k_{2z})(k_{2z} - k_{3z})e^{-2jk_{2z}d}}
\] (2.1)

so that

\[
r = \frac{B}{A} = \frac{r_{12} + r_{23}e^{-2j\phi}}{1 + r_{12}r_{23}e^{-2j\phi}}. \tag{2.2}
\]

In this equation, \(r_{12}\) and \(r_{23}\) are the Fresnel reflection coefficients of the optical wave from medium 1 to medium 2 and from medium 2 to medium 3, respectively. \(\phi = k_{2z}d\) is the phase delay of the optical wave in the film of thickness \(d\). For TE polarization incidence, \(r_{12}\) and \(r_{23}\) are

\[
r_{12} = \frac{k_{1z} - k_{2z}}{k_{1z} + k_{2z}}, \quad r_{23} = \frac{k_{2z} - k_{3z}}{k_{2z} + k_{3z}}. \tag{2.3}
\]

For TM polarization incidence, \(r_{12}\) and \(r_{23}\) are

\[
r_{12} = \frac{n_2^2k_{1z} - n_1^2k_{2z}}{n_2^2k_{1z} + n_1^2k_{2z}}, \quad r_{23} = \frac{n_3^2k_{2z} - n_2^2k_{3z}}{n_3^2k_{2z} + n_2^2k_{3z}}. \tag{2.4}
\]

In the previous two equations, \(k_{1z}\), \(k_{2z}\), and \(k_{3z}\) are the normal components of the wave vectors inside medium-1, medium-2, and medium-3, respectively. They are calculated as

\[
k_{iz} = \frac{2\pi n_i \cos \theta_i}{\lambda}, \tag{2.5}
\]

where \(\theta_i\) is the angle of incidence in medium \(i\), and \(n_i\) is the index of refraction of the medium \(i\) \((i = 1, 2, 3)\). Using boundary conditions for the tangential
components of the wave vectors (i.e., $k_{1x} = k_{2x} = k_{3x}$), $k_{iz}$ can also be found in terms of the incident angle $\theta_i$ as

$$k_{iz} = 2\pi n_i \cos \theta_i / \lambda = \sqrt{k_i^2 - k_{ix}^2}, \quad (2.6)$$

$$\sqrt{k_i^2 - k_{ix}^2} = \sqrt{(2\pi n_i / \lambda)^2 - (2\pi n_1 \sin \theta_1 / \lambda)^2}. \quad (2.7)$$

For unpolarized light, the effective optical reflectance is the average optical reflectance for TE and TM polarizations.

### 2.4.2 Interference and Resonance Condition

At the heart of the Fabry-Perot nanocavity lies the principle of interference. When a monochromatic plane wave of wavelength ($\lambda$) is incident on the nanocavity at an angle $\theta$ with respect to the normal to the metal layer, it undergoes multiple reflections between the metal layers. Interference in these cavities relies on the superposition of light waves reflected within the cavity. The path difference between successive beams, critical in interference, is given by $2nd \cos \theta$, where $n$ is the real part of the refractive index, and $d$ is the thickness.

Two cases apply to define the path difference.

**Constructive Interference and Resonance Condition:** Constructive interference, leading to resonance in the cavity, occurs when the path difference is an integer multiple of the wavelength. The condition for this is expressed as

$$2nd \cos \theta = m\lambda, \quad (2.8)$$
where \( n \) represents the real part of the refractive index for the dielectric spacer, \( d \) is the cavity thickness or length, \( m \) is an integer representing the order of interference, \( \theta \) is the incident angle, and \( \lambda \) is the wavelength of the incident light [108].

**Destructive Interference:** The condition for destructive interference, where the reflected light waves cancel each other out, is

\[
2nd\cos\theta = (m+1/2)\lambda. \tag{2.9}
\]

In both equations, the refractive index \( (n) \) plays a crucial role in determining the phase shift that occurs as light travels through the dielectric medium. The real part of the refractive index alters the effective optical path length, while the imaginary part \( (\kappa) \), if present, indicates absorption within the medium, affecting the intensity of the transmitted and reflected light.

### 2.4.3 Optical Resonant Modes and Free Spectral Range

The resonant modes of the Fabry-Perot nanocavity correspond to the allowed discrete wavelengths for which constructive interference occurs. The free spectral range (FSR) characterizes the spacing between successive resonant frequencies and is defined as

\[
\text{FSR} = \frac{c}{2nd\cos\theta}, \tag{2.10}
\]

27
where $c$ is the speed of light in vacuum. The FSR determines the mode spacing and is a crucial parameter in the characterization of the nanocavity’s optical behavior [108].

2.4.4 Quality Factor and Mode Selectivity

The quality factor ($Q$) of the Fabry-Perot nanocavity is a vital and unitless metric describing the sharpness of its resonances. It is defined as the ratio of the energy stored within the cavity to the energy lost per cycle. A higher $Q$ value indicates a narrower resonance and better mode selectivity. The $Q$ factor is related to the wavelength by the full-width at half-maximum (FWHM) of the resonance peak through the equation:

$$ Q = \frac{\lambda_m}{\text{FWHM}}. $$ \hfill (2.11)

2.5 Classification of Fabry-Perot Nanocavities

In the exploration of Fabry-Perot nanocavities, two prominent architectures emerge, symmetric and asymmetric. These classifications determine the optical characteristics of nanocavities, like resonance behavior, spectral response, and tunability. The following discussion describes the distinctive features and implications associated with each category.
2.5.1 Symmetric Fabry-Perot Nanocavities

Symmetric Fabry-Perot nanocavities are characterized by identical metal layer properties, resulting in equal reflectivities for both metals. Thin metal layers will usually allow some degree of light transmission in addition to reflection. The thin metal configuration is common in optical applications where control is required on both transmission and reflection of light. In such a thin metal layer structure, the resonance condition remains as in any Fabry-Perot cavity

\[ 2nd\cos\theta = m\lambda. \]  

(2.12)

This condition ensures that light of certain wavelengths constructively interferes inside the cavity, resonating at specific modes determined by the integer m.

In an FPN where the second metal is optically thick, the nanocavity becomes highly reflective and allows negligible to no transmission. This configuration shifts the focus of the cavity’s operation to reflection mode rather than transmission. In such a case, the cavity consists of one partially transmissive metal layer and one optically thick metal layer. Light entering through the first metal layer undergoes multiple reflections inside the cavity. The thick second metal ensures that almost all light is reflected into the cavity or out through the first metal layer. The resonance condition in terms of optical path length remains the same. However, resonance is mainly seen in the reflection spectrum.
2.5.2 Asymmetric Fabry-Perot Nanocavities

An asymmetric Fabry-Perot nanocavity is an optical structure characterized by two parallel metal layers that differ in their optical properties. The cavity also contains a dielectric medium situated between the metals. The resonance condition in an asymmetric Fabry-Perot cavity is determined by the optical path length and the phase shifts at each metal layer

\[ 2n d \cos \theta + \phi_1 + \phi_2 = m \lambda. \] (2.13)

Here, \( n \) and \( d \) represent the real part of the effective refractive index and thickness of the dielectric spacer, respectively. The terms \( \phi_1 \) and \( \phi_2 \) represent phase shifts upon reflection from the first and second metal layers, respectively.

When the second metal layer of an asymmetric Fabry-Perot nanocavity is made optically thick, this changes the behavior of the cavity, especially in reflection mode. The optically thick metal layer acts as a highly reflective barrier, preventing light from being transmitted through it, while the other metal layer being partially reflective, allows light to enter the cavity. The resonance condition still depends on the optical path length and the phase shifts at the metal layers. However, resonance is primarily seen in the reflection spectrum.

2.6 Tunable Fabry-Perot Nanocavity

Fabry-Perot nanocavities of metal and dielectric layers can be designed to exhibit wavelength selectivity, applicable to sensing, communications, and quan-
tum optics. This tunability allows tailoring the optical properties for specific requirements in both static and dynamic configurations.

2.6.1 Static Tunable Fabry-Perot Nanocavities

Static tunability refers to changing the optical properties of a Fabry-Perot nanocavity in a controlled manner. This tunability often relies on engineering the geometrical parameters and the dielectric materials. For example, by altering the thickness or refractive index of the layers within the cavity, the resonant wavelengths and the spectral response can be adjusted to achieve the desired performance. The fundamental Fabry-Perot resonance condition, \( 2nd = m\lambda \), is at the core of this static tunability.

**Geometrical Parameters:** Modifying the thickness of the layers within the nanocavity allows control over the cavity’s resonance. By changing the layer thicknesses, it is possible to achieve a specific resonance wavelength. Applications include wavelength-selective filters [2, 109, 110].

**Material Properties:** By selecting the materials with specific refractive indices, absorption characteristics, and reflective properties, and by controlling the physical dimensions of the cavity, the resonant wavelengths and the quality of the resonances can be tailored to specific applications [111, 112].
2.6.2 Dynamic Tunable Fabry-Perot Nanocavities

Dynamic tunability takes the control of Fabry-Perot nanocavities to a new level, allowing for real-time, reversible adjustments. This type of tunability is particularly valuable in applications where rapid adaptability is required. Some of the methods for gaining dynamic tuning include:

**Thermo-optic Effect:** The refractive index of materials changes with temperature. By introducing localized heating, through microheaters, the resonance of the nanocavity can be shifted dynamically. This effect has applications in thermal sensing and reconfigurable photonic circuits [113, 114].

**Optomechanical Tuning:** With deformations induced by external forces, dynamic tuning can be achieved as well. The introduction of nanomechanical elements into the cavity structure allows for precise control over the resonance. Optomechanical cavities have been explored for applications in sensing and quantum information processing [115, 116, 117].

**Electro-optic Effect:** Using the electro-optic effect in specific materials known as Epsilon Near Zero (ENZ) materials, the refractive index can be modulated by applying an electric field. This enables dynamic control of the nanocavity’s resonance, leading to the development of electro-optic modulators and switches. ENZ are semiconductors whose real permittivity value slowly changes sign from positive to negative with wavelength. These materials, such as indium tin oxide (ITO) and n-type doped indium antimonide (n-InSb), are already widely used in the semiconductor industry. ITO, for example, is often used as a transparent con-
ductive layer in display applications. ENZ materials have also received considerable attention as potential electro-optical devices. Researchers have demonstrated narrow band [118, 119] and broad band [120] directional perfect light absorption in nanocavity devices made of ENZ materials.

In the context of ENZ materials, the focus is primarily on the dielectric permittivity ($\epsilon$) which is a complex-valued quantity, where the real part corresponds to the refractive index ($n$) and the imaginary part to the absorption. Mathematically, $\epsilon$ is defined as

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega), \quad (2.14)$$

where $\epsilon_1$ is the real part, $\epsilon_2$ is the imaginary part, and $\omega$ represents the angular frequency.

In typical dielectric materials, $\epsilon_1$ is positive, leading to positive refractive indices ($n > 0$). In contrast, ENZ materials have $\epsilon_1$ close to zero, causing $n$ to approach zero. When $\epsilon_1 \approx 0$, the wavelength of light in the material increases substantially, leading to extreme phase velocities. This unique behavior of ENZ materials at or near $\epsilon_1 \approx 0$ has far-reaching implications in photonics.

The following chapter covers the optical characteristics of ENZ materials, the models used to understand and control ENZ behavior, and how ENZ materials can adjust the spectral response of a Fabry-Perot nanocavity.
Chapter 3. Fabry-Perot Nanocavities: Modeling and Simulation

3.1 Fabry-Perot Nanocavity for Narrow and Broadband Applications

Nanophotonics is the study of light manipulation at the nanoscale, focusing on creating structures that can control light beyond the limits of traditional optics. This field utilizes plasmonic materials and metamaterials to design filters that modify light’s absorption, reflection, and transmission. These changes are due to optical resonances, which occur when light interacts with nanostructures, leading to the possibility of new optical devices.

Several studies have reported the modeling and experimental realization of optical resonance-based nanostructures for mid-infrared and near-infrared (NIR) wavelengths [2, 3, 4, 5, 7, 8, 13]. These resonance conditions such as surface plasmon resonance (SPR) or Fabry-Perot resonance (FPR) rely on the dimensions of the nanostructures utilized. Recent advancements in nanoscale fabrication techniques enable the realization of intricate nanostructures with dimensions suitable for applications in the infrared (IR) wavelength range. However, creating these devices for visible light is difficult. The precision needed for making such small structures is complex and expensive. Although plasmonic structures have a big potential for making high-performance optical filters, their use is limited by the
cost of making them, imperfections from the manufacturing process, and the natural loss of light that happens with plasmonic metals.

In response to these challenges at visible wavelength range, the use of thin-film optical coatings offers a simple way to control light. This method avoids complicated and expensive processes such as lithography for creating tiny patterns on surfaces. Optical coatings, which are layers of non-metal and metal films, are crucial for improving the performance of various optical devices, from simple items like eyeglasses to important parts in advanced imaging systems. The success of structures with multilayer thin-film coatings relies on the Fabry-Perot cavity principle. The thickness of the cavity layer is important as it determines how light inside the cavity will behave, leading to desired effects like reflection, absorption, or transmission. This is done by controlling how light interference takes place within the cavity for different wavelengths. Choosing materials that don’t absorb much light for these cavities is important because it allows more light to move through, making the device work better.

This approach not only makes the manufacturing process easier but also opens up new possibilities, including making narrow and broadband optical filters. By focusing on thin-film optical coatings, efficient and cost-effective optical devices can be realized, expanding the applications of nanophotonics to include applications such as very thin photodetectors and improved color filters.

Recent work by Mirshafieyan et al. showed the use of silicon films (30-60 nm) as a medium in an aluminum-silicon-aluminum Fabry-Perot nanocavity, to create ultra-thin perfect light absorbers using the FPR [121]. Depending on the
thickness of the silicon film from 30 nm to 60 nm, the structure absorbs more than 99% of the incident light at specific wavelengths in 500-800 nm wavelength range. This absorber structure does have a low sensitivity to the angle of incidence because it is made of silicon (a relatively lossy material compared to lossless oxides) as the cavity medium [122]. The other advantage of this structure is that it requires less cavity thickness than a cavity using lower loss films. A similar study by Li et al. demonstrated a narrowband light absorption in visible range by silicon-coated silver thin films [123].

Yang et al. experimentally demonstrated a full-color printing concept based on the interference effect in metal-dielectric-metal Fabry-Perot (FP) cavities. The study employed hydrogen silsesquioxane (HSQ), an organic material with optical parameters similar to silicon dioxide as the cavity medium. The color for printing is determined by the thickness of the dielectric layer in each microscale FP cavity [124]. HSQ films with thickness in the range of 780 - 980 nm were used as the cavity layer between 100 nm and 10 nm thick aluminum and nickel thin films, respectively. The structure provided more than 95% absorption at specific wavelengths in the visible range, generating a vivid full-color image.

In contrast to color filters based on the principle of narrow-band perfect light absorption, the development of lithography-free Fabry-Perot cavities by G Hobadi et al. focuses on narrow-band color reflection [122]. A multilayer-based color filter was realized using a proper series connection of two cavities that exhibit relatively high efficiency, high color purity, and a wide viewing angle. The structure follows a metal-insulator-metal-insulator-semiconductor design to ob-
tain red-green-blue (RGB) band-pass color generation at the reflection mode, a capability that cannot be attained with a conventional metal-insulator-metal FP resonator.

Shurvinton et al. demonstrated a four-layer metal-dielectric-metal-dielectric (MDMD) thin-film stack designed for color control [125]. This MDMD stack included a silicon dioxide film positioned between silver and titanium films, resembling an asymmetric Fabry-Perot (FP) cavity. The design operates as a narrow-band RGB color reflector, offering over 80% reflections in a narrow band and ensuring high color purity. A similar study was presented by Park et al. [126], in which asymmetric Fabry-Perot nanocavities incorporated a platinum film on rigid and flexible aluminum substrates through a lithography-free deposition process. The structure achieved up to 99% absorption at the resonance wavelengths and showed more than 80% reflection for the non-resonant bands.

While narrow-band near-perfect absorption or reflection is easily achieved with highly reflective metal layers and a dielectric spacer forming a Fabry-Perot cavity, broadband absorption can be challenging as it is difficult to find an optical phenomenon that can exist over a wide spectral range. Various approaches have been explored to develop broadband absorbers in visible, near-infrared (NIR), and mid-infrared (MIR) wavelength regions. These include plasmonic resonant structures [127], multi-shape nano units [128], and metal-insulator-metal (MIM) structures incorporating lossy metals like titanium (Ti), tungsten (W), and nickel (Ni) [129]. However, many of these designs only cover a limited portion of the visible or NIR spectrum. Furthermore, some designs heavily rely on electron beam
lithography (EBL), limiting their applicability to large-area devices. To address this limitation, several planar MIM configurations have been proposed that utilize multi-metal configuration to minimize the dependency on EBL [130, 131].

Dereshgi et al. developed an ultra-broadband perfect absorber designed for visible and near-infrared applications [132]. This absorber relies on multilayers of metal-insulator (MI) stacks created through layer deposition. The structure comprises an MIMI configuration, featuring an optically thick tungsten back reflector layer, followed by layers of 80 nm aluminum oxide, 10 nm titanium, and another 80 nm aluminum oxide. This arrangement achieves over 80% absorption across the wavelength range of 600-1400 nm.

Zhong et al. showed broadband absorption using a multiple-metal metamaterial perfect absorber [131]. The structure uses the phenomenon of field penetration and the field absorption for the photons at different wavelength ranges using different metallic layers. In an MIMIM configuration, the use of titanium, nickel, and aluminum with silicon dioxide as an insulator enables near-unity broadband absorption for visible and near-infrared wavelengths.

Such nanoscale narrowband absorbers, reflectors, and broadband absorbers find utility in various optical applications, including color filters [122, 15, 133, 134, 135], colorimetric sensing [136, 137], solar energy harvesting [50, 51, 138], and infrared sensing [55, 56]. However, these structures are typically constructed from materials with static effective refractive index values within a given wavelength range. This means that the optical response of such devices remains fixed for a specific set of structural dimensions. To achieve dynamic tunability in the re-
sponse and gain control over the operating wavelength range, it becomes essential to employ dynamically tunable optical materials.

Semiconductors like indium tin oxide (ITO), indium antimonide (InSb), and indium arsenide (InAs) are categorized as epsilon-near-zero (ENZ) semiconductors. The real part of the dielectric permittivity of these materials becomes negative at a specific wavelength referred to as the ENZ wavelength. Below this wavelength, these materials act as dielectrics, while above it, they exhibit metallic behavior. The ENZ wavelength in such materials is contingent upon the concentration of free electrons within them. Thus, manipulating the number of free electrons offers the means to control the ENZ wavelength dynamically. This, in turn, facilitates dynamic regulation of the transition from dielectric to metallic behavior. Such ability of ENZ materials can be used to develop dynamically tunable nanoscale optical devices.

Feigenbaum et al. demonstrated a unity-order refractive index change in indium tin oxide in visible wavelength region, leading to a tunable Fabry-Perot nanocavity [118]. The research utilized gold - silicon dioxide - indium tin oxide - gold metal-oxide-semiconductor heterostructure with indium tin oxide as an active ENZ layer. Under externally applied field, electron concentrations at the silicon dioxide - indium tin oxide interface increased from $1 \times 10^{21}/\text{cm}^3$ to $2.8 \times 10^{22}/\text{cm}^3$, resulting in a local refractive index change of 1.39 at 800 nm. The structure was utilized as a plasmonic waveguide with dynamic control over plasmonic mode.

Mirshafieyan et al. utilized n-doped indium antimonide to model an electrically tunable Fabry-Perot nanocavity for dynamic color filter and modulation
applications [139]. The nanocavity structure used silver - titanium dioxide - n-doped indium antimony - silver as a metal-oxide-semiconductor-metal nanocavity. Simulations indicated that applying an external voltage to the metal surfaces led to an accumulation of electrons at the oxide - semiconductor interface, resulting in a predicted spectral shift of 40 nm in the resonance wavelength of the nanocavity within the visible range.

Deriving inspiration from the mentioned static and dynamically tunable Fabry-Perot nanocavity structures designed for narrow and broadband applications, this dissertation introduces the modeling, simulations, and realization of the following:

Dynamically tunable Fabry-Perot nanocavities employing epsilon-near-zero (ENZ) semiconductors, specifically n-doped indium antimony and n-doped indium arsenide.

A silicon-enhanced, static tunable narrowband color reflector and a near-infrared (NIR) broadband absorber.

An ultra-broadband absorber spanning the visible to near-infrared (NIR) range, accomplished through the use of an oxide-coated asymmetric Fabry-Perot nanocavity.

Optical tolerance analysis of Fabry-Perot nanocavity using Monte Carlo simulation to assess the impact of design parameters on performance metrics.
3.2 Modeling and Simulation Methods

The modeling of Fabry-Perot nanocavities for both broad and narrowband applications begins with the selection of appropriate materials, including metals, oxides, and semiconductors, to achieve the desired optical properties such as absorption, reflection, and transmission in the wavelength range of interest.

From an extensive review of relevant literature (Chapter 1), noble metals like gold, silver, and aluminum are chosen for their suitability in operating within the visible and near-infrared (NIR) spectral regions. These metals exhibit high absorption coefficients in these wavelength ranges, making them effective as highly reflective metal layers. They are particularly well-suited as optically thick bottom layers, which facilitate the operation of Fabry-Perot nanocavities in reflection mode by blocking transmission. Using the same metal for both the top and bottom layers in a metal-insulator-metal structure results in a narrowband absorber, which is advantageous for absorbing additive colors like red, green, and blue while reflecting subtractive colors such as cyan, magenta, and yellow.

Conversely, to create narrowband color reflectors and broadband absorbers, it is necessary to employ asymmetric Fabry-Perot cavities. These cavities use metals with moderate to low extinction coefficients (κ) as the top metal layer, combined with high κ metals as the bottom (reflector) layer, which enables additive color reflection or broadband absorption in the visible or NIR range. Notably, lossy metals like titanium, nickel, tungsten, and chromium are commonly used as materials with moderate κ values, as identified in the literature review.
The optical performance in terms of reflection or absorption within a specific wavelength range not only depends on the choice of metal layers but also on the type and thickness of the insulator layer utilized. To enhance absorption by the metal layers and allow for multiple reflections between them, lossless oxides such as silicon dioxide, titanium dioxide, or aluminum oxides are valuable. These materials possess low extinction coefficients, meaning they do not significantly absorb light while it travels through the cavity, allowing for multiple reflections between the metal layers and resulting in optical interference within the Fabry-Perot nanocavity.

However, these lossless oxides, while ideal for the cavity medium, have a drawback of high sensitivity to incident angles, especially at angles greater than 60°. Such angles may lead to undesired reflectance or absorptance by the cavity. To overcome this limitation, it is advantageous to incorporate semiconductors with higher refractive indices and extinction coefficients compared to lossless oxides. In addition to reducing angle sensitivity, semiconductor materials offer the capability for dynamic tunability within the Fabry-Perot nanocavities. This is achieved through the metal-oxide-semiconductor-metal architecture, which not only functions as a Fabry-Perot nanocavity but also acts as a metal-oxide-semiconductor capacitor structure. This configuration is renowned for its ability to control the concentration of charge within the semiconductor material. Consequently, semiconductors inherently suitable for operation in the visible or NIR wavelength range or those that can be tuned for such operation prove to be
valuable choices as cavity mediums. Semiconductors like silicon, n-doped indium antimonide, and n-doped indium arsenide are employed in this research.

3.3 Transfer Matrix Method

Once a suitable combination of materials for operating a Fabry-Perot (FP) nanocavity in the desired wavelength range is determined, the transfer matrix method (TMM) becomes a valuable tool for calculating the appropriate layer thicknesses for the cavity medium. Typically, for the FP cavity to function in reflection mode, it requires an optically thick bottom metal layer. In the literature, a thickness of 100 nm for the bottom metal layer is widely considered ideal to achieve zero transmittance through the nanocavity. Regarding the top metal layer, two primary considerations govern its thickness: first, it should be thick enough to enable sufficient field penetration, and second, it should have a minimum thickness to prevent the formation of metal islands during experimental deposition onto the nanocavity. A minimum thickness of 10 nm is necessary to prevent the formation of metal islands during experimental deposition. Additionally, for all the noble and lossy metals considered in this research, their optical penetration depth exceeds 10 nm, ensuring sufficient field penetration for FP resonance to occur.

With initial values of 10 nm for the top layer and 100 nm for the bottom layer, the transfer matrix method (TMM) can be applied to determine the appropriate cavity layer thickness for either narrow or broadband applications. This calculation relies on the refractive index and extinction coefficients of the chosen
cavity material within the desired wavelength range. The TMM uses discrete propagation and transmission matrices to calculate a final transfer matrix \((M)\), and the reflectance at a specific wavelength is determined by two of the transfer matrix elements. The propagation \((P_m)\) and transmission \((D_m)\) matrices are components of the TMM and can be written as:

\[
P_m = \begin{bmatrix}
  \exp(i\phi_m) & 0 \\
  0 & \exp(-i\phi_m)
\end{bmatrix}, \quad \text{where } \phi_m = \frac{2\pi(n_m - ik_m)d_m}{\lambda \cos \theta_t}.
\] (3.1)

For P polarization,

\[
D_m = \begin{bmatrix}
  1 & 1 \\
  (n_m - ik_m) \cos \theta_m & -(n_m - ik_m) \cos \theta_m
\end{bmatrix},
\] (3.2)

and for S polarization,

\[
D_m = \begin{bmatrix}
  \cos \theta_m & \cos \theta_m \\
  (n_m - ik_m) & -(n_m - ik_m)
\end{bmatrix}.
\] (3.3)
Here, $m = 0, 1, 2, 3$ represents air, the top metal layer, the insulator layer, and the bottom metal layer. $n_m$ and $\kappa_m$ are the real and imaginary parts of the effective refractive index ($n_{\text{eff}}$), respectively, $\theta_m$ is the incident angle of light, $d_m$ is the layer thickness, and $\phi_m$ is the phase delay of the optical wave in layer $m$.

The term $\theta_t$ represents the transmitted wave angle; however, in this study, the incident angle for the optical study of all four structures is set to zero. Thus, the $\theta_t$ becomes zero, reducing the denominator of the $\phi_m$ eq. to just $\lambda$. For the given four-layer systems, the $M$ is written as:

$$ M = D_1^{-1}(D_2P_2D_2^{-1})(D_3P_3D_3^{-1})(D_4P_4D_4^{-1})D_5. \quad (3.4) $$

Later, the reflection coefficient $(r)$ and reflectance $(R)$ are calculated using the $M_{21}$ and $M_{11}$ elements of $M$:

$$ R = |r|^2 = \left| \frac{M_{21}}{M_{11}} \right|^2. \quad (3.5) $$

Figure 3.1 displays the reflectance contour derived from TMM calculations for an asymmetric FP nanocavity composed of Ti-SiO$_2$-Ag, varying the thickness of SiO$_2$. It is evident that alterations in SiO$_2$ thickness lead to shifts in the perfect absorption wavelength. In this context, “$m$” denotes the mode of resonance. Notably, when SiO$_2$ thickness exceeds certain values, multiple resonance modes become evident within the visible range.

Similar calculations can be performed for any MIM nanocavity combinations to obtain ideal cavity thickness for perfect absorption at desired wavelength.
Figure 3.1: Contour plot of the visible reflectance spectra of Ti-SiO$_2$-Ag as a function of SiO$_2$ thickness, when the Ti thickness is set to 10 nm.
Thus, the TMM works as an efficient and straightforward tool to model an MIM cavity to target narrow or broadband applications for desired wavelength range.

3.4 FDTD Technique for Optical Response Analysis of Fabry-Perot Nanocavities

The Finite Difference Time Domain (FDTD) method stands as a formidable computational technique in photonics modeling, offering a robust framework for the analysis of electromagnetic wave propagation and interaction with structures. Developed as a numerical solution to Maxwell’s equations, the FDTD method has become a valuable tool for investigating optical responses. The goal, again, is a detailed model of Fabry-Perot nanocavities and their spectral characteristics [140].

3.4.1 Maxwell’s Equations and FDTD Foundation

At its core, FDTD hinges on the discretization of Maxwell’s equations, which govern the behavior of electromagnetic fields. The fundamental equations, in their differential form, can be expressed as follows:

- Gauss’s Law for Electricity:
  \[ \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}. \]

- Gauss’s Law for Magnetism:
  \[ \nabla \cdot \mathbf{B} = 0. \]
• Faraday’s Law of Electromagnetic Induction:
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \]

• Ampère’s Law with Maxwell’s Addition:
\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}. \]

Here, \( \mathbf{E} \) and \( \mathbf{B} \) represent the electric and magnetic field vectors, \( \mathbf{D} \) is the electric displacement field vector, \( \mathbf{H} \) is the magnetic field vector, \( \rho \) is the charge density, \( \mathbf{J} \) is the current density, \( \epsilon_0 \) is the vacuum permittivity, and \( t \) denotes time. Here, \( \mathbf{D} \) is related to \( \mathbf{E} \) and the material properties through \( \mathbf{D} = \epsilon \mathbf{E} \), where \( \epsilon \) is the permittivity of the material.

3.4.2 FDTD Algorithm and Temporal Evolution

The FDTD algorithm represents a numerical method utilized to address Maxwell’s equations concerning the analysis of electromagnetic field dynamics within nanophotonic structures. This discussion explores the details of the FDTD algorithm, concentrating on its discrete formulation and its ability to capture the temporal progression of electromagnetic fields within a Fabry-Perot nanocavity.

3.4.2.1 Discretization of Maxwell’s Equations

Maxwell’s equations describe how electric and magnetic fields interact in space and time. The FDTD algorithm discretizes these equations to operate on a grid in both space and time [140, 141]. Consider the one-dimensional form of Maxwell’s equations:
1. Faraday’s law:

\[ \frac{\partial E_y}{\partial t} = -\frac{\partial B_z}{\partial x}. \]  

(3.6)

2. Ampere’s Law:

\[ \frac{\partial H_z}{\partial t} = -\frac{\partial E_y}{\partial x}. \]  

(3.7)

These equations describe the evolution of the electric field \((E_y)\) and magnetic field \((H_z)\) in the \(y\) and \(z\) directions, respectively.

### 3.4.2.2 Temporal Evolution:

The FDTD algorithm advances the fields through time in discrete steps \((\Delta t)\). The temporal evolution is captured using the finite difference approximation [141]:

1. Updating Electric Field:

\[ E_{y}^{n+1}(x) = E_{y}^{n}(x) - \frac{\Delta t}{\epsilon} \frac{\partial H_{z}^{n}}{\partial x}. \]  

(3.8)

2. Updating Magnetic Field:

\[ H_{z}^{n+1}(x) = H_{z}^{n}(x) + \frac{\Delta t}{\mu} \frac{\partial E_{y}^{n+1}}{\partial x}. \]  

(3.9)

Here, \(n\) represents the discrete time step.
3.4.2.3 Courant-Friedrichs-Lewy (CFL) Stability Condition:

The stability condition in FDTD is determined by the allowed time step ($\Delta t$). An electromagnetic wave propagating in free space cannot go faster than the speed of light. To propagate a distance of one cell requires a minimum time of $\Delta t = \Delta x/c$, where $\Delta x$ is cell size and $c$ is the speed of light in free-space. In two dimensional simulation, the propagation can be considered in orthogonal direction, which brings the time requirement to $\Delta t = \Delta x/(\sqrt{2}c)$. Similarly, in three dimensional simulation $\Delta t = \Delta x/(\sqrt{3}c)$. This is summarized by the Courant–Friedrichs-Lewy (CFL) Stability Condition, popular as “Cournat condition” [141, 142]:

$$\Delta t \leq \frac{\Delta x}{\sqrt{nc}},$$

(3.10)

where $n$ is the dimension of the simulation. Most FDTD simulation software follows the following relation between $\Delta x$ and $\Delta t$,

$$\Delta t = \frac{\Delta x}{2c}.$$  

(3.11)

This is not the best approximation, however for simplicity it is adopted by popular FDTD simulation softwares [143].

3.4.2.4 Incorporating Material Properties:

Incorporating material properties into the FDTD simulation is vital for accurately modeling electromagnetic interactions with various materials within
nanophotonic structures. One fundamental aspect of this incorporation lies in understanding how the electromagnetic fields interact with materials through Maxwell’s equations.

Maxwell’s equations govern the behavior of electromagnetic fields, and within the FDTD framework, equations are discretized in both time and space. Ampere’s Law with Maxwell’s correction and Faraday’s Law as mentioned above are the key equations to incorporate material properties in the FDTD calculations. In the Ampere’s law with Maxwell’s corrections, in the presence of material, the electric displacement field \( \mathbf{D} \) is related to the electric field \( \mathbf{E} \) through \( \mathbf{D} = \varepsilon \mathbf{E} \), where \( \varepsilon \) represents the permittivity of the material. While, for the Faraday’s law, in the presence of materials, the magnetic flux \( \mathbf{B} \) is related to the magnetic field \( \mathbf{H} \) through \( \mathbf{B} = \mu \mathbf{H} \), where \( \mu \) represents the permeability of the material.

Incorporating material properties into FDTD simulations necessitates the discretization and incorporation of these equations into the simulation framework. By specifying the permittivity \( \varepsilon \) and permeability \( \mu \) values that are specific to the materials for each grid cell, precise modeling of electromagnetic wave interactions with different materials becomes achievable. This capability allows for the simulation of nanophotonic structures while considering the actual properties of real-world materials.

3.4.2.5 Perfectly Matched Layers (PML):

To mitigate unwanted reflections at the simulation boundaries, Perfectly Matched Layers (PML) are incorporated. PML acts as an absorbing layer, ef-
fectively damping outgoing waves, and preventing them from reflecting back into the simulation domain. This ensures an accurate representation of the system’s behavior by minimizing artificial boundary effects.

3.4.2.6 Mesh Settings

The success of Finite-Difference Time-Domain (FDTD) simulations hinges on the appropriate meshing of the simulation domain. The spatial grid \((\Delta x, \Delta y, \Delta z)\) and temporal steps \((\Delta t)\) must be carefully chosen to ensure numerical stability and accuracy. The spatial resolution of the mesh is crucial for capturing the fine details of the nanocavity structure.

Exploring Fabry-Perot nanocavities requires meticulous attention to mesh settings. A refined spatial resolution is critical, necessitating precise meshing strategies around the nanocavity structure, especially for features like highly reflective metal surfaces. This precision is paramount when studying resonant modes. To this end, various mesh settings can be utilized, including uniform for simplicity, non-uniform or auto non-uniform for adaptive precision, and sub-grid meshing to capture sub-wavelength features accurately. Moreover, conformal meshing improves accuracy at material boundaries, essential for modeling the intricate geometries of nanocavities. Mesh override regions allow for further customization in specific areas of interest.

Similarly, a small temporal step \((\Delta t)\) is necessary to accurately represent rapid electromagnetic field oscillations within the nanocavity during simulations. This temporal precision is essential for capturing dynamic phenomena. Addi-
tionally, considering material dispersion in FDTD simulations is necessary. Incorporating frequency-dependent permittivity and permeability accounts for the dispersive nature of materials, making the model more physical. These considerations collectively contribute to the precision and reliability of FDTD simulations of Fabry-Perot nanocavities.

### 3.5 Electrical Simulation for Dynamic Optical Control in Fabry-Perot Nanocavities

Achieving dynamic control of Fabry-Perot nanocavities (FPN) through an external electric field necessitates the strategic placement of an epsilon-near-zero (ENZ) semiconductor within the FPN structure. Utilizing an ENZ semiconductor as the medium within the FP cavity enables precise modulation of the phase change induced during wave propagation through the cavity layer. In electronics, metal-oxide-semiconductor (MOS) structures are well-recognized for their applications in cases requiring precise control over semiconductor carrier concentration. Similarly, a metal-oxide-semiconductor-metal (MOSM) nanoscale structure can serve as an FPN. This allows for dynamic changes in the optical characteristics of the FPN by regulating the carrier concentration within the semiconductor layer, which may consist of an ENZ semiconductor for adjustable absorbers.

Within the framework of an MOS capacitor, Poisson’s equation is crucial for understanding how charges and electric fields are distributed within the semiconductor layer. This description assumes a simplified one-dimensional model for illustration.
The Poisson’s equation in one dimension is given by:

\[
\frac{d^2\psi}{dx^2} = -\frac{\rho}{\epsilon}, \tag{3.12}
\]

where \(\psi\) is the electrical potential, \(x\) is the spatial coordinate, \(\rho\) is the charge density, and \(\epsilon\) is the permittivity of the material.

To solve Poisson’s equation, one must initially determine the charge distribution within the semiconductor layer. In an MOS capacitor, the charge distribution \(\rho\) mainly consists of two components:

**Doping Profile \((\rho_d)\):** Due to the introduction of dopant atoms, there is a fixed charge distribution within the semiconductor layer. This can be modeled as a step function, with a sudden increase in charge density at the semiconductor-dielectric interface.

**Mobile Charge \((\rho_{mobile})\):** This component represents the mobile charge carriers, i.e., electrons and holes. The concentration of mobile carriers is influenced by the application of an external voltage.

Considering the charge distribution, the next step is to integrate Poisson’s equation to derive the electric field \((E)\) and potential \((\psi)\):

\[
E = -\frac{d\psi}{dx}, \tag{3.13}
\]

\[
\psi(x) = -\int E\,dx. \tag{3.14}
\]
Solving these equations provides the semiconductor layer’s electric field and potential profiles. The resulting electric field influences the distribution of charge carriers, and changes in the applied voltage will modify this distribution.

For a Fabry-Perot nanocavity resembling an MOS capacitor, the aim is to quantify how changes in charge distribution affect the effective refractive index of the spacer material. Although this problem appears straightforward, the relation between the charge distribution and effective refractive index is not and requires a detailed understanding of optical models useful to relate the charge concentration of material with its permittivity, which relates to the effective refractive index by the following equation,

\[ n_{\text{eff}} = \sqrt{\epsilon_r}, \]  

(3.15)

where, \( \epsilon_r \) represents relative permittivity.

The following section explores optical models that establish a connection between a material’s dielectric permittivity and its effective refractive index. Here, the permittivity value is significantly influenced by the material’s charge concentration.

3.6 Classical Optical Models and ENZ Semiconductors in Nanocavity Optics

The optical properties of a material are described by its dielectric permittivity \( (\epsilon) \). However, the ensemble \( \epsilon \) value of a material depends on its electronic configuration. Electromagnetic (EM) waves passing through a material generally
experience damping. Mathematically, this wave with its amplitude and phase can be described using the following equation:

\begin{equation}
E(x, t) = E_0 \exp\left\{i\left(\frac{n + i\kappa}{c}\right)x - \omega t\right\},
\end{equation}

(3.16)

\begin{equation}
E(x, t) = E_0 \exp\left(-\frac{\kappa\omega}{c}x\right) \exp\left(\frac{n\omega}{c}x - \omega t\right).
\end{equation}

(3.17)

The interaction between distinct electronic configurations and electromagnetic waves is described using the Lorentz and Drude models below.

3.6.1 Lorentz Model

The complex refractive index of a material describes its macroscopic properties and is connected to the material’s microscopic permittivity:

\begin{equation}
n + i\kappa = \sqrt{\epsilon' + i\epsilon''}.
\end{equation}

(3.18)

Here, \(n\) and \(\kappa\) are the real and imaginary parts of the effective refractive index, and \(\epsilon'\) and \(\epsilon''\) are the real and imaginary parts of the relative permittivity; also called the dielectric constant \((\epsilon_r)\), where \(\epsilon = \epsilon_0\epsilon_r\). In general, permittivity \((\epsilon)\) describes how an electric field influences (and is influenced by) a dielectric medium. A high permittivity implies more “resistance” to the propagation of the electric field, leading to reduced electric field flux in the material. These macroscopic/microscopic parameters are interrelated through the polarizability of the material.
Macroscopic description: The fields in a material are related by \( D = \varepsilon_0 E + P \), where \( P, E, \varepsilon_0 \), and \( D \) stand for electric polarization, electric field, the permittivity of free-space, and the electric displacement field, respectively. The electric polarization and electric field are related through the electric susceptibility:

\[
P = \varepsilon_0 \chi E, \quad \text{(3.19)}
\]

\[
D = \varepsilon_0 (1 + \chi) E, \quad \text{(3.20)}
\]

\[
D = \varepsilon_0 \varepsilon_r E. \quad \text{(3.21)}
\]

So, the relative permittivity/dielectric constant of the material is related to the electric susceptibility: \( \varepsilon_r = 1 + \chi \). Here a linear relationship is assumed between \( \varepsilon_r \) and \( \chi \). However, in materials with nonlinear behavior, additional terms or dependencies may be introduced to describe the relationship accurately. For nonlinear dielectric materials, the relationship between \( \varepsilon_r, \chi \), and electric field \( (E) \) can be described using a power series expansion. One commonly used expression is the nonlinear electric displacement (D) as a function of electric field:

\[
D = \varepsilon_0 \varepsilon E + \chi_1 \varepsilon_0 E^2 + \chi_2 \varepsilon_0 E^3 + \chi_3 \varepsilon_0 E^4 + \ldots. \quad \text{(3.22)}
\]

where \( \chi_1, \chi_2, \chi_3 \), etc. are the nonlinear susceptibility coefficients. This equation includes nonlinear terms (second-order and higher) to describe the
behavior of nonlinear dielectric materials under the influence of an electric field. However, in this research, only the linear response of the materials involved is considered.

- **Microscopic description:** A dielectric material is often modeled as atoms having bound electrons. A classical spring represents the hold of the nucleus on these bound electrons. The electron is much lighter than the nucleus, so the EM waves more affect the electron’s motion. The restoring force on the electron counterbalances the force exerted by the EM waves. The description follows Hooke’s law, where the restoring force on the electron is $F = -kx$. $k$ and $x$ are the spring constant and displacement. The time-dependent solution (from Newton’s 2nd law) for displacement $x$ is given by:

$$x(t) = x_0 \cos(\omega_0 t); \quad \omega_0 = \sqrt{\frac{k}{m}}. \quad (3.23)$$

It is possible to connect the microscopic with the macroscopic through the electric dipole moment. The electric polarization ($P$) is related to the electric dipole moment ($p$) as $P = Np$. Here, $N$ is the density of atoms inside the material. The atomic dipole moment $p$ can be rewritten as $p = qr$, where $q$ is the charge and $r$ is the separation between the nucleus and electron. Following the description:

$$P = Nqr. \quad (3.24)$$
The displacement, \( r \) can be understood by balancing the forces that oscillate the electron from its mean position. The forces that affect the position, \( r \) are the restoring force \((-k \, r(t))\), the electric field of the incoming EM waves \((q \, E(t))\), and a damping of the form: \((m \, \gamma \, \frac{\partial r(t)}{\partial t})\). Here, \( k, q, E(t), \gamma, \) and \( m \) are the spring constant, the charge of the electron, the electric field, the damping factor, and the mass of the electron, respectively. Arranging all these quantities into Newton’s 2\textsuperscript{nd} law results in:

\[
\frac{q}{m} E(t) = \frac{\partial^2 r(t)}{\partial t^2} + \gamma \frac{\partial r(t)}{\partial t} + \omega_0^2 r(t). \tag{3.25}
\]

The general solution of this equation for \( E(t) = E_0 \exp(i\omega t) \) is \( r(t) = r_0 \exp(i\omega t) \). The amplitude of the oscillation as a function of frequency is found when these relations are substituted into eq. (3.25):

\[
r_0 = \frac{q}{m} \frac{E_0}{(\omega_0^2 - \omega^2) + i \gamma \omega}. \tag{3.26}
\]

This equation is physically meaningful. For \( \omega < \omega_0 \), the \( r_0 \) and \( E \) are in phase, resulting in a moderate amplitude of the oscillation. At \( \omega = \omega_0 \), the \( r_0 \) and \( E \) are 90\(^\circ\) out of phase. Maximum oscillation amplitude (resonance) results, and for \( \omega > \omega_0 \), the \( r_0 \) and \( E \) are 180\(^\circ\) out of phase, resulting in a minimum oscillation amplitude. Equation (3.24) can be rewritten using \( r_0 \) from eq. (3.26):
\[ P = N q r_0 = \frac{N q^2}{m} \frac{E_0}{(\omega_0^2 - \omega^2) + i \gamma \omega}. \] 

(3.27)

This form of \( P \) can now be used to rewrite some equations from the macroscopic description, such as:

\[ \epsilon_r = 1 + \chi = 1 + \frac{N q^2}{\epsilon_0 m} \frac{1}{(\omega_0^2 - \omega^2) + i \gamma \omega}. \] 

(3.28)

Here, \( \frac{N q^2}{\epsilon_0 m} = \omega_p^2 \) and this is known as the plasma frequency, which will become one of the most important parameters in this research. Equation 3.28 can now be rewritten as:

\[ \epsilon_r(\omega) = 1 + \frac{\omega_p^2}{(\omega_0^2 - \omega^2) + i \gamma \omega}. \] 

(3.29)

Equation (3.29) is complex and can be separated into its real and imaginary parts:

\[ \epsilon'(\omega) = 1 + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}, \] 

(3.30)

\[ \epsilon''(\omega) = \frac{\omega_p^2(\gamma \omega)}{(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}. \] 

(3.31)

The changes in \( \epsilon' \) and \( \epsilon'' \) over the electromagnetic spectrum can be visualized using fig. 3.2 [144].
Figure 3.2: An illustration of the frequency response of various dielectric mechanisms in terms of the real and imaginary parts of the permittivity.
In the narrow visible range $\epsilon'$ and $\epsilon''$ are both relatively small and do not change significantly, so the basic Lorentz model gives an overall useful description of the behavior of dielectrics in this region of interest.

### 3.6.2 Drude Model

The Drude model describes the interaction of light with metals. The primary distinction between a dielectric and a metal is the configuration and motion of electrons. While a dielectric comprises bound electrons, metals are characterized by predominantly free electrons. Consequently, electrons in metals do not encounter a restoring force, as in dielectrics. Nevertheless, the presence of both a damping force and an electric force accounts for the interaction between electrons and electromagnetic waves. The Drude model closely resembles the Lorentz model, differing in the absence of resonance behavior. A solution for $\epsilon_r(\omega)$ is obtained by eliminating $\omega_0$ from eq.(3.29):

$$
\epsilon_r(\omega) = 1 + \frac{\omega_p^2}{i \gamma \omega - \omega^2}.
$$

(3.32)

This equation characterizes the (complex) dielectric function, or relative permittivity, as per the Drude model. The plasma frequency is critical for understanding, the optical characteristics of metals.

- **Metal as free-electron gas:**

  The interaction of light with a free-electron gas does not require the damping factor in $\epsilon_r(\omega)$. Consequently, eq.(3.32) simplifies to the following expression:
\[ \epsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2}. \] (3.33)

This equation can be used to obtain the effective refractive index \( (n_{\text{eff}}) \) as \n\( (n_{\text{eff}}) = \sqrt{\epsilon_r(\omega)}. \)

In this context, two scenarios become apparent, depending on the value of \( \omega \).

1. \( \omega < \omega_p \): In this case, \( \epsilon_r(\omega) \) assumes a negative value, yielding an imaginary solution for \( n_{\text{eff}} \), so that \( n_{\text{eff}} \) is primarily influenced by \( \kappa \), the extinction coefficient, which is intricately linked to the more familiar absorption coefficient. This condition ensures that electrons can respond to the electric field, resulting in the absorption of energy from the field.

2. \( \omega > \omega_p \): This means the solution for \( n_{\text{eff}} \) is real and dominated by the frequency-dependent \( n \) in the relation \( n + i\kappa \). This is normal optical dispersion; the dependence of the index of refraction on frequency (or wavelength). In this case, the electrons cannot move far away from the nucleus and appear to be somewhat bound to it. Even metals can behave as dielectrics when the EM wave’s electric field oscillation frequency is larger than the plasma frequency of the metal.

Reflectivity \( (R) \) is conventionally defined as:

\[ R = \frac{(n - 1)^2 + \kappa^2}{(n + 1)^2 + \kappa^2}. \] (3.34)
For $\omega < \omega_p$, where $\kappa$ dominates and $n$ is approximately 0, the reflectivity ($R$) is equal to 1. This indicates that metals reflect all frequencies less than $\omega_p$. Conversely, for $\omega > \omega_p$, where $\kappa$ is approximately 0, and if $n$ is close to 1, the classical optics expression for reflectivity is attained, leading to $R = 0$, which is a characteristic of dielectrics.

This explanation, while straightforward, is based on the assumption that metals behave as a free-electron gas, simplifying the equation for $\epsilon_r(\omega)$. However, in the case of a real metal thin film, this simplification is not valid. A new damping factor can be introduced into the equation for $\epsilon_r(\omega)$ to account for collisions between electrons and ions. This damping factor ($\gamma$) represents the collision frequency. The Lorentz-Drude model is used to describe this system involving electrons and ions, and the real and imaginary permittivities can be expressed by modifying eqs. 3.30 and 3.31:

\[ \epsilon'(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}, \]  
(3.35)

\[ \epsilon''(\omega) = \frac{\omega_p^2 \gamma}{\omega(\omega^2 + \gamma^2)}. \]  
(3.36)

In eq. (3.35), 1 represents the high-frequency permittivity limit ($\epsilon_{\infty}$), also referred to as $\epsilon_{\text{core}}$ in some references [145]. In eq. (3.35), when $\omega_p^2 = \omega^2$ (with zero or relatively low $\gamma$), the real part of the permittivity approaches zero. In the context of metals, at the plasma frequency ($\omega_p$), $n$ also approaches zero. The frequency at which either $n$ vanishes or becomes nearly zero is recognized as the
epsilon-near-zero (ENZ) frequency. For metals with $\varepsilon_\infty = 1$, the plasma frequency $\omega_p$ and the ENZ frequency ($\omega_{ENZ}$) coincide. However, for semiconductors like Silicon (Si), Indium Arsenide (InAs), Indium Antimonide (InSb), and PbTe, where the $\varepsilon_\infty$ values are 12, 14, 16, and perhaps more than 100, respectively [145], this results in significantly different values for $\omega_p$ and $\omega_{ENZ}$ in these materials.
Chapter 4. Nanoscale Modeling and Experimental Realization: Achieving Dynamically Tunable Planar Narrowband Perfect Absorbers

4.1 Preface

Part of this chapter is based on the following publication: Dixit, K.P., Gregory, D.A. “Nanoscale modeling of dynamically tunable planar optical absorbers utilizing InAs and InSb in metal-oxide-semiconductor–metal configurations.” Discover Nano 18, 100 (2023). Adapted (or “reproduced in part”) with permission from Springer Nature Publishing Group.

4.2 Motivation

Recently, there has been significant progress in the development of spectrally selective optical absorber and modulators, including patterned and unpatterned thin-film structures. These structures find use in a wide range of applications such as biological and chemical sensing [107, 106, 146, 147], structural color printing [148, 149], solar energy harvesting [150, 151], and color filters [152, 153, 122]. However, the incorporation of tunability into these structures has presented a significant challenge. Efficient modification of the
refractive index of the materials employed in the design, as well as the enhancement of light–matter interaction, has remained constant areas of focus in pursuit of tunability. In recent times, researchers have adopted a strategy that involves utilizing an epsilon-near-zero (ENZ) semiconductor as the active layer for developing dynamically tunable optical absorbers/modulators [118, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 119, 165, 139, 166]. Transparent conductive oxides (TCO) and doped semiconductors such as indium tin oxide (ITO) [118, 154, 156, 157, 161, 162, 164, 119, 165], zinc oxide (ZnO) [167], aluminum-doped zinc oxide (AZO) [158], indium oxide (In2O3) [159], cadmium oxide (CdO) [168], indium antimony (InSb) [155, 139], and indium arsenide (InAs) [166, 169] show excellent light modulation performance based on the ENZ effect.

The fundamental concept underlying the operation of many of these modulators revolves around leveraging the influence of an external potential on the majority charge carriers within a heavily doped ENZ semiconductor. This external potential subsequently impacts the plasma frequency ($\omega_p$) of the semiconductor.

The effect of external potential on the plasma frequency is a direct prediction of the classic Drude model for light–matter interaction [170, 171], which describes the relationship between the plasma frequency, relative permittivity ($\epsilon_r$), and the scattering constant ($\gamma$) of a material, as well as the incoming light frequency ($\omega$). As per eq. 4.1 (from the Drude model), the plasma frequency ($\omega_p$) is a function of electron concentration ($N$) and is dependent on various parameters such as the electron’s effective mass ($m^*$), charge ($q$), and vacuum permittivity ($\epsilon_0$).
The change in $\omega_p$ in turn affects the $\epsilon_r$ of the doped semiconductor, through the relationship:

$$
\epsilon_r(\omega) = \epsilon_\infty + \frac{\omega_p^2}{i\gamma \omega - \omega^2}, \quad \text{where} \quad \omega_p = \sqrt{\frac{Nq^2}{m^*\epsilon_0}}. \quad (4.1)
$$

The $\epsilon_r(\omega)$ of a material is a complex function that can be expressed as $\epsilon_r(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$, where $\epsilon'(\omega)$ and $\epsilon''(\omega)$ are real and imaginary components, respectively. The equations for $\epsilon'(\omega)$ and $\epsilon''(\omega)$ can be written as:

$$
\epsilon'(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + \gamma^2}, \quad \epsilon''(\omega) = \frac{\gamma \omega_p^2}{\omega(\omega^2 + \gamma^2)}. \quad (4.2)
$$

The $\epsilon_r$ also determines the effective refractive index ($n_{\text{eff}}$) of a material, as defined by $n_{\text{eff}}(\omega) = \sqrt{\epsilon_r(\omega)}$. This relationship can be written as $n(\omega) + in(\omega) = \sqrt{(\epsilon'(\omega) + i\epsilon''(\omega))}$, where $n$ and $\kappa$ represent the real and imaginary components of the effective refractive index of the material. The real component, $n$, governs the dispersion of light in the material, while the imaginary component, $\kappa$, signifies the absorption of light. From eq. (4.2), it can be seen that for a given value of plasma frequency ($\omega_p$), a high-frequency permittivity ($\epsilon_\infty$), and a scattering constant ($\gamma$), the value of $\epsilon'(\omega)$ becomes zero at a specific frequency ($\omega$). This frequency is known as the ENZ frequency and can be obtained by rearranging the eq. for $\epsilon'(\omega)$ and setting it equal to zero:

$$
\omega_{\text{ENZ}} = \sqrt{\frac{\omega_p^2 - \epsilon_\infty \gamma^2}{\epsilon_\infty}}, \quad \lambda_{\text{ENZ}} = \frac{2\pi c}{\omega_{\text{ENZ}}}. \quad (4.3)
$$
Therefore, the ENZ frequency ($\omega_{ENZ}$) can be considered as a transition point where the real component of the permittivity ($\epsilon'$) changes from positive to negative [172, 173]. This transition also affects the effective refractive index ($n_{\text{eff}}$), as a negative $\epsilon_r$ results in an increase in the imaginary component ($\kappa$), thereby increasing the absorption in the material for all frequencies below $\omega_{ENZ}$. Although the phenomenon of epsilon-near-zero (ENZ) materials is intriguing, it is important to note that free-standing ENZ materials do not exhibit significantly enhanced optical absorption when subjected to normal incident light at frequencies lower than $\omega_{ENZ}$. This lack of enhancement arises from the absence of an electric field component perpendicular to the interface for normal incident light [161]. Therefore, to achieve dynamic tunability in optical modulators and improve absorption, the utilization of ENZ materials alone is insufficient. It is imperative to design the modulator in a manner that enhances the strength of the interaction between light and matter. In essence, both the selection of an appropriate ENZ material and the careful design of the modulator are necessary to achieve the desired enhanced light-matter interaction strength.

In the majority of the tunable electro-optical modulator designs based on the epsilon-near-zero (ENZ) effect, the ENZ effect is primarily confined to an ultrathin layer at the interface between the dielectric and semiconductor materials. As a result, the modulation performance relies on the strength of the interaction between light and the semiconductor, specifically the degree to which light is concentrated within the semiconductor sublayer, thereby enhancing absorption through the ENZ effect [118, 154, 157, 161, 119, 165, 139, 166, 158].
In ENZ material-based tunable optical devices, the modification of the transition frequency ($\omega_{ENZ}$) of the material is crucial in changing its optical behavior. This is achieved by altering the material’s plasma frequency ($\omega_p$), which is highly dependent on the electron concentration ($N$). Thus, generating a charge gradient within a doped semiconductor (with an applied potential bias) is one of the methods to alter $\omega_p$ throughout the material layer [118, 154, 158, 157, 161, 139, 119, 164, 165, 166]. The majority of electrically tunable optical modulators based on epsilon-near-zero (ENZ) materials are meticulously designed to facilitate the coupling between the ENZ region induced by the applied potential and the plasmon resonance mode of the structure. This deliberate coupling is aimed at enhancing the optical absorption capabilities of the modulator [119, 166, 157, 161]. However, such structures do require complex lithography patterning.

In contrast to other designs of dynamically tunable modulators that primarily focus on enhancing absorption within specific wavelength bands or plasmon modes, the proposed research showcases the optical tuning capabilities of a Fabry-Perot nanocavity. This nanocavity is constructed using a metal-oxide-semiconductor-metal (MOSM) structure (see Fig. 4.1) and aims to achieve spectral tuning of a Fabry-Perot resonance within the visible range. The key feature of this design lies in the utilization of an epsilon-near-zero (ENZ) semiconductor as the semiconductor layer within the MOSM structure. This incorporation enables dynamic control and manipulation of the refractive index within the semiconductor sublayer, facilitating precise tuning of the nanocavity’s optical properties.
In general, in a nanocavity composed of two reflecting metal layers separated by a dielectric spacer, the propagation round trip phase delay in the spacer is \( \phi_s = 4\pi nd/\lambda \), and the reflection phase change with top and bottom metal boundaries are \( \phi_{ms} \) (metal-semiconductor) and \( \phi_{om} \) (oxide-metal). For the given MOSM structure, \( d \) is the thickness of the spacer \( (d_{oxide} + d_{semiconductor}) \), \( n \) is the real part of the refractive index of the spacer, and \( \lambda \) is the effective wavelength. The presented study follows the idea of tuning the spectral response of nanocavity by manipulating the refractive index of the semiconductor sublayer using an external potential [139, 167]. Further in the chapter, the effect of this manipulation on the resonance is elaborated upon in detail through the application of the transfer matrix method.

**Figure 4.1:** Schematic structure of metal-oxide-semiconductor-metal Fabry-Perot nanocavity.

In this research, the concept of manipulating the effective refractive index of a doped semiconductor is thoroughly explored using a combination of electronic and optical descriptions. The practical applications of this concept are illustrated
in the design and operation of dynamically tunable FPN models composed of the MOSM architecture. To begin, a modeling methodology employing the transfer matrix method (TMM) for MOSM configurations is developed [153, 122]. The aim was to identify suitable layer thicknesses for metals and oxide materials to be used in conjunction with an ultrathin n-InSb and n-InAs layers for achieving narrow-band perfect absorption within the visible range. Aluminum (Al) and gold (Au) were chosen for the metal layers in constructing symmetric FPNs. Their high extinction coefficients enhances light-matter interaction in the epsilon-near-zero (ENZ) semiconductor. This is achieved by enabling multiple reflections within the MOSM structure. Aiming for operation in reflection mode, a 100 nm thickness for the bottom metal layer was chosen to ensure zero light transmission. To attain dynamic tunability, an external electric potential should be applied to the metal layers. To prevent the oxide layer from easy breakdown due to the high electric field within the FPN, titanium dioxide (TiO$_2$) was selected as the oxide layer due to its high dc dielectric constant [174].

The choice of a 20 nm thickness for the n-InSb and n-InAs semiconductor layers is based on several studies that demonstrates the advantages of using tunable conducting oxides and semiconductors to create dynamically tunable optical absorbers [118, 162, 119, 166, 157, 139]. Dynamic tuning of the FPN incorporating ENZ semiconductors depends on increasing the charge density within a specific region of the semiconductor layer. However, achieving high charge density is feasible only within a few nanometers of the semiconductor layer, limiting the modulation of optical parameters to this thin region. A small ratio between
the thickness of the modulated semiconductor region and the region with regular charge distribution leads to negligible changes in the spectral response of the nanocavity [119, 139, 166]. To ensure a significant effect, the n-InSb and n-InAs layers must be kept as thin as possible. Practical challenges in depositing such ultrathin layers via the sputtering method necessitate a minimum thickness of 20 nm. The top metal layer is designed to be semi-transparent, allowing significant light penetration into the cavity, with a thickness range of 10 - 15 nm.

Based on the modeling results, the MOSM configurations featuring gold (Au), aluminum (Al), titanium dioxide (TiO$_2$), n-InSb, and n-InAs were designed as follows: (1) Au (100 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (17 nm), (2) Al (100 nm) - TiO$_2$ (12 nm) - (n-InSb) (20 nm) - Al (8 nm), (3) Au (100 nm) - TiO$_2$ (10 nm) - (n-InAs) (15 nm) - Au (15 nm), and (4) Al (100 nm) - TiO$_2$ (15 nm) - (n-InAs) (20 nm) - Al (8 nm).

4.3 Modeling and Simulation Approach

The functioning of the dynamically tunable nanocavity is based on a synergistic interaction between electrical and optical processes that take place within the semiconductor layer, particularly at the interface between the oxide and semiconductor materials [118, 154, 163, 157, 159, 160, 158, 161, 165, 166, 139].

4.3.1 Electronic Processes

The structure depicted in Fig. 4.1 closely resembles the metal-oxide-semiconductor capacitor (MOScap) architecture, with the top metal layer serving
solely as an electrical contact. The metal-oxide-semiconductor (MOS) structure is widely utilized for its ability to control charge concentration location inside the semiconductor layer to within a few nanometers. The effect of an applied electric field on charge concentration at the oxide-semiconductor interface has been exploited for a range of practical applications, such as in power electronics [175], sensing devices [176, 177], and memory devices [178, 179]. The nanocavity presented in this work holds the potential to become a new optical application of the MOS structure. The MOScap design is similar to a parallel plate capacitor, with the metal and semiconductor layers serving as the capacitive plates and the oxide serving as the dielectric medium. Upon application of a positive bias to the metal layer (referred to as the gate), the majority charge carriers (electrons) of the n-type doped semiconductor layer accumulate at the oxide-semiconductor interface. This is known as the accumulation mode of a MOScap [180].

The charge density in the accumulation mode is dependent on the electric potential distribution across the semiconductor layer. Poisson’s equation provides a means of evaluating potential differences between different points in such systems. The solution of Poisson’s equation in the surface region of the semiconductor (such as n-InSb or n-InAs in this study) near the oxide-semiconductor interface yields a relationship between the surface potential ($\psi_s$), charge ($q$), and electric field ($E$). In the case of an n-type semiconductor, Poisson’s equation can be expressed as follows:

$$\frac{d^2\psi}{dx^2} = -\frac{dE}{dx} = -\frac{q}{\epsilon_{semi.}}[p(x) - n(x) + N_d(x) - N_a(x)].$$

(4.4)
Figure 4.2: Energy-band diagram near the semiconductor boundary of a MOS device with n-type semiconductor. The band bending potential is defined as positive when the bands bend downward in accumulation mode.

Where $\psi$ is the electrostatic potential, $\epsilon_{\text{semi.}}$ is the permittivity of the semiconductor material, $p(x)$ and $n(x)$ are the densities of holes and electrons at any position $x$ within the semiconductor, respectively, $N_d(x)$ is the donor concentration, and $N_a(x)$ is the acceptor concentration. Many electrostatic parameters in the semiconductor layer can be expressed in terms of this electrostatic potential. With no applied field, a uniformly doped n-type or p-type semiconductor is charge neutral — the right-hand side of the eq. (4.4) is zero, and the potential is constant throughout the semiconductor sample.

To illustrate the impact of the electrostatic potential ($\psi$), the energy band diagram serves as a valuable tool. The potential ($\psi$) is typically defined relative to the intrinsic Fermi level, and can thus be represented as $\psi_i$. In n-type doped semiconductors, the Fermi potential ($\psi_f$) and donor concentration ($N_d$) are also significant electronic parameters. The difference between $\psi_i$ and $\psi_f$ in the band diagram is referred to as $\psi_B$, as depicted in Fig. 4.2.
The relationship between $\psi_B$ and the doping concentration (or the ionized dopant concentration for incomplete ionization) is established through the following:

$$\psi_B = \psi_f - \psi_i = \frac{kT}{q} \ln \left( \frac{N_d}{n_i} \right). \quad (4.5)$$

In this eq., $k$ represents the Boltzmann constant, $T$ represents the ambient absolute temperature and $n_i$ represents the intrinsic carrier density of the semiconductor material. It is worth noting that eq. (4.5) is based on the principle of charge neutrality, and is valid only when the local net charge density, being the sum of the mobile and ionized dopant charge densities, is zero, in the right-hand side of eq. (4.4). In instances where a net charge exists (due to a discrepancy between the mobile and fixed charge densities) and band bending (spatial variations of $\psi_i$ under applied potential) occurs, the carrier densities in relation to the electrostatic potential can be expressed as follows:

$$n = n_i e^{\frac{q(\psi_i - \psi_f)}{kT}}, \quad p = n_i e^{\frac{q(\psi_f - \psi_i)}{kT}}. \quad (4.6)$$

These relations are known as Boltzmann’s relations and are applicable to both n-type and p-type semiconductors in thermal equilibrium.

As illustrated in Fig. 4.2, the potential $\psi(x) = \psi_i(x) - \psi_i(x = \infty)$ represents the degree of band bending at position $x$, with $x = 0$ being the oxide-semiconductor interface and $\psi_i(x = \infty)$ being the intrinsic potential beyond the interface. A positive value of $\psi(x)$ indicates that the band is bent downward.
The boundary conditions are defined as $\psi = 0$ away from the interface, and $\psi = \psi(0) = \psi_s$ at the interface, where accumulation occurs when $\psi_s > 0$. The electron and hole concentrations at any given point $x$ within the semiconductor can be expressed as a function of $\psi(x)$ using $\psi(x) = \psi_i(x) - \psi_i(x = \infty)$ in eq. (4.5). The expressions for $n(x)$ and $p(x)$ in terms of $\psi(x)$ are as follows:

$$n(x) = n_i e^{q(\psi(x) - \psi_B)/kT} = n_0 e^{q\psi(x)/kT}, \quad (4.7)$$

$$p(x) = n_i e^{q(\psi_B - \psi(x))/kT} = \frac{n_i^2}{n_0} e^{-q\psi(x)/kT}, \quad (4.8)$$

where $n_0$ represents the majority carrier density of electrons at $x = \infty$ and $n_i^2/n_0$ represents the minority carrier density of holes at $x = \infty$, respectively.

Therefore, the solution of Poisson’s eq. determines the distribution of electrostatic potential at every point $x$ within the semiconductor layer of the MOScap, which in turn, defines the electron and hole density distributions across the semiconductor (as described in eqs. 4.7 and 4.8) at the applied gate potential.

In this study, the distributions of electrostatic potential and majority carriers for four systems comprising n-InSb or n-InAs semiconductor layers and TiO$_2$ oxide layers have been calculated using the CHARGE solver of the Ansys LUMERICAL software [181]. The solver iteratively solves Poisson’s eq. for the given MOScap system. To achieve precise results, it is important to have a fine enough mesh setting in the solver to sample the carrier distribution curves accurately. The results of this analysis are presented and discussed in detail later.
4.3.2 Absorber Structure and Optical Processes

The proposed FPN (Fig. 4.1) consists of reflective metal layers and a semiconductor with an oxide layer acting as the medium. The thickness of the medium determines the resonance wavelength, which is found to be in the visible range for the four structures presented in Fig. 4.3. The use of TiO$_2$ as the oxide layer increases the dielectric breakdown voltage (due to its high dielectric constant) [182].

The optical behavior of the semiconductors n-InSb and n-InAs is crucial in understanding the optical response to an external electric potential. Carrier concentrations of $N_{1}^{(\text{n-InSb})} = 3.5 \times 10^{17}$/cm$^3$ and $N_{1}^{(\text{n-InAs})} = 1.4 \times 10^{18}$/cm$^3$ were used in the simulation. To understand the effects of free carrier concentration density on the effective refractive index, the results using the calculated parameters $n(\omega)$ and $\kappa(\omega)$ from the Drude model for both semiconductors, with N values
$5 \times 10^{19}/\text{cm}^3$ and $10^{21}/\text{cm}^3$, are presented in Fig. 4.4. One should note that, due to the limitation of solid solubility of the dopant, one cannot physically dope a semiconductor such as InAs with a concentration higher than $10^{19}/\text{cm}^3$ [169]. However, a temporary electron concentration of the order of $10^{21} - 10^{22}/\text{cm}^3$ can be achieved within a sublayer of the semiconductor using the effects of external electric potential on certain types of device architectures as discussed in this article.

As can be observed in Fig. 4.5, with increasing carrier concentration, the $\lambda_{ENZ}$ shifts from the far-infrared (35.14 $\mu$m) to the visible range (0.657 $\mu$m) for n-InSb, and from the mid-infrared (19.61 $\mu$m) to the visible spectrum (0.734 $\mu$m) for n-InAs. The parameters used to calculate the $n(\omega)$ and $\kappa(\omega)$ using the Drude model are listed in Table 4.1 [183].

Table 4.1: Measured optical properties of n-InSb and n-InAs by Spitzer et al. $m_e = 9.1 \times 10^{-31}$ kg (electron rest mass).

<table>
<thead>
<tr>
<th>Material</th>
<th>$\epsilon_\infty$</th>
<th>$m^*$</th>
<th>$\gamma(\text{rad/s})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-InSb</td>
<td>16.8</td>
<td>0.023$m_e^{(a)}$</td>
<td>2.12x10^{12}</td>
</tr>
<tr>
<td>n-InAs</td>
<td>14.6</td>
<td>0.033$m_e^{(a)}$</td>
<td>2.63x10^{12}</td>
</tr>
</tbody>
</table>

Using Figs. 4.4 and 4.5, two ranges of wavelength ($\lambda$) can be observed: 1) $\lambda < \lambda_{ENZ}$ and 2) $\lambda > \lambda_{ENZ}$. For wavelengths that fall under the first case, it is evident that the real part of the refractive index plays a dominant role in determining the optical behavior, leading the material to act like a dielectric. On the other hand, for wavelengths that follow the second case, the imaginary
Figure 4.4: Calculated (A) Real and imaginary parts of the relative permittivity of n-InAs and n-InSb for $N = 5 \times 10^{19}/\text{cm}^3$, (B) real and imaginary parts of the relative permittivity of n-InAs and n-InSb for $N = 1 \times 10^{21}/\text{cm}^3$, (C) real and imaginary parts of the effective refractive index of n-InAs and n-InSb for $N = 5 \times 10^{19}/\text{cm}^3$, and (D) real and imaginary parts of the effective refractive index of n-InAs and n-InSb for $N = 1 \times 10^{21}/\text{cm}^3$. 
part of the effective refractive index becomes dominant as the real part of the permittivity becomes negative. This leads the material to behave optically like a metal.

In the proposed MOSM structures, when an external potential is applied, it follows the electrostatic potential distribution described in the earlier section. This results in a noticeable charge gradient ($\Delta N$) in the n-InSb and n-InAs semiconductors due to the majority charge distribution generated by the applied potential. As a result, n-InSb and n-InAs show different values of $\lambda_{ENZ}$ across the layer when an external potential is applied.

To actively modify the optical performance of the proposed FPNs, it is crucial to manipulate the effective refractive index of the n-InSb or n-InAs layers through changes in the electron concentration gradient.
The transfer matrix method (TMM) is a theoretical tool that can uncover the overall optical effect of the refractive index gradient in the proposed optical cavities, resulting in a global relationship between the electric-field vectors of the incident, reflected, and transmitted electromagnetic waves [108]. Mathematically, the TMM is a 2x2 matrix that incorporates information about all partial reflections and transmissions within a multilayer thin film structure. The TMM uses propagation and transmission matrices to calculate a final transfer matrix ($M$), and the reflectance at a specific wavelength can be determined by two of the transfer matrix elements. The propagation ($p_m$) and transmission ($D_m$) matrices are components of the TMM and can be written as

$$P_m = \begin{bmatrix} \exp(i\phi_m) & 0 \\ 0 & \exp(-i\phi_m) \end{bmatrix},$$

where $\phi_m = \frac{2\pi(n_m - i\kappa_m)d_m}{\lambda \cos \theta_t}$. \hfill (4.9)

For TE polarization,

$$D_m = \begin{bmatrix} 1 & 1 \\ (n_m - i\kappa_m)\cos \theta_m & -(n_m - i\kappa_m)\cos \theta_m \end{bmatrix},$$

and for TM polarization,
Here, \( m = 0, 1, 2, 3, 4 \) represents air, the top metal layer (Au or Al), the semiconductor layer (n-InSb or n-InAs), the oxide layer (TiO\(_2\)), and the bottom metal layer (Au or Al). \( n_m \) and \( \kappa_m \) are the real and imaginary parts of the effective refractive index, \( \theta_m \) is the incident angle of light, \( d_m \) is the thickness, and \( \phi_m \) is the phase delay of the optical wave in layer \( m \). The manipulation of the \( \phi_m \) by introducing a refractive index change is the key for dynamically tuning the resonance wavelength of the proposed FPNs. The term \( \theta_t \) represents the transmitted wave angle; however, in this study, the incident angle for the optical study of all four structures is set to zero. Thus, the \( \theta_t \) becomes zero, reducing the denominator of the \( \phi_m \) eq. to just \( \lambda \). For the given four-layer systems, the \( M \) is written as:

\[
M = D_m^{-1}(D_2P_2D_2^{-1})(D_3P_3D_3^{-1})(D_4P_4D_4^{-1})D_5. \tag{4.12}
\]

Later, the reflection coefficient \( (r) \) and reflectance \( (R) \) are calculated using the \( M_{21} \) and \( M_{11} \) elements of \( M \),

\[
R = |r|^2 = \left| \frac{M_{21}}{M_{11}} \right|^2. \tag{4.13}
\]
The results obtained using the TMM are dependent on the parameters $n$, $\kappa$, and $d$ of the multilayer thin film structure. For a given layer thickness ($d$), the values of $n$ and $\kappa$ determine the $M$. In the absence of an applied potential, the effective refractive index values are constant across the semiconductor layer. However, when an external potential is applied, the effective refractive index values become different across the semiconductor layer, creating sublayers with different effective values of $d$, which leads to variations in $M$ and hence, the $R$.

4.4 Results from Simulation and Modeling

The electric potential and electron concentration distributions in the n-InSb and n-InAs layers of the four systems (as depicted in Fig. 4.3) were determined using the CHARGE solver of the Ansys LUMERICAL software [181]. The CHARGE solver utilizes material parameters from its built-in library, which includes the work functions of 5.1 eV for Au and 4.28 eV for Al and a relative dielectric permittivity of 80 for TiO$_2$ [145, 174]. For the semiconductors InSb and InAs, the solver uses DC permittivities of 16.8 and 14.6, work functions of 4.71 eV and 5.08 eV, and intrinsic carrier densities of $1.92 \times 10^{16}/\text{cm}^3$ and $7.24 \times 10^{14}/\text{cm}^3$, respectively [145, 183]. The user can set the doping concentration of the semiconductor using the doping tool provided in the solver.

The doping tool was set to n-type doping with constant concentrations of $3.5 \times 10^{17}/\text{cm}^3$ and $1.4 \times 10^{18}/\text{cm}^3$ for n-InSb and n-InAs, respectively. The solver uses Poisson’s equation to calculate the electric field, potential, and charge distribution across the semiconductor. For the simulation, the gate metal layer
Figure 4.6: Electric potential ($\psi$) distribution in semiconductor layers of (A) Au (100 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (17 nm), (B) Al (100 nm) - TiO$_2$ (12 nm) - (n-InSb) (20 nm) - Al (8 nm), (C) Au (100 nm) - TiO$_2$ (10 nm) - (n-InAs) (15 nm) - Au (15 nm), and (D) Al (100 nm) - TiO$_2$ (15 nm) - (n-InAs) (20 nm) - Al (8 nm).
Figure 4.7: Electron distribution in semiconductor layers of (A) Au (100 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (17 nm), (B) Al (100 nm) - TiO$_2$ (12 nm) - (n-InSb) (20 nm) - Al (8 nm), (C) Au (100 nm) - TiO$_2$ (10 nm) - (n-InAs) (15 nm) - Au (15 nm), and (D) Al (100 nm) - TiO$_2$ (15 nm) - (n-InAs) (20 nm) - Al (8 nm).
(bottom metal layer) was set to 0 V, 5 V, 10 V, and 15 V, while grounding the top metal layer. These voltage levels were chosen to significantly increase electron density at the oxide-semiconductor interface. Figure 4.5 shows that the epsilon-near-zero (ENZ) wavelength for n-InSb and n-InAs shifts into the visible range at an electron concentration of $10^{21} - 10^{22}/\text{cm}^3$. A study by Riedel et al. demonstrated a charge accumulation in the range of $10^{18}$ to $10^{21}$ for a similar MOSM structure incorporating ITO as ENZ semiconductor [165]. The study used a voltage sweep of 1-5 volts with a step size of 1 V. The primary goal of their study was to identify the minimum voltage needed to achieve significant charge accumulation, thereby enabling dynamic tunability in the Fabry-Perot nanocavity (FPN). Drawing on these findings, the present study opts for a step size of 5 V instead of 1 V.

In this study, at 0 V, the observed electric potentials at the oxide-semiconductor interface of all four systems were due to the difference between the metal and semiconductor Fermi energy, resulting in a band bending. As depicted in Fig. 4.6, a fraction of the total external voltage is dropped across the semiconductor layer with a $\psi_s$ value less than 0.5 V. With a 5 V increment, the $\psi_s$ value roughly increases by 0.02 V for all four systems. Fig. 4.7 illustrates that the electron concentration at the interface can reach as high as $\sim 10^{22}/\text{cm}^3$ and exhibit an exponential decline across the semiconductor layer, eventually reaching the doped concentration of $3.5 \times 10^{17}/\text{cm}^3$ for n-InSb and $1.4 \times 10^{18}/\text{cm}^3$ for n-InAs near the edge of the semiconductor layer.
Figure 4.8: (A) Real and (B) imaginary refractive index gradient in n-InAs layer of Au - TiO$_2$ - (n-InAs) - Au structure at 10V applied voltage.

The calculated $\Delta N$ across the semiconductor layer can be imported into the Ansys LUMERICAL software’s FDTD solver using the “np density” attribute [143]. The FDTD, a finite-difference time-domain routine, then applies the Drude model to calculate the refractive index using the charge distribution from the np density over every 1nm sublayer of the semiconductor. Figure 4.8 displays the calculated gradient in the real and imaginary parts of the effective refractive index for the n-InAs layer of Au- TiO$_2$ - (n-InAs) - Au with a 10 V applied voltage (for the visible range), as calculated by the FDTD. Similar calculations are performed for all four systems at external voltages of 0, 5, 10, and 15 volts.

As shown in Fig. 4.8, the refractive index near the TiO$_2$ - (n-InAs) interface exhibits high $\kappa$ values and low $n$ values. This implies that, under the influence of the applied voltage, up to 2 nm of the n-InAs material facing the TiO$_2$ layer should exhibit a different phase delay compared to the remaining part of the layer. To ascertain the optical impact of this change, the absorbed optical power
Figure 4.9: Absorbed power contour plot for (A) Au - TiO₂ - (n-InAs) -Au structure at 0V (B) Au - TiO₂ - (n-InAs) -Au structure at 10V (C) n-InAs layer from TiO₂-(n-InAs) interface of Au - TiO₂ - (n-InAs) -Au structure at 0V (D) n-InAs layer from TiO₂-(n-InAs) interface of Au - TiO₂ - (n-InAs) -Au structure at 10V.

The calculated absorption profile of the Au- TiO₂-(n-InAs)-Au structure as a function of wavelength is presented in Fig. 4.9. It is evident that the metal layers absorb a majority of the incident light. However, the application of potential leads to a change in the power absorbed by the n-InAs layer closest to the TiO₂ layer for a depth up to 2 nm (Fig. 4.9 (D)).

The optical impact of the refractive index gradient can be further elucidated by analyzing the reflectance spectrum of FPN structures. The TMM was
utilized to calculate the reflectance spectrum of all four FPN structures under normal incidence. For TMM calculations the refractive indices of Au, Al, and TiO$_2$ were obtained from previously published data by Gao et al. [185], McPeak et al. [186], and Sarkar et al. [187], respectively. As previously mentioned, the refractive indices of n-InSb and n-InAs at various applied voltages were obtained using the Drude model in the FDTD index perturbation tool. The thickness of each layer for all four FPN structures used in TMM calculations is given in the introduction section of this chapter as well as in Fig. 4.3. The obtained reflectance spectra at different applied potentials for all four FPN structures under investigation using TMM are shown in Fig. 4.10.

At a potential of 0 V, the Au - (n-InSb) and Al - (n-InSb) structures predict perfect absorption at wavelengths of 602 nm and 480 nm, respectively. For the Au - (n-InAs) and Al - (n-InAs) structures, the corresponding wavelengths are 546 nm and 467 nm. By adjusting the thickness of the n-InSb and n-InAs layers in the structures, it is possible to shift the wavelengths of perfect absorption to longer wavelengths within the visible and infrared ranges. Application of a potential of 15 V to the structures results in spectral shifts of 47 nm, 37 nm, 33 nm, and 22 nm for the proposed Au - (n-InSb), Al - (n-InSb), Au - (n-InAs), and Al - (n-InAs) structures, respectively.

In the examined set of four structures, the Au - (n-InSb) combination produced the largest spectral shift. The use of Au as a reflective metal in FPNs caused a greater spectral shift compared to FPNs that employed Al. This effect can be attributed to the Fermi energy gap, also known as the flat-band potential,
Figure 4.10: Reflectance spectrum of (A) Au (100 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (17 nm), (B) Al (100 nm) - TiO$_2$ (12 nm) - (n-InSb) (20 nm) - Al (8 nm), (C) Au (100 nm) - TiO$_2$ (10 nm) - (n-InAs) (15 nm) - Au (15 nm), and (D) Al (100 nm) - TiO$_2$ (15 nm) - (n-InAs) (20 nm) - Al (8 nm) for 0, 5, 10, and 15 volts applied potential.
between the metal (Au or Al) and semiconductor (n-InSb or n-InAs) materials. The work-function of Au (5.1 eV) is higher than that of n-InSb (4.71 eV) and n-InAs (5.08 eV). As a result, at 0 V applied potential, the depletion of holes arises at the oxide-semiconductor interface to maintain a constant Fermi energy between the metal and semiconductor. This hole depletion is created by the lack of electrons in that region (see Figs. 4.7(A) and 4.7(C)). Applying a potential of 15 V to the gate metal (Au) results in a significant increase in the number of accumulated electrons in n-InSb and n-InAs semiconductors. Specifically, in n-InSb, the number of accumulated electrons increases by a factor ranging from $10^8$ to $10^{10}$, while in n-InAs, the increase is a factor of $10^6$ to $10^7$. (see Figs. 4.7(A) and 4.7(C)).

In FPNs that utilize Al (with a work-function of 4.28 eV) as the gate metal, the work-function difference between the metal and semiconductor is of the opposite sign to that of FPNs with Au as the gate metal. As a result, at 0V applied potential, the MOS structure generates a small accumulation of electrons at the oxide-semiconductor interface in order to maintain a constant Fermi energy. However, with the application of a positive potential to the gate metal, this accumulation increases by a factor of approximately $10^2$ in the first few nanometers of n-InSb and n-InAs (see Figs. 4.7(B) and 4.7(D)). Therefore, owing to the relatively greater change in electron concentration among the proposed structures, FPNs utilizing Au as the gate metal exhibit a higher spectral shift compared to those employing Al as the gate metal.
The limitation of the dynamic spectral shift, in either case, is determined by the potential limit, which is, in turn, determined by the breakdown voltage. It has been found that the breakdown strength of titanium dioxide is approximately $1.6 \times 10^7$ V/cm [174]. Based on this, the MOS architectures proposed can withstand 16-24 V. The breakdown voltage can be enhanced by increasing the thickness of the oxide layer. However, any variation in the thickness of the oxide layer can have an effect on the optical response of the FPN.

### 4.5 Experimental Realization

#### 4.5.1 Device Fabrication

Figure 4.11 provides a schematic of the fabricated MOSM FPN structure. This structure comprises a sequence of (n-InSb) and TiO$_2$ layers, sandwiched be-
tween Au as top and bottom layers. The bottom Au film, with its considerable thickness, effectively prevents light from reaching the substrate. During the device fabrication process, a 100 nm thick Au film was initially sputtered onto a microscope slide. This was accomplished using a Denton sputtering system, operating at 200 W DC power, an argon plasma pressure of 5 mTorr, a pre-deposition conditioning duration of 60 seconds, and a deposition time of 230 seconds. The deposition rate for the Au film was determined to be 0.43 nm per second, a measurement obtained using a Wyko NT1100 white light interferometer from Veeco. The Au deposited slide served as substrates for the subsequent deposition of a 10 nm thick TiO$_2$ layer, a 20 nm n-InSb layer, and a 17 nm thick top Au layer. The power settings, argon plasma pressure, and pre-sputtering times for TiO$_2$ layer was consistent with those used for Au deposition. For deposition of n-InSb layer, a custom made sputtering target with doping concentration of $1 \times 10^{18}$/cm$^3$ doping density was utilized. The sputtering power for n-InSb layer deposition was set to 200W RF with 4.85 m Torr argon pressure. The calibrated deposition rates for TiO$_2$ and n-InSb, as measured by the white light interferometer, were 0.03 nm per second and 0.17 nm per second, respectively.

4.5.2 Optical Characterization

The optical reflectivity of the sample within the visible spectrum was measured using a broadband halogen light source alongside an optical spectrometer (Ocean Optics Flame Miniature Spectrometer). A normal reflection/backscattering probe, supplied by Ocean Optics, was used to assess light
reflection at normal incidence from the structure. Dynamic tunability was examined by connecting a voltage supply to the top and bottom metal layers of the FPN with micromanipulators. A high resolution microscope was utilized to observer the placement of micromanipulator contact on the metal surface.

Figure 4.12 presents the reflectance spectra for the fabricated Au-TiO$_2$-(n-InSb)-Au FPN structure with 0V and 5V applied. A spectral shift of approximately 20 nm was noted upon applying a 5V gate voltage. The samples could not withstand voltages above 5V, with the deposition-related impurities in the TiO$_2$ layer being a significant limitation. A CIE1931 chromaticity diagram, generated by the Ocean Optics spectrometer, is shown in fig. 4.13 to illustrate the color change. The reflectance spectra reveal that the absorption at the resonance wavelength deviates from the simulation predictions, showing a redshift. This discrepancy is likely due to errors in deposition thickness. Measurements of each layer’s thickness by white light interferometer showed a deviation of ±2 nm from the targeted thicknesses.

4.6 Summary

This study describes the modeling, simulation and experimental realization of dynamically tunable optical absorbers utilizing n-doped InSb and InAs as epsilon-near-zero (ENZ) semiconductors. The absorber structure models consist of nano-scale metal and semiconductor layers arranged in a metal-oxide-semiconductor-metal (MOSM) configuration. The MOSM architecture bears similarities to an MOS capacitor, which is effective in obtaining electrical control over
Figure 4.12: Measured reflectance spectra for Au-(n-InSb)-TiO$_2$-Au FPN structure at 0 and 5 volts input voltage.
Figure 4.13: Measured CIE1931 chromaticity diagram for Au-(n-InSb)-TiO$_2$-Au FPN structure at 0 and 5 volts input voltage.
charge distribution in the semiconductor layer. Optically, the MOSM structure serves as a Fabry-Perot nanocavity (FPN) that enables wavelength-selective light absorption. The selection of appropriate materials and thicknesses for each layer in the MOSM configuration provides perfect narrowband light absorption in the visible region, which renders the optical absorbers useful as color filters. The MOSM configuration is voltage-controlled, where the application of voltage results in charge accumulation in the n-InSb and n-InAs layers, thereby regulating the dielectric constant. The accumulated sublayers of n-InSb and n-InAs lead to a variation in the refractive index, which affects the effective phase delay of the semiconductor spacer. Such a phenomenon results in a change in the FPNs’ resonance in the visible range. The electro-optical modeling and simulation predicted a spectral shift of up to 47 nm with an applied voltage of 15 V, provided the materials and layer thicknesses are optimized. For the experimental realization of the same a layer by layer deposited FPN consisting n-InSb as ENZ semiconductor was fabricated. This fabricated FPN structure sustained voltages up to 5 volts and exhibited a spectral shift of approximately 20 nm in the visible range. The degree of spectral shift in the absorbed color depends on both the applied voltage and the specific mix of metal and semiconductor materials used. The findings indicate that integrating an ENZ semiconductor within an MOSM configuration can enable a lithography-free, dynamically tunable, all-solid-state narrowband optical color filter.
Chapter 5. Silicon-enhanced Narrowband Color Reflectors to Broadband Absorbers: Modeling and Experimental Investigations

5.1 Preface

Part of this chapter is based on the following publication: Dixit, K. P., Houtman Z. B., and Gregory, D. A. “Reflective Color Filter Using Series Connection of Semiconductors in Asymmetric Fabry-Perot Nanocavity”. In Proceedings of 2023 IEEE Photonics Conference (IPC), pp. 1-2. IEEE, 2023. Adapted (or “reproduced in part”) with permission from IEEE.

5.2 Motivation

In recent years, nanostructured color filters have garnered significant attention owing to their compact design, superior performance relative to pigment-based color dyes, and high efficiency in terms of color reflection, transmission, and absorption [152, 125, 122, 126]. These devices may become crucial in the advancement of display technology, imaging, sensing, and photovoltaics [188, 189, 190, 191, 192, 193, 194, 195, 196]. Despite their impressive capabilities in these applications, certain structural and material constraints limit the full real-
ization of their potential. Additionally, the nano-patterning processes essential for their fabrication limit their scalability, particularly in the context of large-scale device production. To address these challenges, lithography-free planar structures have gained attention. Such structures typically employ a metal-insulator-metal (MIM) configuration, comprising plasmonic materials or specially designed metamaterials to modulate light reflection, transmission, or absorption. These MIM configurations resemble Fabry-Perot nanocavities, which are known for their spectrally selective color absorption and transmission properties [126, 125, 122]. Nanoscale color filters that couple the incident wave to the fundamental Fabry-Perot resonance mode have been a hot topic recently. Fabry-Perot nanocavities (FPN) that include a dielectric or semiconductor medium sandwiched between two reflecting metal surfaces are well-known architectures for color filters [121, 2, 153, 139]. One of the major reasons for the popularity of FPNs is the straightforward architecture that does not require special nanopatterning. This makes such architectures a great choice for nanoscale device applications where a large surface area is required, as in many sensing applications. Although FPNs are great contenders for color filter application their utility is in preventing a wavelength band from being reflected, while reflecting a non-resonant wavelength band. This property makes FPNs a great filter where red-green-blue (RGB) colors are required in transmission or subtractive colors such as cyan-magenta-yellow (CMY) are required in reflection. Thus, FPNs are also known as transmissive color filters rather than reflective ones. For the creation of FPN-based color filters, noble metals such as gold, silver, and aluminum are popular because they
provide high reflection and low absorption throughout the visible band. Such noble metals in combination with a dielectric spacer having low absorption can create perfect subwavelength transmissive color filters. Various approaches have been identified to develop color filters in reflection mode using the combination of Fabry-Perot cavities in a way that they complement each other [122], where the second cavity absorbs the light transmitted by the first cavity and the reflected result is just the wavelength band ignored by both cavities. While some approaches use a specific metamaterial layer in combination with noble metals and dielectrics to create reflective color filters [15, 126], most of these resemble an architecture where the substrate follows the metal-dielectric-metal configuration where both metals have different reflectivities and extinction coefficients. Such architectures are known as asymmetric Fabry-Perot nanocavities (AFPNs). In AFPN the top and bottom metals have different optical characteristics to make them complimentary reflectors and absorbers for different bands in the visible range. AFPN with a combination of lossy metals such as titanium (Ti), nickel (Ni), chromium (Cr), and tungsten (W) with noble metals such as gold (Au), silver (Ag), and aluminum (Al) are also useful in developing broadband absorbers [13, 15, 16, 39, 197]. Using lossy metals widens the absorption bandwidth.

In addition to color transmission and reflection-based devices, nanoscale devices can be useful for broadband absorption. These devices are useful in diverse fields: biomedical optics, antenna systems, thermal emitters, and thermal photovoltaics [39, 58, 59, 146]. The engineering of a broadband absorber is significantly different from a narrowband one. Nanoscale devices incorporating pat-
terned metallic gratings on dielectrics and plasmonic resonant structures have been explored for broadband absorption, but the scalability of such devices is limited by the required nanopatterning, particularly for large surface area applications. Consequently, AFPNs with an anti-reflection (AR) coating have emerged as a promising solution [14, 126]. In an AFPN, it is crucial that metals with specific optical properties be used. The AR coating plays a crucial role in this architecture. In some instances, AR coatings are engineered with a refractive index that lies between that of the surrounding medium and the Fabry-Perot nanocavity material. This gradation in the refractive index reduces the contrast in the refractive index at the interfaces, subsequently decreasing reflected light. AR coatings exploit interference effects, relying on destructive interference. These coatings are tailored to a thickness that is one-quarter of the wavelength of the targeted light transmission. When light reflects from the coating’s top surface and the interface between the coating and the cavity material, the out-of-phase nature of these reflections leads to destructive interference, effectively neutralizing the reflected waves and minimizing reflection. This determines the performance of AR coatings for enhancing the efficiency of broadband absorbers.

Considering the recent developments in MIM architecture-based color reflectors, the use of AFPN is very popular. Optimal material combinations for such devices have been identified, involving metals like platinum (Pt), bismuth (Bi), Ni, and Ti, paired with noble metals such as Au, Al, and Ag [126, 14, 153, 125]. These devices typically consist of two metal layers separated by a dielectric or semiconductor material such as silicon dioxide (SiO₂), lithium fluoride (LiF), aluminum
Figure 5.1: (A) Schematic diagram of Ti-SiO$_2$-Ag asymmetric Fabry-Perot nanocavity. (B) Contour plot of the visible reflectance spectra of Ti-SiO$_2$-Ag as a function of SiO$_2$ thickness, when the Ti thickness is set to 10 nm.

Shurvinton et al. explored an AFPN with Ag and Ti layers using SiO$_2$ as a spacer for achieving high-chroma color coatings in the visible [125]. Similarly, Park et al. conducted a study using Pt and Al with a TiO$_2$ spacer [126]. Both studies leveraged the resonance properties of the AFPNs to achieve color reflection. In the Ti-SiO$_2$-Ag structure, the reflection spectra in the visible range, as a function of the SiO$_2$ spacer thickness are illustrated in fig. 5.1 (B). The contour plot reveals that a thicker SiO$_2$ layer can accommodate multiple resonance wavelengths. This reduces the free spectral range between resonance wavelengths, as shown in fig. 5.2. These findings suggest that fabricating AFPNs with varied SiO$_2$ thicknesses can result in efficient reflection of RGB colors without the need for complex nanopatterning.
Figure 5.2: Reflectance spectra of Ti (10 nm) - SiO$_2$ (120 nm, 350 nm, and 215 nm) - Ag (100 nm) nanocavity structure for red, green, and blue peak reflectance wavelengths.

Figure 5.3: Reflectance spectra of Ti (10 nm) - SiO$_2$ (335 nm) - Ag (100 nm) for S-polarized incident wave at angles ($\theta$) = 0°, 20°, 40°, and 60°.
Figure 5.4: Reflectance spectra of Ti (10 nm) - SiO$_2$ (335 nm) - Ag (100 nm) for P-polarized incident wave at angles ($\theta$) = 0°, 20°, 40°, and 60°.

While the previous structure achieves high chroma color coating, the ratio of the SiO$_2$ thickness to the peak reflected wavelength is notably high. For the red spectrum, this ratio stands at approximately 1/3.3, 1/1.6 for green, and 1/3.75 for blue. This elevated ratio implies that effecting a substantial shift in the resonance wavelength requires a more substantial alteration in the thickness of the dielectric spacer. The utilization of SiO$_2$, a lossless material, contributes significantly to these elevated ratios. Previous studies on narrowband absorbers have shown that replacing the spacer with a relatively lossy material can substantially decrease the spacer thickness requirement. Additionally, such structures exhibit enhanced sensitivity to changes in spacer thickness.

The use of a lossless material like SiO$_2$ not only results in a high spacer thickness to peak wavelength ratio but also increases the structure’s sensitivity
to incident angles other than normal. Under oblique illumination, the extended optical path within the cavity induces a blue shift in the resonance wavelength, a phenomenon more pronounced in reflection mode due to the lengthier optical path of light. To address this issue, various methods have been explored. Achieving an angle-insensitive resonance response involves increasing the refractive index and reducing the cavity thickness. Incorporating a relatively lossy material, like a semiconductor as the cavity medium can alter the phase upon reflection at the metal-semiconductor or dielectric-semiconductor interface, allowing for Fabry-Perot resonance at the desired wavelength with thinner layers [121, 122]. This adjustment would result in a minimal optical path length difference between normal and oblique incident light. A caveat of this approach is light absorption by the cavity’s semiconductor layer, potentially diminishing the color filter’s efficiency. This effect is particularly significant at shorter wavelengths, where the semiconductor’s extinction coefficient ($\kappa$) is higher [121]. Therefore, substituting a lossless dielectric layer entirely with a lossy semiconductor may not be the preferred strategy.

In consideration of these factors, the present study introduces a planar, scalable, and lithography-free reflective color filter, demonstrating substantial efficiency in color reflection. The proposed architecture utilizes a Metal-Dielectric-Semiconductor-Dielectric-Metal (MDSDM) cavity structure. The layers of this cavity are sequentially composed of Ag as the bottom metal, SiO$_2$ as a dielectric layer, silicon (Si) as a semiconductor layer, SiO$_2$, and Ti as the top metal layer. The strategic placement of a Si layer, sandwiched between two SiO$_2$ lay-
ers, significantly reduces both the spacer thickness and the angle sensitivity of the reflector. Furthermore, the Si layer not only contributes to the effectiveness within the visible spectrum but also creates considerable broadband absorption in the near-infrared (NIR) range. This enhanced performance is attributed to the multilayer configuration of the three materials (Ag, Si, and Ti), each with distinct $\kappa$, effectively targeting regions of both the visible and NIR wavelength spectra. Silicon’s higher $\kappa$ at lower wavelengths attenuates these wavelengths, while titanium and silver suppress higher wavelengths [198, 199, 200]. The rationale behind choosing silicon as a spacer material is twofold. Firstly, silicon is one of the most abundant elements on earth, offering cost-effectiveness compared to other semiconductor materials. Secondly, the deposition of ultrathin silicon films uses established techniques, such as radio-frequency (RF) sputtering and chemical vapor deposition (CVD). There are no inherent optical constraints preventing the substitution of silicon with other materials that exhibit a similar trend in $\kappa$ values to provide an efficient reflection phase change at the dielectric-semiconductor interface for creating color reflectors.

5.3 Experimental and Simulation Methods

5.3.1 Device Fabrication

Figure 5.5 provides a schematic of the MDSDM asymmetric nanocavity structure. This structure comprises a sequence of $\text{SiO}_2$-$\text{Si}$-$\text{SiO}_2$ layers, sandwiched between a Ti layer on top and a substantially thick Ag film at the bottom. The
bottom Ag film, with its considerable thickness, effectively prevents light from reaching the substrate. During the device fabrication process, a 100 nm thick Ag film was initially sputtered onto six microscope slides. This was accomplished using a Denton sputtering system, operating at 200 W DC power, an argon plasma pressure of 5 mTorr, a pre-deposition conditioning duration of 60 seconds, and a deposition time of 556 seconds. The deposition rate for the Ag film was determined to be 0.51 nm per second, a measurement obtained using a Wyko NT1100 white light interferometer from Veeco. The Ag deposited slides served as substrates for the subsequent deposition of a 10 nm thick SiO$_2$ layer, a Si layer for 5 nm, 10 nm, and 20 nm, an 80 nm SiO$_2$ layer, and a 10 nm thick Ti layer, all applied onto three Ag-coated substrates. The remaining three substrates (slides) received
identical layering, with an additional 80 nm thick SiO$_2$ layer serving as an anti-reflection (AR) coating for exploration of the broadband absorption aspect of the presented AFPN. This resulted in a Metal-Dielectric-Semiconductor-Dielectric-Metal-Dielectric (MDSDMD) structure, specifically Ag (100 nm) - SiO$_2$ (10 nm) – Si (5 nm, 10 nm, and 20 nm) - SiO$_2$ (80 nm) – Ti (10 nm) - SiO$_2$ (80 nm). The power settings, argon plasma pressure, and pre-sputtering times for all layers except for Si were consistent with those used for Ag deposition. For Si the sputtering power was set to 200W RF with 4.85 m Torr argon pressure. The calibrated deposition rates for SiO$_2$, Si, and Ti, as measured by the white light interferometer, were 0.02 nm per second, 0.34 nm per second, and 0.15 nm per second, respectively.

5.3.2 Simulations and Measurements

The modeling of the MDSDM and MDSDMD structures was performed using the transfer matrix method (TMM) [108]. In addition to this modeling, optical simulations were conducted using commercial finite-difference-time-domain (FDTD) software, Ansys Lumerical FDTD [143]. These simulations were three-dimensional (3D) in nature. A plane-wave source was employed, spanning the desired wavelength range of 400–1600 nm. For the boundary conditions, periodic settings were applied in the lateral (x and y) directions, while the vertical (z) direction (AFPN thickness) was configured with a perfectly matched layer (PML) to effectively absorb outgoing waves and prevent reflections.
The optical reflectivity within the visible spectrum of the sample was experimentally measured using a broadband halogen light source in conjunction with an optical spectrometer (Ocean Optics Flame Miniature Spectrometer). For the assessment of normal incidence light reflection from the structure, a normal reflection/backscattering probe, also provided by Ocean Optics, was employed. In all of the measurements, the obtained reflection values are normalized with the reflection data from a thick Ag-coated sample. The real and imaginary parts of the refractive index of the SiO$_2$, Si, and Ti layers within the visible wavelength range were determined using a J.A. Woollam Alpha-SE Spectroscopic Ellipsometer. For the near-infrared wavelength range, the refractive index data for Ag, Si, and Ti thin films were obtained from the studies by Ciesielski et al. [200], Pierce et al. [198], and Palm et al. [199].

5.3.3 Structure Modeling

To achieve effective color reflectors and broadband absorbers, the selection of materials for each layer within the stack plays a crucial role. The application of the TMM modeling approach assists in determining the optimal thickness for each layer, thereby achieving the desired reflectance in the visible spectrum and broadband absorption in the near-infrared range. Chapter 3 of this dissertation provides an in-depth discussion of the mathematical formulation of the transfer matrix method.

In the present study, Ag and SiO$_2$ coatings are the chosen materials. Ag is preferred as the thick bottom reflector metal due to its high reflectivity in the
visible range, making it a suitable choice for developing a color reflector in reflection mode. SiO$_2$, characterized as a lossless material, enhances multiple beam reflections within the Fabry-Perot cavity which helps increase light absorption in the metal layers.

Above the SiO$_2$ coating, Si is introduced as the third layer as a material with a relatively higher extinction coefficient, especially when compared to SiO$_2$. As previously discussed, the higher extinction coefficient of Si in the lower range of visible wavelengths aids in suppressing reflectance within that spectral region. Additionally, the inclusion of Si reduces the angular sensitivity of incident waves by decreasing the overall spacer thickness (especially in the reflection mode). To mitigate a relatively higher reflection phase change at the metal-semiconductor (Ti-Si) interface, an SiO$_2$ layer is added atop the Si film. The uppermost layer consists of Ti to establish an asymmetric Fabry-Perot cavity. A schematic structure for the AFPN is presented in fig. 5.5.

The initial phase of the study involved calculating the round trip phase delay for the Ti-SiO$_2$-Si-SiO$_2$-Ag structure, targeting a reflection wavelength of 600 nm. The purpose was to fine-tune the thickness of the SiO$_2$-Si-SiO$_2$ combination to induce destructive interference at wavelengths outside the vicinity of 600 nm. Numerical simulations employing the TMM were utilised, incorporating the refractive indices for each layer. The thicknesses of the Ag, bottom SiO$_2$, top SiO$_2$, and Ti layers were fixed at 100 nm, 40 nm, 40 nm, and 10 nm respectively, while the Si layer’s thickness was varied to determine the optimal value. The reflection contour plot for varying Si thicknesses within the Ti-SiO$_2$-Si-SiO$_2$-Ag
Figure 5.6: The contour plots of the reflectance spectra for different (A) Ti thickness (B) Si thickness (C) top SiO₂ thickness, and (D) bottom SiO₂ thickness.

MDSDM cavity configuration is presented in fig. 5.6(B). It is evident that a minor alteration in Si thickness results in a significant shift in the peak reflection wavelength.

Variations in the Ti layer thickness (fig. 5.6(A)) demonstrates that while such adjustments do not significantly shift the peak reflected wavelength, they contribute to narrowing the bandwidth of the reflected spectrum, thereby enhancing color purity. The choice of Ti thickness must account for its absorptive
properties, ensuring the thickness does not exceed the metal’s optical penetration depth. Adjustments to the top SiO$_2$ layer thickness (fig. 5.6(C)) result in a notable shift in the peak reflected wavelength across the visible spectrum. However, alterations to the thickness of the bottom SiO$_2$ layer (fig. 5.6(D)) are less effective.

To develop a silicon-enhanced AFPN color reflector, the top Ti layer’s thickness was set at 10 nm. This parameter allows Ti to function as a layer with partial reflectivity and transmissivity and represents an optimal thickness for thin film deposition, avoiding the complexities associated with depositing ultra-thin nanofilms (3-7 nm). The top SiO$_2$ layer was assigned a thickness of 80 nm, achieving a narrow peak reflection band at greater thicknesses (fig. 5.6(C)). The bottom SiO$_2$ layer’s thickness was chosen to be 10 nm, selected for producing a narrow peak reflection band (fig. 5.6(D)). To achieve a spectral transition from blue to red, as illustrated in Figure 5.7, the thickness of the silicon layer was methodically varied between 5 nm and 25 nm, in increments of 5 nm. Figures 5.8, 5.9, 5.10, 5.11, 5.12 and 5.13 illustrate the modeled reflectance spectra for AFPNs under S and P polarized incident waves. These spectra are analyzed at incident angles of 20°, 40°, and 60°, corresponding to silicon thicknesses of 5, 15, and 25 nm, respectively. Comparing these figures with Figures 5.3 and 5.4, it becomes evident that the silicon-enhanced AFPNs have reduced sensitivity to the angle of incidence, as was anticipated.

Focusing on the near-infrared (NIR) spectrum, the implementation of silicon as a spacer medium in the cavity is observed to limit NIR wavelength re-
flection to below 30% for wavelengths up to 1600 nm. Figures 5.14(A) and (B) depict the reflectance and absorptance in the NIR region for the Ti-SiO\textsubscript{2} -Ag, Metal-Dielectric-Metal (MDM) cavity with 350 nm thick SiO\textsubscript{2} layer (represented as green in the RGB colour reflector) developed by Shurvinton et al. In Figure 5.14(B), the absorptance (A) is governed by the relationship A+R = 1-T, where R is reflectance and T is transmittance. Given that the cavity operates in reflection mode with zero transmittance, the relationship simplifies to A = 1-R. Figure 5.15 presents the R and A plots for the Ti-SiO\textsubscript{2} Si-SiO\textsubscript{2} -Ag cavity with Si at 15 nm, in the NIR range up to 1600 nm, respectively. The relationship between A and R is consistent with the previously mentioned cavity.

A cavity comprised solely of SiO\textsubscript{2} as the layer spacer extends resonance modes into the NIR range. In contrast, the SiO\textsubscript{2} -Si-SiO\textsubscript{2} cavity suppresses NIR range reflection more effectively. The layered arrangement of Ti, Si, and Ag is critical here, where the incorporation of a central Si layer bifurcates the cavity into Metal-Dielectric-Semiconductor (MDS) and Semiconductor-Dielectric-Metal (SDM) configurations. Treating these as separate entities, the Ti-SiO\textsubscript{2} -Si cavity decreases reflectance significantly, resulting in 30-50% absorption and 20-30% transmission for the Si-SiO\textsubscript{2} -Ag segment within the 800-1600 nm wavelength range. The power absorption for each layer of the Ti-SiO\textsubscript{2} -Si-SiO\textsubscript{2} -Ag cavity, computed using the Finite-Difference Time-Domain (FDTD) method, is shown in Figure 5.16. The Ti layer absorbs the most power, with the Si and Ag layers contributing to this effect, while SiO\textsubscript{2}, as a lossless material, does not absorb power in the range observed for the metal and semiconductor layers. Conse-
quently, the inclusion of Si in the cavity significantly reduces reflected light by enhancing absorption in the Ti-SiO$_2$-Si section, and transmits a reduced amount to the reflective Ag layer of the Si-SiO$_2$-Ag section, thereby creating a broadband absorber in the NIR range.

To further enhance absorption and extend the coverage across a broader range of the near-infrared (NIR) spectrum, an anti-reflective (AR) coating can be applied to the top of the Ti (10 nm) - SiO$_2$ (80 nm) - Si (15 nm) - SiO$_2$ (10 nm) - Ag (100 nm) AFPN structure. Suitable dielectric materials for the AR coating include SiO$_2$, aluminum oxide Al$_2$O$_3$, and zinc oxide (ZnO). In this research, SiO$_2$ was chosen for the AR coating to limit the number of different materials used in the single AR coated-AFPN structure. This AR coating reduces reflection by preventing direct air-to-metal contact, thereby minimizing the reflection phase shift at the air-metal interface caused by the significant refractive index gradient between air and metal. Additionally, an optimized thickness of the AR coating can lower reflectance by restricting the reflection of wavelengths that produce destructive interference due to round-trip phase delay at the air-dielectric boundary.

The AFPN structure serves not only as a broadband absorber in the NIR but also as a color reflector in the visible range. Therefore, determining the SiO$_2$ AR coating thickness should also take into account its influence on resonance modes within the visible spectrum. Figure 5.17(A) displays a reflectance contour plot for the Ti-SiO$_2$-Si-SiO$_2$-Ag AFPN with a 15 nm Si layer and varying top SiO$_2$ (AR coating) thicknesses. A thickness range of 70-90 nm for the AR coating
appears to be optimal for both color reflection and broadband absorption in the AFPN. As shown in Figure 5.17(B), the reflectance in certain NIR wavelength regions can be reduced significantly, approaching zero, so that the AR-coated AFPN is an effective broadband absorber in the NIR spectrum.

5.4 Results and Discussion

The device under discussion, shown in fig.5.5, is based on an asymmetric Fabry-Pérot (F-P) nanocavity (AFPN), incorporating a sequential arrangement of SiO₂-Si-SiO₂ layers, acting as a spacer, situated between Ag and Ti layers. Figure 5.18 is a picture of the prepared thin film samples for the intended color reflection and NIR absorption. A 100 nm thick Ag layer forms the base of the structure to ensure high reflection across the visible spectrum and prevent trans-
Figure 5.8: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (5 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for S-polarized incident wave.

Figure 5.9: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (5 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for P-polarized incident wave at various angles.
Figure 5.10: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (15 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for S-polarized incident wave.

Figure 5.11: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (15 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for P-polarized incident wave at various angles.
Figure 5.12: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (25 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for (A) S-polarized incident wave.

Figure 5.13: Reflectance spectra for Ti (10 nm)-SiO$_2$ (80 nm)-Si (25 nm)-SiO$_2$ (10 nm) - Ag (100 nm) for P-polarized incident wave at various angles.
Figure 5.14: (A) Reflectance and (B) Absorptance spectrum for Ti (10 nm) - SiO₂ (350 nm) - Ag (100 nm) AFPN for part of the NIR wavelength range.

Figure 5.15: Reflectance and Absorptance spectrum for Ti (10 nm) - SiO₂ (80 nm) - Si (15 nm) - SiO₂ (10 nm) - Ag (100 nm) AFPN for part of the NIR wavelength range.
Figure 5.16: Absorbed power contour plot for Ti (10 nm) - SiO$_2$ (80 nm) - Si (15 nm) - SiO$_2$ (10 nm) - Ag (100 nm) AFPN for part of the NIR wavelength range.

Figure 5.17: (A) Reflectance contour plot as a function of AR coating (SiO$_2$) thickness for AR coating - Ti (10 nm) - SiO$_2$ (80 nm) - Si (15 nm) - SiO$_2$ (10 nm) - Ag (100 nm) structure. (B) Reflectance spectra for AR coating (SiO$_2$) (80 nm) - Ti (10 nm) - SiO$_2$ (80 nm) - Si (15 nm) - SiO$_2$ (10 nm) - Ag (100 nm) AFPN for visible and NIR wavelength range.
mission through the device. The resonance wavelength of the F-P nanocavity is determined by the cavity’s thickness \((d)\), and the spectral response is fine-tuned by varying the Si layer’s thickness within the cavity: 5 nm, 10 nm, and 20 nm. The optical characteristics of the Metal-Dielectric-Semiconductor-Dielectric-Metal (MDSDM) stack were investigated by measuring reflection profiles at normal incidence, using a broadband halogen light source in conjunction with an Ocean Optics FLAME miniature spectrometer and a reflection/backscattering probe. Figure 5.19 provides a comparison between the experimentally measured reflectance spectra of the fabricated devices and the theoretical reflectance, computed using the transfer matrix method (TMM) at normal incidence for differently colored MDSDM samples. Here, slight variations are observed in the measured reflectance spectra compared to the calculated spectra. This indicates variations in the number density and damping factor within the silicon layer of the deposited samples compared to ideal calculations. As described in the simulation and measurement section, a planar, thick Ag layer serves as a reference for normalizing the measured reflectance spectra. These results demonstrate that the design concept, which relies on integrating a relatively lossy material within the cavity layer, can offer a straightforward, lithography-free route for creating efficient reflective RGB color filters. This architecture differs from other Fabry-Perot-based multilayer designs. While other designs absorb only a narrow frequency range and reflect the rest of the spectrum, this one serves as a narrowband reflective filter.

An important factor limiting the practical utility of a color filter is its angular response under various angles of incident light. Figures 5.20, 5.21, 5.22,
5.23, 5.24, and 5.25 illustrate the angular response of the fabricated thin film reflectors for S and P light polarizations, with incident angles $\theta = 20^\circ$, 40°, and 60°. For all samples, the peak position undergoes a blue shift for both polarizations. As the angle of incident light widens, leading to light refraction at different interfaces, the optical path lengthens, resulting in the expected blue shift for the samples when illuminated with angled light. In this planar configuration, varying Fresnel reflection coefficients for S and P polarizations result in predictable angular responses.

To evaluate the broadband response of the constructed sample in the near-infrared (NIR) region, a broadband visible to NIR light source was employed along with the Ocean Optics Flame NIR miniature spectrometer. Measurements were conducted exclusively at normal incidence and are depicted in fig. 5.19. The spectral range of the NIR spectrometer extends from 970 to 1640 nm, whereas the visible spectrometer spans 200 to 830 nm. This results in a data collection gap in the 830-970 nm wavelength range. However, this absence of data does not impact the research objectives, as the experimental investigation of fabricated AFPNs as color reflectors is limited to the 400-800 nm range, and the broadband NIR absorption is expected to be substantial within 900-1250 nm (as shown in figs. 5.15 and 5.17(B)). The experimental results agree well with the predicted response of the AFPN and the AR-coated AFPN in the NIR spectrum, as illustrated in fig. 5.26.
Figure 5.18: The optical image of the fabricated MDSDM designs operating in different wavelengths in the visible regime. In all samples, the bottom metal (Ag) layer thickness is 100 nm, bottom dielectric SiO$_2$ thickness is 10 nm, semiconductor (Si) thickness is 5 nm (blue film), 10 nm (green film), and 20 nm (orange film).

Figure 5.19: Comparison of measured reflectance spectra from the fabricated blue, green and orange colored devices with theoretically calculated reflectance using the TMM method.
Figure 5.20: Blue colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for S-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.

Figure 5.21: Blue colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for P-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.
Figure 5.22: Green colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for S-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.

Figure 5.23: Green colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for P-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.
Figure 5.24: Red colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for S-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.

Figure 5.25: Red colored filters under different incidence angles (i.e. 20°, 40°, and 60°) for P-polarization. In all samples, the reflection shows a blue shift for wider viewing angles.
5.5 Summary

This study investigates the unique optical response of an asymmetric Fabry-Perot nanocavity (AFPN), that incorporates a series of dielectric-semiconductor-dielectric layers as a spacer medium in the design of deep subwavelength resonant cavities. Employing a Transfer Matrix Method (TMM)-based modeling approach, the optical response of the nanocavity in both the visible and near-infrared (NIR) ranges was initially determined, focusing on the use of a semiconductor to augment the dielectric material in the cavity spacer. Unlike other designs that utilize dielectric materials as cavity spacers and have problems with low spectral shift sensitivity and high angular sensitivity issues, the inclusion of silicon within the cavity spacer noticeably enhances the spectral shift sensitivity to changes in Si thickness and significantly reduces the angu-
lar sensitivity of the color reflector compared to AFPNs using standard dielectric spacers. Furthermore, the structure was also predicted to function as a broadband absorber in the NIR range.

Numerical simulations were then conducted to identify optimal geometries for achieving peak performance. Characterization of the fabricated samples revealed that the Metal-Dielectric-Semiconductor-Dielectric-Metal (MDSDM) cavities exhibit both broadband absorption and narrowband color reflection. It was also observed that the spectral position of the reflection peak could be tuned by varying the thickness of the silicon layer. The planar structure demonstrated the ability to absorb over 80% of incident light in a broadband regime ranging from 800 nm to 1300 nm. This absorption can be extended up to 1600 nm with the addition of an anti-reflection coating less than 100 nm thick atop the AFPN.

In conclusion, the findings of this study offer a cost-effective method for creating planar nanoscale optical structures capable of serving as RGB color filters in reflection mode, while simultaneously acting as broadband absorbers in the NIR range. This dual functionality makes the design efficient for color filtering and sensing applications in the visible spectrum, as well as for photovoltaic and communication systems operating in the NIR wavelength range.

6.1 Preface

Part of this chapter is based on the following publication: Dixit, K. P., James, E. E., and Gregory, D. A. “Ultra-Broadband Visible to Near-Infrared Absorber Using Oxide-Coated Asymmetric Fabry-Perot Nanocavity.” In Laser Science (pp. JTu4A-46). Optica Publishing Group, 2023. Adapted (or “reproduced in part”) with permission from Optica Publishing Group.

6.2 Motivation

The confinement of light in subwavelength-thickness structures is an established technique for achieving highly efficient light absorption. This absorption can be tailored to specific optical applications, either narrowband or broadband. While narrow-band near-perfect absorption is easily achieved with highly reflective metal layers and a dielectric spacer forming a Fabry-Perot cavity [121, 139, 152]. Broadband absorption can be challenging as it is difficult to find any useful optical phenomenon that exists over a wide spectral range.
Thus, broadband absorption requires special considerations. Various approaches have been explored to develop broadband absorbers in visible, near-infrared (NIR), and mid-infrared (MIR) wavelength regions. These include plasmonic resonant structures [39, 201], multi-shape nano units [57], and metal-insulator-metal (MIM) structures incorporating lossy metals like titanium (Ti), tungsten (W), and nickel (Ni) [153, 3]. However, these designs only cover a limited portion of the visible or NIR spectrum. Furthermore, some designs heavily rely on electron beam lithography (EBL), limiting their applicability for large-area devices. To address this limitation, several planar MIM configurations have been proposed to minimize the dependency on EBL [197, 131]. The planar broadband absorber of the present investigation draws inspiration from the work by Dereshgi et al. and Zhong et al. [132, 197], which demonstrated near-unity broadband absorption in the visible spectrum using a multi-metal configuration. The studies showed that the use of (metal-insulator)_N (MIMI_N) multilayers with proper thicknesses can provide light absorption in a broad wavelength range. The absorption edge can be extended toward longer wavelengths by increasing the number of pairs. This design configuration does not require any nano patterning, which increases production feasibility. Following this basic design, several experimental techniques have been exploited to fabricate a perfect ultra-broadband absorber based on an MI multilayer. Different types of metal and insulators have been employed to attain ultra-broadband absorption using these multilayer stacks. Tungsten-Aluminum oxide (W-Al_2O_3) [202], tungsten-silicon oxide (W-SiO_2) [203], and nickel-silicon oxide (Ni-SiO_2) [130] are some examples of these
MI pairs that can be fabricated to obtain perfect broadband absorption. Incorporating metals with diverse extinction coefficients ($\kappa$ values) in the (MI)$_N$s creates absorption over a wide wavelength range. The study presented in this chapter employs a similar approach but with an altered structural layout. The fundamental principle of the devices presented here revolves around constructing an asymmetric Fabry-Perot nanocavity (AFPN), integrating metals that possess optimum extinction coefficients across the visible to near-infrared (NIR) spectrum.

This study proposes a simplified planar metal-dielectric-metal-dielectric (MDMD) configuration employing two metals with favorable optical properties for creating broadband near-perfect to perfect absorption in visible and NIR wavelength ranges. The physics and design of this proposed multi-metal structure are based on the different extinction coefficients ($\kappa$) for different metallic materials. The arrangement of these two metals (from moderate to high extinction coefficient) can create efficient absorption over the desired wavelength ranges. This is not surprising since an absorbing material with a moderate $\kappa$ value is the most suitable for structured perfect absorbers taking advantage of field penetration. Excessively large $\kappa$ value leads to reflections, while insufficient $\kappa$ value means low absorption [197, 130]. Most metallic materials have strong wavelength dispersion, so choosing a single metal for broadband absorption may be impossible.

6.3 Modeling Approach

Although, the basic cavity configuration seems simple, choosing the right combination of materials can be challenging since the cavity structure is nothing
but a dielectric-coated asymmetric Fabry-Perot nanocavity (a Fabry-Perot cavity with metals of different reflectivities). An asymmetric Fabry-Perot nanocavity (AFPN) is not only useful as a broadband absorber but also as a color reflector in the visible range, as discussed in Chapter 5 of this dissertation. Thus, finding the right combination of metals that provides broadband absorption requires parameter optimization in using the transfer matrix method (TMM). In this approach, the bottom metal and the dielectric layer are both fixed. Following a literature review regarding feasible metal-dielectric combinations for broadband absorption [2, 132, 197, 202, 203], the present research uses aluminum (Al) as the bottom metal and aluminum oxide (Al$_2$O$_3$) as a dielectric. Figure 6.1 shows the layer arrangement for modeling this structure.

Figure 6.1: Schematic representation of the MDM design used for the TMM model.
The bottom metal is thick (to avoid transmission of the light), the dielectric layer thickness is varied from 80-100 nm. A relatively thicker dielectric coating is used to establish a clear definition between the aluminum and the aluminum oxide layers. To determine the ideal top metal for the cavity, the transfer matrix method is utilized as described below. The TMM uses discrete propagation and transmission matrices to calculate a final transfer matrix (M), and the reflectance at a specific wavelength is determined by two of the transfer matrix elements. The propagation ($P_m$) and transmission ($D_m$) matrices are components of the TMM and can be written as:

$$P_m = \begin{bmatrix}
exp(i\phi_m) & 0 \\
0 & exp(-i\phi_m)
\end{bmatrix}, \text{ where } \phi_m = \frac{2\pi(n_m - i\kappa_m)d_m}{\lambda \cos \theta_t}.$$  \hspace{1cm} (6.1)

For P polarization,

$$D_m = \begin{bmatrix}
1 & 1 \\
(n_m - i\kappa_m)\cos \theta_m & -(n_m - i\kappa_m)\cos \theta_m
\end{bmatrix}, \hspace{1cm} (6.2)$$

and for S polarization,
Here, $m = 0, 1, 2, 3$ represents air, the top metal layer, the dielectric layer, and the bottom metal layer. $n_m$ and $\kappa_m$ are the real and imaginary parts of the effective refractive index, respectively, $\theta_m$ is the incident angle of light, $d_m$ is the layer thickness, and $\phi_m$ is the phase delay of the optical wave in layer $m$. To achieve optimal broadband absorption characteristics, a top metal layer thickness of 10 nm was selected. This choice assures optical penetration while also ensuring practical fabrication processes. Thickness values were set to 10 nm for the top unknown metal layer, 100 nm for the (Al$_2$O$_3$) layer, and 100 nm for the Al layer, respectively. The transfer matrix method (TMM) calculation used the refractive index ($n$) and extinction coefficient ($\kappa$) values from Palik’s data for the Al and (Al$_2$O$_3$) layers. However, for the top metal layer, a parameter range was used, varying the values of $n$ and $\kappa$ within the range of 0.01 to 7. This iterative approach was undertaken to generate a reflectance contour map for the range of $n$ and $\kappa$ values. The purpose of this analysis was to determine the optimal complex refractive index parameters for the top metal layer. Figure 6.2 shows the reflectance contour plot at 700 nm wavelength ($\lambda$) for different combinations of $n$ and $\kappa$ for the top metal layer. Similar calculations are also done for the 400-1000 nm range.
Figure 6.2: Contour plot showing the reflection value at the wavelength of 700 nm for a 10 nm thick top mental ideal material as a function of n and κ.

The reflectance contour plots identify an optimal range of n and κ to achieve less than 10% reflection throughout the 400-1000 nm wavelength range. The ideal range for n and κ values, calculated in this study, is illustrated in fig. 6.3. The shaded region denotes the preferred wavelength spectrum. The figure also compares these values to those of lossy metals like titanium (Ti), nickle (Ni), and chromium (Cr), reflective metals such as gold (Au) and aluminum (Al), and the semiconductor silicon (Si) [185, 199, 197, 198]. The n and κ values for Cr and Ti align closely with the shaded region indicating an ideal combination of n and κ that results in less than 10% reflection. This translates to more than 90% absorption over a wide wavelength range, according to the relation $A + R + T = 1$, where $A$ represents absorptance, $R$ is reflectance, and $T$ denotes transmittance.
Figure 6.3: Calculated $n$ and $\kappa$ values suitable for near perfect absorption for 10 nm top layer thickness in Ideal metal (10 nm) - Al$_2$O$_3$ (100 nm) - Al (100 nm).

In this context, the bottom metal layer is optically dense, preventing any light transmission, leading to $A = 1 - R$.

In this study, chromium (Cr) was selected as the top layer in the design of an AFPN for broadband absorption. To determine the optimal layer thicknesses for maximum absorption, the base layer of aluminum (Al) is fixed at a thickness of 100 nm, and a 100 nm thick Al$_2$O$_3$ spacer is used. The reflectance contour for the Cr - Al$_2$O$_3$ (100 nm) - Al (100 nm) assembly was calculated for Cr thicknesses ranging from 10 to 30 nm. Results are shown in fig. 6.4(B). The contour plot indicates that the cavity achieves maximum broadband absorption when the Cr layer is less than 15 nm thick.

Maintaining the 100 nm thickness for the Al layer and setting the Cr layer thickness at 10 nm, a reflectance contour for varying Al$_2$O$_3$ thicknesses was calculated to identify the optimum thickness for broadband absorption in both the visible and NIR (fig. 6.5(A)). With the aim of more than 90% absorption
over a broad wavelength range, the Cr (10 nm) - Al₂O₃ (100 nm) - Al (100 nm) is near-perfect, but does not provide complete absorption over the target wavelength range.

To enhance absorption, an anti-reflection (AR) coating, consisting of an oxide layer, was tried. This coating is intended to reduce the reflection phase change at the air-Cr interface and create destructive interference at certain wavelengths at the air-dielectric boundary [126]. Incorporating an Al₂O₃ AR coating with a thickness matching that of the dielectric spacer further reduces reflectance, as shown in fig. 6.5(B). With the addition of the AR coating, the structure functions as an oxide-coated AFPN. A schematic diagram is given in fig. 6.4(A).

Finally the calculated absorption spectrum for the oxide-coated asymmetric Fabry-Pérot nanocavity (AFPN) structure is presented. This section predicts the structure’s response for varying angles of incidence, accounting for both S and
P polarizations. The finite-difference-time-domain (FDTD) method is then used to calculate the absorbed power of the structure.

6.4 Results and Discussion

In the design of an oxide-coated AFPN, the integration of a high-extinction metal, Al, with the moderate-extinction coefficient metal, Cr, shows promising absorption over a broad spectrum, from the visible to the NIR, depending on the spacer thickness. To validate the theoretical predictions, numerical simulations were conducted using the Ansys Lumerical finite-difference-time-domain (FDTD) software. The absorption spectrum for the Cr (10 nm) - Al$_2$O$_3$ (100 nm) - Al (100 nm) configuration at a normal incident angle (covering the visible and part of the NIR spectrum) is illustrated in fig. 6.6(B). The absorption is broad, above 90% for some ranges. Absorption in the 400-500 nm wavelength range is not ideal compared to the rest of the spectrum. This is consistent with the calculated
refractive index \((n)\) and extinction coefficient \((\kappa)\) parameters shown in fig. 6.3, where the values for Cr do not closely match the ideal parameters in the 400-500 nm range. Despite achieving significantly higher absorption over a wider wavelength range (500-1400 nm), there is a potential for improving the absorption efficiency of this structure. With that goal an anti-reflection oxide coating is added over the Cr (10 nm) - Al\(_2\)O\(_3\) (100 nm) - Al (100 nm) configuration. The thickness of the AR coating is contained from the AR layer thickness contour calculated using the TMM method (fig. 6.5(B)). For an Al\(_2\)O\(_3\) AR coating thickness in the range 70-100 nm in the 500-1400 nm wavelength range, perfect absorption \((\geq 97\%)\) is possible in the wavelength range shown in fig. 6.7 (B). The addition of Al\(_2\)O\(_3\) as an AR coating increases the absorption efficiency of the structure over a broad wavelength range.

To achieve a broad wavelength coverage in the NIR, adjustments can be made to the thickness of both the dielectric spacer (Al\(_2\)O\(_3\)) and the anti-reflection (AR) coating. The metallic layer thickness can remain unchanged because the ultra-thin metal layer thickness is the key to field penetration and absorption in the periodic dielectric-metallic layered structure. By increasing these layers to a thickness of 150-200 nm, a redshift in the broadband absorption spectrum for normal incidence can be attained. The absorption spectrum for an Al\(_2\)O\(_3\) (170 nm) - Cr (10 nm) - Al\(_2\)O\(_3\) (170 nm) - Al (100 nm) structure in the 1000-2000 nm wavelength range is given in fig. 6.8(B). The increase in Al\(_2\)O\(_3\) thickness provides a significant redshift in the absorption spectrum while maintaining absorptance close to unity for a broad wavelength range.
The absorbed power profiles for two nanocavity configurations, Al₂O₃ (100 nm) - Cr (10 nm) - Al₂O₃ (100 nm) - Al (100 nm) and Al₂O₃ (170 nm) - Cr (10 nm) - Al₂O₃ (170 nm) - Al (100 nm), were modeled with the FDTD software. These profiles, covering wavelength ranges of 400-1400 nm and 1000-2000 nm, respectively, are displayed in fig. 6.9. An analysis of the figure indicates that the Cr layer acts as the principal power absorber in this nanocavity structure. The Al layer also plays a role in absorbing power to a certain extent. The choice of a material with a moderate extinction coefficient, such as Cr, is critical in this context. Employing materials with higher extinction coefficients, like Al or Au, as the top layer is less effective for broadband absorption. They reflect more light, even when applied as ultra-thin films.

Constructing an AFPN with ultra-thin layers of high-extinction metals requires advanced deposition techniques like atomic layer deposition (ALD) or molecular beam epitaxy (MBE), especially for thicknesses below 5 nm. Standard methods such as e-gun evaporation or sputtering are not practical for such minute thicknesses. Conversely, materials like Cr, Ni, or Ti, which possess moderate extinction coefficients, offer lower reflectance and easier penetration of the electromagnetic field through the films. As shown in fig. 6.9, a Cr layer with a thickness of 10 nm efficiently absorbs power, more than the bottom Al layer. Furthermore, depositing a 10 nm thick metal layer using sputtering is a feasible and practical approach.

Figures 6.10 and 6.11 illustrate the spectral absorbance as a function of wavelength for the proposed cavities, designed to operate in the visible-NIR and
Figure 6.6: (A) Schematic diagram of Cr-Al$_2$O$_3$-Al AFPN for visible to NIR broadband application. (B) Absorption spectrum for Cr (10 nm) - Al$_2$O$_3$ (100 nm) - Al (100 nm) nanostructure at normal incidence.

Figure 6.7: (A) Schematic diagram of Al$_2$O$_3$-Cr-Al$_2$O$_3$-Al AFPN for visible to NIR broadband application. (B) Absorption spectrum for Al$_2$O$_3$ (100 nm) - Cr (10 nm) - Al$_2$O$_3$ (100 nm) - Al (100 nm) nanostructure at normal incidence.
Figure 6.8: (A) Schematic diagram of Al₂O₃-Cr-Al₂O₃-Al AFPN for NIR broadband application. (B) Absorption spectrum for Al₂O₃ (170 nm) - Cr (10 nm) - Al₂O₃ (170 nm) - Al (100 nm) nanostructure at normal incidence.

Figure 6.9: Absorbed power contour for (A) Al₂O₃ (100 nm) - Cr (10 nm) - Al₂O₃ (100 nm) - Al (100 nm) and (B) Al₂O₃ (170 nm) - Cr (10 nm) - Al₂O₃ (170 nm) - Al (100 nm) nanostructures.
NIR regions, respectively, for oblique incidence angles. High broadband absorption is maintained even at large incident angles. However, there is a noticeable decrease in absorptance, ranging between 0.8 and 0.9, for an incidence angle of 60° for both S and P polarization.

The minimal reduction in absorbance at oblique angles is attributed to the fact that high broadband absorption is principally due to field penetration and absorption in ultra-thin metal films. This effect is not significantly altered by changes in the incident angle, resulting in consistently high absorption across broad angles. The slight reduction in absorption at larger incident angles is due to the increased effective path length of photons in the metal-dielectric multilayer structure, leading to an effectively greater perceived metal thickness.

In conclusion, adopting a modeling approach that identifies the optimal range of refractive index (n) and extinction coefficient (κ) is crucial for achieving the targeted absorptance. This study further highlights the necessity of using materials with low to moderate extinction coefficients as the top metal layer in nanocavity designs. Such materials allow field penetration and extended absorption across a broader wavelength range, thereby creating an effective asymmetric Fabry-Pérot nanocavity. The use of an anti-reflection coating can also elevate the absorptance, nearing complete absorption, which makes them useful as nanoscale broadband absorbers.
Figure 6.10: Absorption spectra for $\text{Al}_2\text{O}_3$ (100 nm) - Cr (10 nm) - $\text{Al}_2\text{O}_3$ (100 nm) - Al (100 nm) structure at different incident angles for (A) S-polarization and (B) P-polarization.

Figure 6.11: Absorption spectra for $\text{Al}_2\text{O}_3$ (170 nm) - Cr (10 nm) - $\text{Al}_2\text{O}_3$ (170 nm) - Al (100 nm) structure at different incident angles for (A) S-polarization and (B) P-polarization.
6.5 Summary

In this study, a planar nanoscale broadband absorber is introduced, based on an asymmetric Fabry-Perot nanocavity design. This approach is advantageous due to its lithography-free and etching-free fabrication, facilitating scalability in both device fabrication and wavelength. The transfer matrix method is employed for parameter optimization to identify the ideal refractive index ranges (real and imaginary parts) for developing these absorbers for various wavelength ranges. Additionally, the proposed broadband absorber structure provides more than 80% absorption for oblique angle incidences up to 60 degrees. Numerical analysis indicates that combining a high-extinction coefficient metal at the bottom layer with a moderate-extinction coefficient metal at the top enhances broadband absorption. Traditional high-extinction metals like gold (Au), silver (Ag), or aluminum (Al) tend to reflect excessively, even at minimal thicknesses. Conversely, chromium (Cr), a moderate-extinction coefficient material, reduces reflection and increases field penetration, thereby extending absorption across a broader wavelength spectrum. Finite-difference-time-domain (FDTD) simulations support the numerical findings, confirming the absorptive efficiency of the proposed Cr-Al$_2$O$_3$-Al structure. This structure achieves over 90% absorption in the 600-1400 nm range, which can be shifted to longer wavelengths in the near-infrared spectrum by increasing the thickness of the Al$_2$O$_3$ dielectric spacer. To further boost absorption near 100%, an anti-reflective oxide coating can be applied atop the asymmetric Fabry-Perot nanocavity. The resultant Al$_2$O$_3$-Cr-Al$_2$O$_3$-Al configuration shows
more than 95% absorption across a wide wavelength range. The straightforward, lithography-free design of this broadband absorber makes it an attractive candidate for thermal photovoltaic applications where high absorption over large areas is essential.
Chapter 7. Analysis of Sensitivity in Fabry-Perot Nanocavities: Impacts of Layer Refractive Index and Thickness on Optical Reflectance Spectrum

7.1 Preface

Fabry-Perot nanocavities (FPN) are key elements in the field of nanophotonics, essential in creating a variety of optical devices. These structures are miniature versions of the classical Fabry-Perot interferometer, characterized by their ability to produce distinct interference patterns through multiple reflections between two parallel, highly reflective surfaces. Unlike their macroscopic counterparts, the reflective boundaries in nanocavities are made up of metal layers having high reflectivities or Bragg reflectors, scaled to nanometric dimensions. This miniaturization enables the confinement of light within volumes much smaller than the wavelength of light. The operational principle of FPNs centers on optical resonance. This phenomenon occurs when light of specific wavelengths constructively interferes after bouncing back and forth within the cavity, creating standing wave patterns. The wavelengths that experience resonance are directly related to the cavity’s physical length and the refractive index of the material.
within, satisfying the resonance condition [108]:

\[ d = \frac{m \lambda}{2n \cos \theta}. \]  (7.1)

Here, \( d \) denotes the physical cavity length, \( m \) is an integer representing the mode number, \( \lambda \) is the wavelength of light in vacuum, and \( n \) is the effective refractive index of the medium inside the cavity. The resonance wavelength condition is usually obtained in the transmission mode. However, if an FPN is set up with a semi-transparent metal layer and a second, optically thick metal layer, it does not allow any light pass through; it has zero transmittance. In this case, the FPN reflects light instead of transmitting it. The wavelengths of light that do not reflect, but instead get fully absorbed, are the resonant wavelengths in this context. The formula to determine which wavelengths will undergo this destructive interference is as follows [108]:

\[ d = \frac{(m + 1/2) \lambda}{2n \cos \theta}. \]  (7.2)

The condition \((m+1/2)\) accounts for the phase shift that leads to destructive interference, as it ensures that the path difference between interfering waves corresponds to an odd multiple of half the wavelength. This formula is crucial for designing FP nanocavities intended to operate as reflective filters or perhaps sensors, allowing for precise control over which wavelengths are reflected and which are absorbed or otherwise not transmitted, based on the cavity’s specific design and material composition. This resonant behavior employed in devices like lasers, sensors, and optical filters engineered on the nanoscale. By adjusting the length
of the cavity and the materials used, it is possible to control which wavelengths of light are enhanced or suppressed. The refractive index of each layer in an FPN, the real and imaginary parts, determines the cavity’s optical behavior. The real part of the refractive index dictates the phase change upon reflection. The imaginary part relates to material absorption. Both determine the transmission and reflection characteristics of the cavity. The thickness of these layers is equally important, as it directly impacts resonance conditions and the constructive or destructive interference of light waves.

Palik’s database is widely recognized for its value in optical modeling [45]. However, its applicability is limited when dealing with ultrathin films, particularly those less than a few tens of nanometers in thickness. This is because of the (extensively recorded) effect that the thickness of the film has on its optical properties. It has been established through various studies that the optical properties of thin films, especially those made of noble metals and semiconductors, are strongly influenced by their thickness. Research by Liang et al. shows a significant relationship between film thickness and optical constants in absorbing metal materials [204]. Gong et al. confirms that the optical properties of silver (Ag) films vary with thickness [205]. Nakamura et al. discovered that the optical dielectric constant of silicon (Si) ultrathin films approaches the experimental bulk value as the film thickness increases [206]. Jolivet et al. found a significant correlation between the optical properties of titanium dioxide (TiO₂) thin films and (both) the deposition temperature and substrate type [207]. Yakubovsky et al. conducted an extensive experimental investigation into the optical and electrical
characteristics of thin polycrystalline gold (Au) films across a thickness range of 20 to 200 nm, revealing that the dielectric function of the metal is influenced by its structural morphology and that this can significantly vary with thickness, even when films are produced under identical conditions [208]. Figures 7.1 and 7.2 provide the n and \( \kappa \) data, respectively, obtained by Yakubovsky et al. for different thicknesses of Au films deposited using electron-beam evaporation.

These findings pose a significant challenge for modeling nanoscale optical devices. Simulations based on Palik’s data for bulk materials often diverge from experimental investigations using thin films. This discrepancy is particularly seen when modeling multilayer structures such as Fabry-Perot nanocavities (FPNs), where the optical performance depends on a delicate balance of refractive index, extinction coefficient, layer thickness, and incident angle. Even minor variations in layer thickness at the nanoscale can lead to significant changes in the overall optical response of an FPN. This makes it essential to precisely understand how layer thickness affects reflection or transmission through the FPNs.

In this context, optical tolerancing of FPN using a sensitivity analysis becomes a powerful tool, offering a quantitative understanding of how slight variations in optical and structural parameters affect the device’s performance. These studies are essential for optimizing cavity design, especially for applications requiring precise control over the spectral characteristics of light, as in narrow-band filtering.
Figure 7.1: Measured real part of the refractive index (n) for different thicknesses of gold (Au) films deposited by the same method by Yakubovsky et al.
Figure 7.2: Measured imaginary part of the refractive index ($\kappa$) for different thicknesses of gold (Au) films deposited by the same method by Yakubovsky et al.
7.2 Theory of Optical Tolerancing in Fabry-Perot Nanocavities

Optical tolerancing refers to defining acceptable limits for a device’s physical and optical parameters, ensuring its performance remains within specified boundaries despite variations in manufacturing [209]. In the context of FPNs, these parameters include dimensions like the physical length of the cavity (to determine the resonance condition), the physical thickness of each layer involved in fabricating an FPN, and the refractive index of materials. This concept is crucial in nanophotonics, where precise control over parameters like layer thickness and refractive index is essential for achieving intended optical behaviour. In the context of FPNs, optical tolerancing is particularly significant for maintaining the device’s operational limits. Variations in layer thickness or refractive index will lead to deviations in resonant wavelengths, reflectance, and transmittance, directly impacting the device’s usefulness in fields such as telecommunications and quantum computing [139, 119, 2].

To address these challenges, this research employs a sensitivity analysis using Monte Carlo simulation and the law of large numbers [210]. This approach quantitatively assesses how uncertainties in the FPN’s parameters, specifically errors in the refractive indices or layer thickness, affect the device’s reflectance. The analysis uses the transfer matrix method (TMM) for modeling the optical behavior of the FPN. TMM provides a framework for calculating the light transmission and reflection through the layered structures (multiple reflections and transmissions at each interface).
The Monte Carlo method, useful to handle complex systems with multiple uncertain variables, is applied to perform the sensitivity analysis. By generating a large number of random variations in the refractive indices and layer thicknesses within specified tolerance ranges, the method simulates a wide array of possible manufacturing outcomes. This method uses randomness to explore how changes in the refractive indices and layer thicknesses might affect the FPN’s performance, offering insights into the device’s sensitivity to fabrication errors. The following section provides details on the modeling approach.

7.3 Modeling Approach

The objective of this analysis is to evaluate how variations in the physical and optical properties of each layer within FPNs affect their reflectance across the wavelength range of 400 to 1000 nm. The approach is detailed as follows:

Defining the Wavelength Range and Step Size
The analysis covers a wavelength range from 400 nm to 1000 nm, with a step size of 5 nm. This selection ensures comprehensive coverage across the visible to near-infrared spectrum.

Variable Specification for Each Layer
For each layer in the FPNs, three variables are critical:
1) Layer thickness (d),
2) Real part of the refractive index (n), and
3) Extinction coefficient (κ).
At each wavelength step, these variables are considered to potentially vary,
reflecting the inherent uncertainties in the fabrication process.

**Error Boundary Setting**

An error boundary percentage is manually defined for each of the three variables across all layers. This boundary specifies the acceptable range of variation from the actual value, establishing upper and lower limits for the generation of random samples.

**Generation of Random Samples**

Utilizing the defined error boundaries, a pool of 1000 random sample values is generated for each variable of every layer. This pool represents the potential variations in layer thickness, refractive index, and extinction coefficient that could arise during manufacturing.

**Reflectance Calculation Using TMM**

TMM is then applied to calculate the reflectance spectra of the FPNs. For this purpose, the method uses the pools generated random numbers as inputs. This calculation is performed 1000 times (iterations) for each wavelength step, incorporating the different combinations of sample values for the layer properties.

**Statistical Analysis of Reflectance Data**

From the 1000 iterations of reflectance calculations at each wavelength step, the mean reflectance value is determined, along with an error margin that reflects the variability observed across the iterations. This error margin provides insight into the sensitivity of the FPN’s optical performance to the variations in layer properties.
Here, all the above-mentioned steps are performed for Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN structure. The structural parameters, refractive indices, and reflectance spectrum of this FPN are discussed in detail in Chapter 4 of this dissertation. In the Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) structure, the resonance wavelength with measured $n$, $\kappa$, and the thickness values of each layer of the fabricated samples is $\sim$600 nm. This FPN behaves as a narrowband color filter and the resonance wavelength of this structure heavily depends on the thickness and refractive index of the cavity medium. Here the combination of TiO$_2$ and (n-InSb) works as the cavity medium. Table 7.1 provides the error % used for each layer’s thickness and refractive indices.

If a variation of $\pm 5$ nm in layer thickness (d) results in a variation of $\pm 0.05$ in both the $n$ and $\kappa$ values for each layer (as observed in several studies [205, 207, 208]), this can be expressed as a percentage error based on the actual values of $n$ and $\kappa$. For metals like Au and Ag, the $n$ remains below 1 across a wide range in the visible and NIR spectra, while the $\kappa$ typically falls within the range of 2 to 7 [200, 208]. Therefore, a variation of 0.05 in the $n$ value represents a significantly high percentage error, whereas the same variation equates to a 5% error for $\kappa$ values due to their inherently large magnitudes. However, in lossless materials such as SiO$_2$, and semiconductors like TiO$_2$, Si, and n-InSb, the $n$ values are comparatively higher than the $\kappa$ values [211, 198, 139], resulting in a higher percentage error for $n$ and a lower percentage error for $\kappa$ for a variation of 0.05.
Table 7.1: Utilized n, κ, and d value error % for each layer of Au (17 nm) - TiO\textsubscript{2} (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN structure to calculate reflectance (R) error.

<table>
<thead>
<tr>
<th>Layer</th>
<th>n error % (±0.05)</th>
<th>κ error % (±0.05)</th>
<th>d error % (±5 nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au (17 nm)</td>
<td>15%</td>
<td>5%</td>
<td>35%</td>
</tr>
<tr>
<td>TiO\textsubscript{2} (10 nm)</td>
<td>5%</td>
<td>15%</td>
<td>50%</td>
</tr>
<tr>
<td>n-InSb (20 nm)</td>
<td>5%</td>
<td>15%</td>
<td>25%</td>
</tr>
<tr>
<td>Au (100 nm)</td>
<td>15%</td>
<td>5%</td>
<td>5%</td>
</tr>
</tbody>
</table>

These percentage errors help establish the boundaries for generating a list of random values for n, κ, and d. For instance, the n value of Au at 630 nm is reported as 0.324 for a 9 nm thin film [208]. Due to the deposition thickness error of ±5 nm, a variation of ±0.05 can be expected in the n value. This translates to a ±15% error in the n value. This yields a range of 0.274 to 0.374 with an actual value of 0.324 as the center value for generating 1000 random samples as inputs for the n-value of the gold layer across multiple iterations of TMM. The similar process is repeated for appropriate error % of κ, and d for the Au layer.

An error of 15% may seem relatively high compared to a 5% error, but when considering the absolute values of n and κ for the specific material, it doesn’t appear to be significantly large. For visualizing the error range for data sampling, Figures 7.3, 7.5, and 7.6 show the actual n values used from the dataset of Au, TiO\textsubscript{2}, and n-InSb thin films [208, 187, 139], with respective error margins of 15%, 5%, and 5%, as mentioned in Table 7.1. Figure 7.4 shows the actual κ value used from the dataset of Au with error margins of 5%. The κ value and errors of the
Figure 7.3: The real part of the refractive index (n) for Au thin film with a 15% error margin from the actual value.

TiO$_2$ and n-InSb layers are not presented as they are very close to zero for the 400 - 1000 nm wavelength range.

Figure 7.7 presents the calculated reflectance spectra for Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN structure by TMM method, presenting narrowband absorption. The reflectance spectrum is obtained for the 400 - 1000 nm wavelength range with a wavelength step size of 5 nm. The resonance wavelength is 590 nm.

7.4 Sensitivity Analysis With Inclusion of Errors

In a symmetric Fabry-Perot nanocavity, like the Au (17 nm) - TiO$_2$ (10 nm) - n-InSb (20 nm) - Au (100 nm) structure, the resonance response significantly
Figure 7.4: The imaginary part of the refractive index ($\kappa$) for Au thin film with a 5% error margin from the actual value.

Figure 7.5: The real part of the refractive index (n) for TiO$_2$ thin film with a 5% error margin from the actual value.
Figure 7.6: The real part of the refractive index (n) for n-InSb thin film with a 5% error margin from the actual value.

depends on the optical parameters and physical thickness of the cavity or spacer material, as discussed in chapters 2 and 4. The phase shift caused by the cavity material is crucial in determining the resonance wavelength. In this specific cavity, the combination of TiO$_2$ and n-InSb acts as the cavity spacer. Therefore, changes in the optical parameters or thickness of these materials are expected to notably influence the resonant band, while having a minimal impact on the nonresonant band. Conversely, the metal layers contribute to the reflection phase shift, an important factor, but their influence on the resonance band is less pronounced compared to the cavity layers.

To validate this, initially, the refractive index and thickness errors for both Au layers were assumed to be zero, focusing solely on the errors in the cavity layer
Figure 7.7: Calculated Reflectance spectrum of Au (17 nm) - TiO\textsubscript{2} (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN structure by TMM without error consideration.
parameters as listed in table 7.1. The impact of these errors on the reflectance spectrum of the Au (17 nm) - TiO₂ (10 nm) - n-InSb (20 nm) - Au (100 nm) structure is shown in fig. 7.8. A significant standard deviation in the reflectance values was observed in the resonance band, indicating that errors in the cavity layer parameters notably affect this band. In contrast, the nonresonant band’s reflectance response showed minimal change due to these errors.

In the second scenario, errors were set to zero for the cavity layers, while errors in the parameters of both Au layers were introduced. The resulting standard deviation in the reflectance spectra, as depicted in fig. 7.9, were not as significant as those caused by errors in the cavity layers. Although metal layers are essential for defining the resonance band by inducing a reflection phase shift, only a slight variation in absorption at the resonance wavelength was noted. This underscores the predominant role of the cavity layers in determining the resonant behavior of the structure. Figure 7.10 displays the reflectance spectrum, including the standard deviation resulting from variations in the optical parameters and thicknesses of all layers in the cavity. The magnitude of the standard deviation is comparable to that caused solely by variations in the cavity layers’ parameters. This indicates that introducing errors in the metal layers, along with errors in the cavity layer, does not substantially impact the nanocavity’s optical performance. Instead, the cavity layer has the most significant role in determining the optical characteristics of the Fabry-Perot nanocavity.

Here, it is noted that even a slight error in deposition thickness, such as 5 nm, can lead to approximately a 5% variation in the perfect absorption at
**Figure 7.8:** Calculated reflectance spectrum of Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN incorporating cavity layer errors.
Figure 7.9: Calculated reflectance spectrum of Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN incorporating metal layer errors.
Figure 7.10: Calculated reflectance spectrum of Au (17 nm) - TiO$_2$ (10 nm) - (n-InSb) (20 nm) - Au (100 nm) FPN incorporating errors in all layers.
the resonant wavelength. While a 5% change in absorption might appear minor, in applications requiring complete absorption of a specific wavelength, this 5% reflection can significantly reduce the device’s overall efficiency. Therefore, it is crucial during the fabrication of a Fabry-Perot nanocavity to deposit each layer, particularly the cavity layer, with precise thickness control. Additionally, when modeling the photonics of such resonance-based devices, relying on optical constants derived from bulk materials is not advisable, as these do not accurately reflect the device’s performance at the nanoscale.

7.5 Summary

This study has investigated how cavity layer properties (such as the refractive index’s real and imaginary parts and thickness) affect the optical performance of Fabry-Perot nanocavities (FPNs). This highlights the challenges of using Palik’s database for simulating nanoscale devices. This database relies on bulk materials and does not account for the effects of film thickness on optical properties. Several studies have shown that the optical characteristics of thin films, particularly those composed of noble metals and semiconductors, vary significantly according to thickness. This variation presents a challenge in designing FPNs incorporating these materials. While a deposition error resulting in a thickness variation of 5-10 nm might seem minor at a larger scale, such discrepancies can alter the optical characteristics of ultrathin layers in FPNs. To quantify the impact of thickness variations on device performance, this study uses a Monte Carlo simulation in reflectance calculations via the transfer matrix. By comparing results
from studies showing the dependence of refractive indices on film thickness, an error margin for each layer parameter of a metal-oxide-semiconductor-metal FPN structure was established. This method generates data sets for optical parameters and layer thicknesses that reflect thickness variation’s effects on thin films’ optical properties, leading to more realistic modeling. The findings indicate that a deposition thickness error as low as 5 nm in the oxide and semiconductor layers of the nanocavity can seriously affect the resonance wavelength’s absorption. The present study highlights the importance of using optical parameters that represent the properties of amorphous or polycrystalline thin films for more accurate estimations of resonance-based nanoscale optical devices. Future research could explore the effects of variations in charge density (N) and damping factor (γ) within doped semiconductor or metal layers on the overall reflectance spectrum.
Chapter 8. Conclusions and Future Work

In this research, Fabry-Perot nanocavities as color filters and perfect absorbers have been explored for narrow-band and broadband applications. The first of these included the modeling and experimental realization of a dynamically tunable Fabry-Perot nanocavity as a narrowband color filter incorporating epsilon-near-zero (ENZ) semiconductors as active layers in the cavity. The modeling outlined the development of dynamically tunable optical absorbers that use n-doped InSb and InAs as materials with epsilon-near-zero (ENZ) properties. These absorbers were engineered by arranging nano-scale metal and semiconductor layers in a metal-oxide-semiconductor-metal (MOSM) configuration conceptually similar to an MOS capacitor. This design enabled electrical modulation of charge distribution within the semiconductor layer. From an optical standpoint, the MOSM structure functioned as a Fabry-Perot nanocavity (FPN), allowing for selective light absorption at specific wavelengths. The selection of materials and layer thicknesses within the MOSM framework allowed narrowband absorption in the visible spectrum, making these devices suitable for color filters.

In the MOSM configuration, an application of voltage causes charge accumulation in the n-InSb and n-InAs layers, changing the dielectric constant. This charge accumulation results in changes in the refractive index of the semicon-
ductor layer, changing the effective phase delay, which leads to changes in the
FPN resonance within the visible spectrum. The electro-optical analysis indi-
cated that, with the right choice of materials and layer dimensions, the MOSM
structure could achieve a reversible spectral shift of up to 47 nm with an applied
potential of 15 V. This shift in the absorption wavelength, affecting the observed
color, was found to be a function of the applied voltage and the specific metal-
semiconductor material combinations. The four MOSM configurations studied
exhibited spectral shifts ranging from 22 to 47 nm. One of the four modeled FPN
structures was built. An FPN consisting of gold layers as reflective metal layers,
with titanium dioxide and n-type doped indium antimonide as the cavity spacer
materials was deposited on a glass substrate using RF/DC sputtering. The fab-
ricated FPN configuration withstood up to 5 volts and displayed a spectral shift
of about 20 nm within the visible spectrum. This suggests that incorporating an
ENZ semiconductor into an MOSM setup could create a lithography-free, dynam-
ically tunable, all-solid-state narrowband optical color filter. These dynamically
tunable narrowband perfect absorbers have applications in optical communica-
tions, sensors, dynamic display technology, and stealth technology. The results of
this study have been published in Discover Nano, vol. 18, pp. 100 (2023).

The second topic in this research involved a lithography-free approach
for developing planar nanoscale optical devices that function as red-green-blue
(RGB) color filters in reflection mode and as broadband absorbers in the near
infrared. The research took advantage of the distinctive optical behavior of
an asymmetric Fabry-Perot nanocavity (AFPN), that integrated a sequence of
dielectric-semiconductor-dielectric (DSD) layers as spacers in creating ultra-thin resonant cavities. Using a Transfer Matrix Method (TMM) for modeling, the study first evaluated the nanocavity’s optical performance across the visible and near-infrared, highlighting the role of a semiconductor as the cavity’s spacer. In contrast to conventional designs using dielectric spacers with low spectral sensitivities and high angle sensitivity, the addition of silicon as the spacer enhanced the sensitivity to changes in thickness. This modification also decreased the angle sensitivity of the color reflector compared to AFPNs that employ standard dielectric spacers. This structure was predicted to act as a broadband absorber in the near infrared.

Optical characterization of the fabricated samples showed that the metal-dielectric-semiconductor-dielectric-metal (MDSDM) cavities could achieve both wide-range absorption and narrow-range color reflection. It was found that adjusting the silicon layer’s (semiconductor layer’s) thickness can modify the reflection peak’s spectral location. The planar design proved to be capable of absorbing more than 80% of incoming light across a wide spectrum from 800 nm to 1300 nm, with a potential expansion up to 1600 nm with the addition of an anti-reflection layer less than 100 nm thick deposited on the AFPN. The proposed MDSDM AFPN design serves a dual purpose: an effective nanoscale device for color filtering and a sensor within the visible spectrum. Additionally, the technology may be useful in photovoltaic and communication systems that operate at NIR wavelengths. Initial results of this research have been published in proceedings of the 2023 IEEE Photonics Conference (IPC), pp. 1-2 (2023).
The third area of this research involved an investigation of a planar nanoscale broadband absorber utilizing an AFPN. This approach offers several advantages, notably its lithography-free and etching-free design, facilitating scalability in both device production and wavelength coverage. TMM was used in parameter optimization, identifying the ideal refractive index ranges (real and imaginary parts) for developing these absorbers across various wavelength ranges.

The proposed broadband absorber structure provided over 80% absorption even at oblique angle incidences up to 60 degrees. Numerical analysis confirmed the effectiveness of combining a high-extinction coefficient metal at the bottom layer with a moderate-extinction coefficient metal at the top for enhancing broadband absorption. Traditional high-extinction metals like gold (Au), silver (Ag), or aluminum (Al) tended to reflect, even for minimal thicknesses. Conversely, chromium (Cr), with its moderate extinction coefficient, reduced reflection, and increased field penetration, extending absorption across a broader wavelength spectrum.

Finite-difference-time-domain (FDTD) simulations corroborated the numerical findings, confirming the absorptive efficiency of the Cr-Al$_2$O$_3$-Al structure. This configuration predicted more than 90% absorption in the 600-1400 nm range, with the potential for an extension into the near-infrared spectrum by adjusting the thickness of the Al$_2$O$_3$ dielectric spacer. To optimize absorption up to 100%, an anti-reflective oxide coating can be applied atop the asymmetric Fabry-Perot nanocavity. The resulting Al$_2$O$_3$-Cr-Al$_2$O$_3$-Al configuration predicts more than 95% absorption across a wide wavelength range.
The straightforward, lithography-free design of this broadband absorber makes the structure an appealing candidate for thermal photovoltaic applications, particularly where high absorption over large physical areas is necessary. Initial results of this research have been published in *Frontiers in Optics + Laser Science 2023* (FiO, LS), Technical Digest Series (Optica Publishing Group, 2023), paper JTu4A.46.

The final topic of this research involved an investigation into the influence of cavity layer properties on the optical performance of Fabry-Perot nanocavities (FPNs), focusing on their resonance behavior. Limitations in using Palik’s database for simulating nanoscale devices were seen. Bulk materials do not consider the effects of film thickness on optical properties. Thin films, especially those made of noble metals and semiconductors, exhibit varying optical characteristics depending on their thickness.

The present study ultimately utilized Monte Carlo simulation and the law of large numbers to assess how thickness variations impact device performance, particularly in reflectance calculations that use the transfer matrix method. By comparing results from studies providing the refractive index’s dependence on film thickness, the present study has established error margins for each layer parameter for a metal-oxide-semiconductor-metal FPN structure. The approach generated datasets for optical parameters and layer thicknesses, reflecting the effects of thickness variation in thin films’ optical properties, improving modeling accuracy. Even minor deposition thickness errors (e.g., 5 nm) in the oxide and semiconductor layers significantly affected the absorption of resonance wavelength. The study
revealed the importance of using optical parameters that represent the properties of amorphous or polycrystalline thin films for modeling resonance-based nanoscale optical devices.

In future studies, integrating ENZ semiconductors, like n-InSb, n-InAs, or ITO, as active layers should be considered in narrowband color reflector designs. This can lead to the creation of dynamically tunable red-green-blue (RGB) color filters operating in the reflection mode.
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Appendix

PUBLICATIONS RESULTING FROM THIS RESEARCH

Journal Paper


Conference Papers


4. **K. P. Dixit**, Z. B. Houtman, E. E. James and D. A. Gregory,