Amorphous photonic structures

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AMORPHOUS PHOTONIC STRUCTURES

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For my family and friends

Abstract

This thesis concerns the study of amorphous photonic crystal structures: disordered photonic lattices possessing short-range but not long-range order.

In the first part of the thesis, I study amorphous structures intended for electrically-pumped random quantum cascade lasers (QCLs). Random lasers are a class of lasers which, unlike traditional lasers, have no well-defined and well-structured cavity; lasing takes place through multiple scattering from a random medium. I design and analyze amorphous lattices of dielectric rods, joined by dielectric veins, which support high quality factor (Q factor) lasing for transverse magnetic (TM) modes. Simulations show that these structures can achieve 2D Q -factors of as large as 10^5 , which is not possible using previous designs based on air holes etched in dielectric slabs.

In the second part, I perform a numerical study of an amorphous variant of a “photonic topological insulator” (PTI). PTIs are photonic crystal structures with band structures analogous to topological insulator materials, supporting robust electromagnetic edge states that propagate unidirectionally along the edge. Although the existence of these edge states is justified by theoretical arguments that assume long-range order, I show that similarly robust edge states exist in amorphous lattices, which possess only short-range order. This study opens new possibilities for studying disorder in PTIs.

In the third and final part, I develop a computational method called “FLAME-slab”, which is capable of efficiently solving the wave scattering problem for amorphous slab structures, where scattering elements are distributed within a slab with short-range order. Compared to standard finite element or finite difference methods, the FLAME-slab method allows for much coarser meshes, with as few as three grid layers spanning the thickness of the slab. Solutions are generated based on the Flexible Local Approximation Method (FLAME), using Rigorous Coupled Wave Analysis (RCWA) as a subroutine to generate local basis functions.

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Contents

List of Figures	viii
List of Tables	x
1 Introduction	17
1.1 Photonic crystals	17
1.2 Disordered photonic lattices	19
1.3 Amorphous photonic lattices	21
1.4 Topics in this thesis	27
2 Optimization of TM modes for amorphous slab lasers	30
2.1 Introduction	30
2.1.1 Random lasers	30
2.1.2 TE and TM modes in random slab lasers	34
2.2 Design of the amorphous photonic structures	39
2.3 Electromagnetic properties	43
2.3.1 Amorphous lattice of unconnected dielectric rods	43
2.3.2 Amorphous lattice of connected rods	46
2.4 Field distributions	49
2.5 Discussion and Conclusion	51

3 Robust Edge States in Amorphous Gyromagnetic Photonic Lattices	53
3.1 Introduction	53
3.1.1 Overview of Photonic Topological Insulators	53
3.1.2 Time reversal ($\mathcal{T}$) symmetry	56
3.1.3 Non reciprocal photonic crystals	58
3.2 Band structure of a gyromagnetic triangular photonic crystal	63
3.3 Generating the amorphous lattices	65
3.4 Bulk states and Edge states	68
3.4.1 Calculation of the spectral weight	68
3.4.2 Calculation of isolation ratio	70
3.5 Group velocity and penetration depth	73
3.6 Conclusion	77
4 The FLAME-slab Method for Electromagnetic Wave Scattering in Slab Structures	79
4.1 Introduction	79
4.1.1 Electromagnetic wave scattering in slab structures	79
4.1.2 Rigorous Coupled Wave Analysis (RCWA)	82
4.1.3 The FLAME approach	88
4.2 Finite-difference scheme for slab geometry	91
4.2.1 Grid layout	91
4.2.2 Organization of stencil coefficients	93
4.2.3 Implementation of scattering boundaries	95
4.2.4 Assembling the finite-difference matrix equation	98
4.3 Generation of FLAME stencil coefficients	99
4.4 Results	103

4.4.1	Calculation of scattered electric and magnetic fields	103
4.4.2	Calculation of reflectance	105
4.5	Error Analysis	107
4.6	Conclusion	109
5	Conclusions and Future Directions	111
	References	114

List of Figures

1.1	2D Photonic Crystal	18
1.2	DOS and Q factor enhancement	22
1.3	2D spatial Fourier transform	23
1.4	Hyperuniform structures	25
2.1	Regular vs. random laser	31
2.2	Low spatial coherence of random laser	32
2.3	Examples of TE and TM random laser	35
2.4	TM band structure of triangular lattice of rods and air holes	37
2.5	Method of generating amorphous structures	40
2.6	Unconnected disordered honeycomb structure	42
2.7	Q factor for unconnected structure	44
2.8	Connected disordered honeycomb structure	45
2.9	Q factor for connected structure	47
2.10	Q vs. vein width w	48
2.11	E_z field plots for random lasers	50
3.1	Photonic Topological Insulators examples	55
3.2	TR symmetry in Photonic crystals	60
3.3	Robustness of edge states against localized defects	62
3.4	TM band structure for gyro and non-gyro PhC	64

3.5	Molecular dynamics schematic	66
3.6	Correlation function $C(\Delta r)$	67
3.7	Schematic for calculating spectral weight and isolation ratio	69
3.8	Spectral weight and isolation ratio calculation	71
3.9	Robustness of edge states in amorphous PTI	73
3.10	Group velocity (v_g calculation)	75
3.11	Intensity decay (β calculation)	76
4.1	Schematic for a typical RCWA calculation	82
4.2	Run time vs N_G for the S^4 RCWA solver	87
4.3	Schematic for 1D FLAME calculation	90
4.4	Setup for Flame-slab calculation	92
4.5	Breakdown of 9 point stencil patch into three subpatches	93
4.6	Schematic of a slab consisting of dielectric rods placed randomly on a flat dielectric substrate, surrounded by air	100
4.7	Real parts of the scattered electric field $E_{y,s}$ and magnetic field $H_{x,s}$	104
4.8	Reflectance R versus frequency for the slab structure	106
4.9	Consistency error ξ versus N_G	107
4.10	Consistency Error ξ versus N_x	108

List of Tables

2.1 Concentration factor $\mathcal{C}$ for modes 51

Chapter 1

Introduction

1.1 Photonic crystals

Photonic crystals (PhCs) are artificial periodic dielectric structures which can be used to manipulate the propagation of light. Though it has long been known that periodic dielectric structures in one dimension (1D) could act as mirrors or Bragg reflectors [1, 2], the generalization of this idea to two dimensions (2D) and three dimensions (3D) came only in 1987, with the seminal papers of S. John and E. Yablonovitch [3, 4]. The idea is that in either 1D, 2D, or 3D, we can engineer periodic dielectric structures—PhCs—so that the propagation of electromagnetic waves is forbidden within a certain range of frequencies, known as the photonic band gap (PBG). Photonic band gaps arise from destructive Bragg interference, in a manner similar to how electronic band gaps (between the valence and conduction bands) arise in crystalline insulating solids [5]. Fig. 1.1, shows the transverse magnetic (TM) (i.e. magnetic field is in the plane and electric field points out of plane) band structure and photonic band gap for a 2D square photonic crystal composed of dielectric rods in air.

PhCs have found numerous applications in optical devices, including lasers,

Figure 1.1: Transverse magnetic (TM) band structure for a 2D square photonic crystal of dielectric rods ($\varepsilon = 8.9$) in air ($\varepsilon = 1$). The rods have radius $r = 0.2a$, where a is the lattice constant. The band structure was calculated using the frequency domain solver MPB [6], and exhibits a photonic band gap, highlighted in yellow. Inset: Brillouin zone (left), and spatial structure with rods shown in black (right).

wave-guides, solar cells, optical circuits, etc. [7–11]. Because the PBG and other important properties of PhCs arise from interference, it is usually considered important that the periodicity (or crystallinity) of the PhC is maintained. In other words, disorder is usually considered detrimental to the operation of the PhC.

On the other hand, disorder in photonics is not merely an uninteresting source of imperfections. A variety of interesting phenomena can be observed in disordered and/or aperiodic photonic structures, including the localization of photonic modes and random lasing.

1.2 Disordered photonic lattices

One of the most important phenomena in disordered systems is Anderson localization, which refers to wavefunctions becoming “localized” to a finite region of space (i.e., falling exponentially to zero outside that region), because of the destructive interference of waves passing through the random medium. (By contrast, periodic lattices support Bloch states, whose wavefunctions are “extended” throughout the lattice.) Although first predicted by P. W. Anderson in 1958 [12], the observation of Anderson localization has proven difficult to achieve in electronic systems [13]. The previously-mentioned 1987 paper of S. John [3] was motivated, in part, by the desire to demonstrate Anderson localization, by using electromagnetic modes in place of electronic wavefunctions. The most extensive and successful experimental studies of Anderson localization, in 1D and 2D, have been performed using light [14, 15]. In 3D, there have also been reports of Anderson localization of light [16, 17] in strongly-scattering granular media such as powdered gallium arsenide, but there is controversy over whether this localization was truly due to Anderson localization or simply optical absorption [18].

Anderson localization is strongly dimension-dependent. In 3D, it is predicted

that wavefunctions below a certain energy (the “mobility edge”) are localized, while those above that energy are extended. In 1D and 2D, all wavefunctions are predicted to become localized as soon as disorder is introduced into a system. However, 2D is a “marginal” case: the localization lengths (i.e., the length scales over which the wavefunctions are trapped) can be very long, and if the size of the sample is smaller than the localization length, then localization will not be observed. (Also, as discussed in Chapter 3, Anderson localization can break down in 2D disordered systems that lack time-reversal symmetry.)

As previously mentioned, Anderson localization is not the only effect that can lead to localization. Loss, such as the dissipation of light in optically-absorbing media, also induces an exponential falloff of wave propagation; in fact, one of the complicating factors in observing Anderson localization is the difficulty of distinguishing it from absorption [13, 18]. Moreover, as described in the next section, disordered systems that have some residual *short-range* order can exhibit photonic band gap (PBG)-like effects that also lead to localization.

In the photonic context, one of the most interesting consequences of disorder is the phenomenon of random lasing [19]. Whereas a regular laser involves a well-defined optical cavity filled with a uniform (or well-ordered) gain medium, a random laser consists of a random-scattering gain medium, with the lasing modes arising from multiple scattering within the medium [18, 20, 21]. In some random lasers, the modes are Anderson localized; in others, the localization length is longer than the system size, and the modes are confined by the boundaries of the random medium; alternatively, the modes can also be localized by the PBG-like effects of short-range order, as discussed in the next section.

An important feature of the random lasers is that they are often multimodal and possess low spatial coherence [22]. The low spatial coherence comes from the fact that modes with different frequencies are emitted from different regions of the

disordered media, which are not coupled to each other. Because low-coherence light is free of speckle artifacts, a highly promising application of random lasers is in the imaging of biological tissues and other complex media [22–24]. Moreover, because random lasers can emit in many directions, they may be useful for display applications and as “laser paints” [18]. One advantage of random lasers, compared to traditional ordered photonic structures, is that we do not need very high-precision methods to fabricate them [18].

1.3 Amorphous photonic lattices

Disordered lattices can possess an important property known as *short-range* order, meaning that the positions of nearby lattice sites are correlated with one another. Such lattices are said to be “amorphous”. In solid-state physics, a well-known example of an amorphous material is amorphous silicon, in which the atoms form a random network; and almost all the silicon atoms have fourfold coordination with almost the same tetrahedral bonds, but the lattice as a whole lacks crystallinity.

The presence of short-range order can have dramatic effects on wave propagation within a lattice. In the photonic context, an important study of disordered structures with short-range order was performed by the Cao group in 2010 [25]. This paper looked at 2D photonic structures consisting of a dielectric medium embedded with amorphous patterns of air holes, as shown in Fig. 1.2(a)–(c). Such structures can represent air holes drilled into a dielectric slab, with electromagnetic modes confined to the plane of the slab [26]. The air holes are placed using a molecular dynamics simulation which contains an adjustable “polydispersivity” parameter, p . For increasing p , the system goes from a polycrystalline system (with differently-ordered local domains) to a fully amorphous system.

The transverse electric (TE) modes (i.e., modes polarized so that the electric

Figure 1.2: (a)–(c) Amorphous 2D structures consisting of air holes (white) in dielectric (black). From left to right, structures generated with different values of the “polydispersity” parameter p , which controls the level of short-range order. (d) Density of states versus frequency for disordered structures with different values of p , where $p = 0$ is the perfectly-ordered triangular lattice, the refractive index for the background medium is $n = 3.4$. (e) DOS for amorphous structure (upper panel) of air holes with polydispersity $p = 0.5$, with background refractive index, $n = 1.4$. Even though the dip in DOS is barely visible, the maximal Q -factor Q_m (lower panel) shows a three fold increase at the centre of the dip. Figures reproduced from Ref. [25].

Figure 1.3: (a) A triangular lattice of 400 dielectric rods in a unit square cell, with radius of rods $r \approx 0.15a$, where a is the lattice constant. (b) 2D spatial Fourier transform of the structure shown in (a), showing Fourier peaks forming a symmetric lattice in reciprocal lattice. (c) A highly disordered system, consisting of 400 randomly-placed dielectric rods with the same radius as in (a). (d) 2D spatial Fourier transform of (c), showing a broad Fourier peak centered at the origin $k = 0$. Note that in (b) and (d), the pixel intensity exactly at $k = 0$ has been set to zero, in order to make the other pixel intensities more clearly visible.

field lies parallel to the 2D plane) were then calculated numerically. It was found that the PBGs of the ordered system (a triangle lattice of air holes) survives into the polycrystalline regime. As the system becomes amorphous, the PBGs evolve into “dips” in the photonic density of states (DOS), occurring within the same range of frequencies. These DOS dips gradually diminish as the short-range order is decreased, as shown in Fig. 1.2(d). However, even when the short-range order is so weak that the DOS dips have almost disappeared, it is still possible to observe an enhancement of light confinement (showing up as an enhancement in the Q -factors) near the relevant frequency range, as shown in Fig. 1.2(e).

The spatial Fourier transform is a powerful tool to classify whether a system is ordered, amorphous, or fully random. It maps the real space structure to reciprocal (k) space. Fig. 1.3(a) shows an ordered triangular lattice of dielectric rods, and Fig. 1.3(b) its corresponding 2D Fourier transform. The peaks in the spatial Fourier transform are observed to form an ordered lattice in k space. For comparison, Fig. 1.3(c) shows a highly disordered system consisting of randomly-placed dielectric rods, while Fig. 1.3(d) shows the corresponding 2D spatial Fourier transform, which forms a broad isotropic peak around $k = 0$. For an amorphous lattice the spatial Fourier transform forms one or more rings (similar to Fig. 1.4(b), which will be discussed below). The existence of these rings is an indicator of the presence of short-range order and the absence of long-range order: the pattern is peaked away from $k = 0$ because there is an average length scale over which neighboring lattice sites appear, but it is isotropic because, unlike in a true crystal, there are no “preferred” spatial directions.

“Hyperuniformity” is a concept strongly related to short-range order, which has recently come into prominence in part of the photonics literature [27–31]. In a hyperuniform structure, the number variance of the lattice sites, $\sigma^2(R) \equiv \langle N_R^2 \rangle - \langle N_R \rangle^2$, within a spherically sampling window of radius R , varies more slowly than

Figure 1.4: (a) Dielectric hyperuniform structure of rods connected by veins (black, $\epsilon = 11.56$), with air as the background medium. (b) 2D spatial Fourier transform of the structure, showing a series of concentric rings. Figs. (a)–(b) reproduced from Ref. [27]. (c) Arbitrary shaped waveguide made out of a hyperuniform structure. (d)–(e) : Calculated transmission (T) (blue curve) and calculated DOS (green curve) for TE and TM polarizations respectively. A complete band gap opens up for both polarizations around frequency $0.4c/a$ as indicated by the black broken lines. Figs. (c)–(e) reproduced from Ref. [28].

R^d where d is the dimension of the system [27]. Steinhardt and co-workers [27, 28] investigated hyperuniform structures consisting of dielectric rods connected by dielectric veins, as shown in Fig. 1.4(a). The 2D spatial Fourier transform, shown in Fig. 1.4(b), consists of concentric rings, indicating that the structure is directionally isotropic and possesses strong short-range order.

This type of 2D hyperuniform structure was investigated for the capability to exhibit PBGs for both transverse electric (TE) and transverse magnetic (TM) modes [28]. To achieve this, a relatively high dielectric function ($\varepsilon = 8.76$) was chosen for the material. The theoretically calculated transmission (T) and DOS for a hyperuniform structure with rods and veins (for a similar structure as shown in Fig. 1.4(a)), are shown in Fig. 1.4 (d) and (e), for TE and TM polarization respectively, revealing a deep PBG [28]. The rod radius was set to be $r = 0.188a$ and vein thickness $t = 0.028a$, where a is the average intercell spacing. A complete band gap opens up for both TE and TM polarizations as indicated by the frequency region between the black broken lines. An important feature of the PBG is that it is isotropic (as evidenced by the 2D spatial Fourier transform). As a result, arbitrarily-shaped waveguides can be embedded within the structure, as shown in Fig. 1.4(c).

In fact, as Pérez and co-workers have recently shown [32], the concept of hyperuniformity is essentially equivalent to short-range order. A hyperuniform structure necessarily possesses short-range order, and conversely various types of amorphous structures (e.g., structures generated through the jammed packing of hard disks) may be shown to satisfy the number variance condition given above, which is the formal definition of hyperuniformity.

1.4 Topics in this thesis

In the Chapter 2, I will present a numerical study of 2D honeycomb-like amorphous photonic structures consisting of dielectric rods where nearest neighbors are connected by veins. The purpose of this study is to design a structure that is suitable for realizing a random laser that can exhibit multi-mode lasing in the transverse magnetic (TM) polarization. I will explain why multi-mode random quantum cascade lasers (QCLs) require a design of this sort, rather than structures of air holes embedded in dielectric studied in previous works [25, 26]. I seek to determine how the amorphous rod-vein structures can be optimized to enhance the quality (Q) factors of the random resonant modes. The results show that even for relatively thick vein widths, Q factor enhancements of several orders of magnitude can be achieved. Most of the material presented in this chapter was previously published in the journal *Optics Express* [33].

In Chapter 3, I will study the interesting case of amorphous photonic structures that break time-reversal symmetry, due to being fabricated out of magneto-optic (gyromagnetic) materials. In ordinary photonic structures, the permittivity (ϵ) and permeability (μ) are both real scalars, giving rise to the symmetry known as “time-reversal symmetry”, $\mathcal{T}$, for electromagnetic waves. This symmetry states, for example, that for every wave propagating in one direction along a waveguide, there must be a reverse wave propagating in the opposite direction. In 2005–2008, Raghu and Haldane [34, 35] suggested that it would be interesting to study photonic crystals (PhCs) which break $\mathcal{T}$ via the inclusion of magneto-optic materials. The reason was that such PhCs could potentially exhibit “topologically nontrivial” PBGs that are qualitatively distinct from conventional PBGs: within the frequency range of such a gap, the PhC supports exotic “topological edge states” analogous to the edge states of topological insulating materials [36], which

move unidirectionally along the edge without back-scattering. This type of PhC was subsequently designed and experimentally realized by Wang *et al.* [37, 38], using a gyromagnetic material (yttrium-iron-garnet), whose permeability tensor μ has non-vanishing imaginary off-diagonal terms. This started a new sub-field of photonics known as “topological photonics” [39].

Thus far, almost all studies within topological photonics have been based on PhCs. In Chapter 3, I show numerically that robust, non-reciprocal edge states (which have essentially all the properties of topological edge states) can be realized in amorphous lattices of gyromagnetic rods. This shows that topologically nontrivial band gaps can be supported by short-range order, without long-range (crystalline) order. I will discuss the implications of these findings for the theory of localization in $\mathcal{T}$ -broken 2D systems. Part of the material in this chapter is available as a preprint manuscript, and is currently under review [40].

In Chapter 4, I will discuss a new computational method, called “FLAME-slab”, which is optimized for solving the wave scattering problem for amorphous photonic slabs. For PhCs, standard computational or numerical methods (e.g., finite element and finite difference methods) can be used to solve the wave scattering problem efficiently. However, these methods become computationally expensive when applied to systems that have no long-range order, because the lack of periodicity means that the computational domain cannot be truncated to a small unit cell. My approach is based on a numerical method called FLAME (the Flexible Local Approximation Method) [41, 42], coupled with the RCWA (Rigorous Coupled Wave Analysis) method running as a subroutine for generating basis functions [43, 44]. I will show that the wave scattering problem can be efficiently solved in a 2D disordered photonic slab structure, with relatively coarse discretization (containing just three layers of grid points). In the future, it is hoped that the FLAME-slab method can be used as an efficient computational method for studying any type of

amorphous slab structure in 2D or 3D. This work was done in collaboration with Prof. Igor Tsukerman from the University of Akron, the original inventor of the FLAME method [41].

Chapter 2

Optimization of TM modes for amorphous slab lasers

Most of the material presented in this chapter was previously published in the journal Optics Express [33]. Wherever figures and materials from other sources have been taken, the authors have been given due credits.

2.1 Introduction

2.1.1 Random lasers

A traditional laser is based on a well-defined resonant cavity containing a gain medium. One example of such a cavity is a pair of partially-reflecting mirrors on opposite sides of a gain medium, as shown in Fig. 2.1(a). The light is multiply reflected between the mirrors, and is amplified by the gain medium; when the total gain is large enough to equal the total loss (including out-coupling loss), lasing takes place.

Random lasers, on the other hand, are a class of lasers that do not have a

Figure 2.1: Regular laser vs random lasers. (a) A regular laser consists of a well-defined cavity, with optical feedback provided by a pair of partially-reflecting mirrors placed at opposite ends of the cavity. Lasing takes place through multiple reflections of light between the mirrors, and amplification from the gain medium. (b) In a disordered medium, such as a colloidal distribution of scattering particles, random lasing can occur without the existence of a well-defined cavity. The lasing mode arises from multiple scattering of light through the disordered medium. (c) Schematic of an electrically-pumped random laser in the slab geometry. A dielectric slab (quantum cascade wafer) is etched with randomly-distributed air holes, and sandwiched between two gold plates that serve as leads for electrical pumping. Panels (a) and (b) reproduced from Ref. [21]; panel (c) reproduced from Ref. [45].

Figure 2.2: Effect of spatial coherence on imaging artifacts. (a)–(b) Emission spectrum of a random laser for (a) a regime with relatively few lasing modes, and (b) the strongly multi-mode regime. Note that in (b), there are so many lasing peaks that they are not individually discernable. (c)–(d) Illumination pattern after the random laser light is passed through a Young's double slit setup. (c) In the few-mode regime, interference fringes are observed; (d) in the strongly multi-mode regime, there are no fringes. Reproduced from Ref. [46].

spatially regular, well-defined cavity [18, 19, 47, 48]. The mechanism of lasing in random lasers is different from traditional lasers; as shown in Fig. 2.1(b), the lasing modes arise from resonances induced by the multiple scattering of light from randomly-distributed particles in the medium [21]. Originally predicted by Letokhov in 1968 [19], random lasers have been realized in many different settings, including colloids infiltrated with laser dye [49], semiconductor powders [20, 50, 51], and semiconductor slabs with etched holes acting as scattering centers [26]. Random lasers can be used to study a variety of interesting phenomena, such as light localization [52], and have promising technological applications as speckle-free (low spatial coherence) light sources for imaging [22, 53] and chemical sensing [45, 54, 55].

For device applications, it is highly advantageous to focus on random lasers in the “slab” geometry, where the scattering takes place within a 2D plane, with vertical index confinement, as shown in Fig. 2.1(c) [45]. The laser light can be emitted along the plane of the slab (“edge emission”) or out-of-plane (“vertical emission”). The slab geometry allows for electrical pumping, and ease of integration with other photonic devices.

One of the most technologically promising features of random lasers is that they can provide bright light with low spatial coherence [46]. This is useful for imaging applications such as optical coherence tomography, because ordinary laser light (which has high spatial coherence) tends to produce “coherent artifacts” such as speckle spots, which reduce the image quality. Light sources with low spatial coherence are needed to suppress these artifacts. (Moreover, the intensity of random laser light can be substantially higher than lamps and other traditional sources of spatially incoherent light.) For this purpose, it is desirable to reach the “strongly multi-mode” regime, in which the number of lasing modes is large. This is demonstrated in Fig. 2.2, which is reproduced from Ref. [46]. The authors

in this paper studied an exemplary random laser consisting of optically-pumped laser dye solution containing polystyrene spheres as scattering centres. Fig. 2.2(a) shows the lasing spectrum when the number of lasing modes is relatively few, while Fig. 2.2(b) shows the spectrum in the strongly multi-mode regime; the laser could be adjusted between these two regimes by tuning the spot size of the pumping beam. The spatial coherence was then measured through a Young's double slit setup. In the few-mode regime, an interference pattern with clear interference fringes (i.e., coherent artifacts) was observed, as shown in Fig. 2.2(c). In the strongly multi-mode regime, however, the interference fringes were absent, as shown in Fig. 2.2(d).

2.1.2 TE and TM modes in random slab lasers

Random slab lasers can be divided into two categories based on the polarization of the 2D modes they support: transverse electric (TE) or transverse magnetic (TM) modes. In the TE polarization, the electric field lies in the x - y plane and the magnetic field points in the z -direction (out-of-plane). In the TM polarization, the magnetic field lies in the x - y plane and the electric field points in the z -direction. In both cases, the electromagnetic modes are effectively two-dimensional due to being index-guided to the plane of the slab; we assume that higher-order transverse modes are negligible.

As discussed in Chapter 1, Cao and co-workers used an amorphous packing of air hole structures [25] to design and realize a TE random slab laser [26]. This laser operated at a wavelength of around $1\ \mu\text{m}$, in the near-infrared regime. The laser efficiency was enhanced by designing the structure so that lasing occurred at a frequency coinciding with a dip in the photonic density of states (DOS), which was induced by short-range order in the amorphous structure. It was found that the Q -factor (defined as $Q = \omega_r/2|\omega_i|$, where ω_r and ω_i are the real and imaginary parts of the resonance frequency) was dramatically enhanced in such a frequency

Figure 2.3: (a) SEM image of a “photonic network laser” based on a trivalent network structure fabricated in GaAs membrane (the scale bar is 2 μm in length; a schematic of a typical vertex is shown inset). The network arms consist of dielectric material, surrounded by air. (b) Calculated photonic DOS versus normalized frequency for a trivalent network structure (blue broken line), and for an amorphous structure of air holes with the same FF and effective refractive index. Figs. (a)–(b) reproduced from Ref. [56]. (c) SEM image of a mid-infrared QCL based on an air-hole structure, with air holes of radius $\approx 3 \mu\text{m}$ (black circles) etched into a QCL wafer. (d) Emission spectra of the laser for 30% FF, at different driving currents (I). With increasing I , we observe up to 3–4 lasing peaks at around 985 cm^{-1} . Figs. (c)–(d) reproduced from Ref. [54].

region, even if the actual DOS dip is small [25, 26]. The maximum Q -factor was reported to be of the order of 10^3 . Later, the same group reported another TE random slab laser based on a trivalent network structure, shown in Fig. 2.3(a). Here, the Q -factor was found to be as high as 10^5 [56], due to a similar dip in the photonic DOS. A high Q -factor results in better trapping of the light, and hence lowers the lasing threshold. These works demonstrated that as a general rule, it is advantageous to design amorphous slab lasers so that the operating frequency range of the gain medium coincides with a DOS dip of the photonic structure.

The studies of Cao *et al.* were focused on transverse electric (TE) modes [25, 26, 56]. This is because most lasing media, including semiconductor laser diodes, emit in the TE polarization. However, transverse magnetic (TM) emission dominates in some lasers, including strained quantum well lasers [57] and quantum cascade lasers (QCLs) [58].

QCLs are notable for being among the only high-power light sources available in the mid-infrared (mid-IR) to terahertz frequency range [59]. Recently, the first random laser operating at mid-IR frequencies was demonstrated by Liang *et al.*. This device was based on a QCL slab with etched air holes [54], similar to the design of Ref. [26]. It was shown that the Q -factor increases with the filling fraction (FF) of the air holes in the QCL slab. Fig. 2.3(c) shows the SEM image of the fabricated laser. The refractive index of the QCL medium is 3.4, and the radius of the air holes was chosen to be $\approx 3 \mu\text{m}$, comparable to the operating wavelength (which is around $10 \mu\text{m}$ in air). The device, however, exhibited rather low Q -factors. Fig. 2.3(d) shows the emission spectra of the laser [54]; with air hole FF 30%, it can be observed that increasing the driving current I increases the number of lasing peaks, but no more than 3–4 lasing peaks can be seen. The device therefore did not reach the desired strongly multi-mode regime discussed in Section 2.1.1,

In this chapter, I present a numerical study of TM mode confinement in amor-

Figure 2.4: TM band structures for perfectly-ordered triangular lattices of air holes or dielectric rods. The structures are shown inset, with air and dielectric regions shown in white and black respectively; the air regions have refractive index $n = 1$ while the dielectric regions have refractive index $n = 3.35$ [54]. (a) Lattice of air holes with hole radius $r = 0.2876a$ (air hole FF=30%), where a is the lattice constant. In this case, there is no TM band gap. (b) Lattice of air holes with radius $r = 0.4233a$ (air hole FF=65%). There is a small band gap (yellow region, frequency $f \approx 0.4c/a$), of relative width $\Delta\omega/\omega \approx 3.15\%$. (c) Lattice of dielectric rods, with radius $r = 0.2876$ (dielectric FF=30%). There are two prominent TM band gaps, at $f \approx 0.28c/a$ and $f \approx 0.48c/a$; the relative gap widths are $\Delta\omega/\omega \approx 34.38\%$ and $\Delta\omega/\omega \approx 23.75\%$ respectively. The band structures were calculated using the MPB software package [6].

phous photonic structures, with the goal of guiding the design of QCL random slab lasers. Previous studies of mode confinement in amorphous structures dealt with TE modes in structures of air holes in a dielectric medium [25], or a network of dielectric veins [56]; and, as we have mentioned, the random QCL realized by Liang *et al.* also used an air hole design [54]. A subsequent numerical study of the modal properties of a random slab laser with air holes was performed by Molardi *et al.* [60, 61].

However, air hole structures are fundamentally unsuitable for manipulating TM modes! This principle can be observed in 2D (non-disordered) photonic crystals, where TM bandgaps are easily opened by having “isolated” high-dielectric regions [7], as shown in Fig. 2.4. Here, I have calculated the TM band structures for three different triangular lattices: (a) small air holes, (b) large air holes, and (c) small dielectric rods. From Fig. 2.4(a)–(b), we observe that there is no TM band gap until the air hole FF is very high ($\approx 65\%$). Even then, the gap is relatively narrow, with gap-midgap ratio $\Delta\omega/\omega \approx 3.15\%$, and is thus easily destroyed by positional disorder. In Fig. 2.4(c), however, we observe that in a triangular lattice of isolated dielectric rods, there are prominent TM band gaps; here, the lower band gap has gap-midgap ratio $\Delta\omega/\omega \approx 34.38\%$.

Likewise, in the disordered regime, previous studies have found strong dips in the TM DOS in amorphous photonic structures consisting of unconnected dielectric rods [62, 63]. We verify this basic result below for an amorphous structure consisting of unconnected rods arranged in a disordered honeycomb-like lattice. Near the gap edge, the TM modes indeed experience substantial Q -factor enhancements, of up to three orders of magnitude.

However, a design consisting of unconnected dielectric rods is problematic for realizing an electrically pumped random laser, such as a random QCL. This is because the pumping current needs to be passed through the entire dielectric

medium, which acts as the gain medium. To resolve this difficulty, we turn to a “connected” structure consisting of dielectric rods joined by dielectric veins. This is quite similar to the structure studied by Steinhardt and co-workers [27, 28, 30]; those authors, however, were primarily concerned with achieving deep and complete (TE and TM) bandgaps, rather than enhancing bulk mode Q -factors for lasing.

Here, we demonstrate that connected amorphous structures can exhibit Q -factor enhancements induced by a DOS dip. For relatively high vein width, comparable to the rod radius, we find a weak dip in the DOS, but the TM Q -factors are enhanced by around two orders of magnitude. Notably, this is a much larger enhancement than what was previously reported for TE modes [25]. When the vein width is further increased, however, the structure becomes similar to a network of dielectric veins [56], and the TM Q -factor enhancement disappears. Our study provides a guide for the design of future TM-polarized electrically-pumped amorphous slab lasers, and particularly QCLs operating in the technologically important mid-infrared to terahertz regimes.

2.2 Design of the amorphous photonic structures

The process for generating the 2D amorphous structures is shown in Fig. 2.5. A set of 1025 disks is jam-packed (into a large circular region) using a molecular dynamics simulation [25]. Using bidisperse disks with radius fraction 1:1.2, we can achieve packed configurations with $FF \approx 0.7$. The disk centers, which form an amorphous lattice locally similar to a triangular lattice, are then connected by Delaunay triangulation, as shown in Fig. 2.5(a)–(b). The incenters of each triangle form an amorphous honeycomb-like lattice, and are used as the center-points of dielectric rods (disks) of radius r . (The original disks that were used for packing are now discarded; the packing procedure ensures that the lattice points are well-

Figure 2.5: Generation of the amorphous photonic structure: (a) An ensemble of bidisperse disks (blue and black circles) is close-packed. The disk centers (red circles) form an amorphous triangle-like lattice. (b) Delaunay triangulation of the disk centers (green lines). (c) The triangle incenters (black circles) form an amorphous honeycomb-like lattice of dielectric rods. (d) Nearest neighbor rods are joined by dielectric veins to form a connected lattice. The packing is performed within a circular region, resulting in an approximately circular sample [see Fig. 2.6(a)]; these plots show a close-up of part of the lattice.

separated and form an amorphous lattice.)

The result is shown in Fig. 2.5(c). As a final step, we connect nearest-neighbor rods using veins of width w , as shown in Fig. 2.5(d).

In the following, the dielectric rods have radius $r = 0.3655a$, where a is the mean nearest-neighbor distance between rod centers. In the absence of the veins, the FF of the dielectric regions is around 0.30. The refractive index of the rods is set to $n_{\text{rods}} = 3.35$, consistent with QCL media [58, 59]; the surrounding medium is air with refractive index 1.

Fig. 2.6(a) shows a typical realization of an amorphous structure generated by the above procedure. The 2D spatial Fourier transform of this structure is shown in Fig. 2.6(b); it forms clear rings, indicating that the structure possesses strong short-range order but no long-range order. The short-range order is also evident from the fact that nearly all the rods have three almost-equidistant nearest neighbors.

In Fig. 2.6(c), we show the ensemble-averaged plot of the 2D spatial correlation function, defined as

$$C(\Delta r) = \langle \Theta(r + \Delta r) \Theta(r) \rangle / \langle \Theta(r) \rangle^2 - 1, \quad (2.1)$$

where $\Theta(r) = 1$ inside the rods, and $\Theta = 0$ outside. The average was taken over 100 independent realizations of the structure, using the same structure parameters. The first peak is around $\Delta r \approx a$, where a indicates the nearest neighbor distance. The second correlation peak occurs around $\Delta r \approx \sqrt{3}a$, which coincides with the next-nearest neighbor distance for the disordered honeycomb lattice structure. The correlation peaks decrease in amplitude with increasing Δr , implies that the disordered structure possesses only short-range order and no long-range order.

If we target a mid-infrared free-space operating wavelength of $10 \mu\text{m}$, then for DOS dips occurring at frequencies around $0.2c/a$ (see below), the rod radius will

Figure 2.6: (a) Schematic of a disordered unconnected lattice, consisting of ≈ 1950 unconnected dielectric rods in a honeycomb-like pattern. The rod radius is $r = 0.366a$, where a is the mean distance between the centers of nearest-neighbor rods. Here, the computational cell for a DOS calculation is depicted: the lattice occupies a finite circular region, with a Gaussian point source at its center (yellow star), and is surrounded by perfectly matched layers (PMLs) to absorb the emitted waves. (b) 2D Fourier transform of the lattice. (c) Ensemble averaged, 2D spatial correlation function $C(\Delta r)$ vs $\Delta r/a$. The red vertical line represents the position of the nearest neighbor (n.n.) and the green vertical line represents the position of the next nearest neighbor (n.n.n.).

be $r \approx 0.75 \mu\text{m}$ and the mean lattice constant will be $a \approx 2.1 \mu\text{m}$. For comparison, this choice of rod radius is approximately half the radius of the etched hole features in the QCL random laser reported by Liang *et al.* [54]

2.3 Electromagnetic properties

2.3.1 Amorphous lattice of unconnected dielectric rods

To determine the optical properties of the amorphous photonic structure, we performed finite-difference time-domain (FDTD) simulations using the MEEP program [64]. Fig. 2.7(a) shows the TM DOS spectrum, averaged over 100 disorder realizations. The setup for this calculation is shown in Fig. 2.6(a); the lattice occupies a finite circular region, surrounded by air, with perfectly matched layer (PML) boundary conditions at the edges of the computational domain. The structure is excited with a Gaussian point source placed at the center of the structure (shown by yellow star), with frequency center $f_0 = 0.2462c/a$ and frequency width $\Delta f = 0.1911c/a$. The results show an extremely strong gap (3 orders of magnitude dip in the DOS) around $f \approx 0.25c/a$. This frequency corresponds almost perfectly with the photonic bandgap of a honeycomb lattice of dielectric rods having the same nearest-neighbor lattice constant a .

In Fig. 2.7(b)–(c), we show the Q -factors of the TM modes. These are again obtained from FDTD simulations, using the response to a broad-band TM source [64]. As expected, there are no modes present in the gap; the modes just below the gap, however, have extremely high Q -factors which are enhanced by up to 3 orders of magnitude relative to the other modes.

Figure 2.7: (a) Transverse-Magnetic (TM) Density of States (DOS) of the disordered lattice, computed using 100 disorder realizations (dark blue). The TM DOS of a honeycomb photonic crystal with the same a is shown for comparison (gold). (b) Q -factors of the TM modes for a single disorder realization, computed using 2D finite-difference time-domain (FDTD) simulations. (c) Average Q -factors versus frequency for the TM modes, calculated from 100 disorder realizations and taking the mean Q -factor in each frequency bin.

Figure 2.8: (a) Schematic of a disordered connected lattice, consisting of dielectric rods in a honeycomb-like pattern. The rods have radius $r = 0.366a$, and are connected by dielectric veins of width $w = 0.9r$. (b) 2D Fourier transform of the lattice.

2.3.2 Amorphous lattice of connected rods

Next, we consider *connected* structures, which are generated by joining nearest-neighbor rods with dielectric veins of width w . (The rods and veins have the same refractive index.) As described in Section 2.1.2, it is desirable to use such connected structures for electrically pumped TM slab lasers. Relatively thick veins are desirable in order to reduce Ohmic heating from electrical pumping, and to maximize the area of gain material available.

Fig. 2.8(a) shows a connected structure with vein width $w = 0.9r$. For the equivalent honeycomb lattice, the dielectric FF (i.e., the relative area covered by the dielectric region) can be estimated to be

$$\frac{2}{\sqrt{3}} \left\{ 2 \left[\frac{\pi}{3} - \sin^{-1} \left(\frac{w}{2r} \right) \right] \left(\frac{r}{a} \right)^2 + \frac{w}{a} \left[1 - \sqrt{\left(\frac{r}{a} \right)^2 - \left(\frac{w}{2a} \right)^2} \right] \right\}.$$

For our chosen rod radius ($r = 0.3655a$), this gives $\text{FF} \approx 0.43$.

For the amorphous lattice, we numerically determine the filling fraction to be approximately 0.4220 ± 0.0003 . The spatial Fourier transform, shown in Fig. 2.8(b), exhibits a strong primary Bragg ring, indicating the presence of short-range order. The TM DOS is shown in Fig. 2.9(a). The presence of the moderately wide veins has strongly suppressed the TM gap, compared to the unconnected case [Fig. 2.7(a)]; this is consistent with the principle that TM gaps require well-isolated high-dielectric regions. However, there remains a small dip at $f \approx 0.2c/a$. Around this frequency, we find that the TM modes have strongly enhanced Q -factors, up to 2 orders of magnitude larger than the modes at other frequencies. This is shown in Fig. 2.9(b)–(c).

The presence of the DOS dip and the Q -factor enhancements do require the veins to be narrower than the rod diameter. In Figs. 2.9(a) and (c), we also show the case of $w = 2r$. In this case, the rods are not “visible”, and the lattice becomes

Figure 2.9: (a) TM DOS for moderate vein width ($w = 0.9r$) and large vein width ($w = 2r$). (b)–(c) Q -factors of the TM modes. In (c), the results are obtained by taking the mean in each frequency band over 100 disorder realizations. The $w = 0.9r$ case still exhibits a two order of magnitude enhancement in Q -factors at $f \approx 0.2c/a$, near the DOS dip.

Figure 2.10: Mean Q -factor versus vein width w . The Q -factors are sampled using modes in the frequency range $0.198c/a < f < 0.226c/a$, over 50 disorder realizations.

a network of veins similar to that studied in [56], by Noh *et al.* As can be seen, the TM modes now all have similar Q -factors.

This Q -factor enhancement is quantified in Fig. 2.10. Here, we calculate the mean Q -factors, averaging over 50 disorder realizations and sampling modes in the frequency range $0.198c/a < f < 0.226c/a$ [which is roughly the range in which the Q -factor enhancement occurs, as shown in Fig. 2.7(c) and Fig. 2.9(c)]. As can be seen, as we increase the vein width w , the Q -factors decrease from $\sim 10^5$ in the unconnected structure ($w = 0$) to the background level $\sim 10^3$ when the vein width equals the rod diameter ($w = 2r$).

It can be noted that changing the vein width w will also change the dielectric FF, since the rod radius r is fixed. Specifically, increasing w from 0 to $0.9r$ will increase the FF from ≈ 0.3 to ≈ 0.42 . This causes the upper “band edge” of the DOS dip to move towards the left (to lower frequencies). However, the lower band edge shows only a very slight frequency shift, remaining more or less fixed at $f \approx 0.21c/a$. The high Q -factor modes are mostly clustered around the lower band edge, and are thus largely unshifted by an increase in w . The shift in frequency δf ,

as w was increased between 0 and $0.9r$, is estimated as $\delta f/f \approx 0.0324$ (i.e. $\approx 3\%$). Similar behavior can be observed in the bandstructure of an *ordered* honeycomb lattice, in which increasing vein width barely shifts the frequency of the band edge.

2.4 Field distributions

Fig. 2.11 shows the field distributions in exemplary unconnected and connected structures. These fields are produced by Gaussian sources of central frequency $f_0 = 0.21c/a$, closely matched to the frequencies of the high- Q modes. We can see that the excited modes are not extended over the entire structure, but are localized to regions that are multiple lattice spacings in size. In the unconnected structure, Fig. 2.11(a), the modes are strongly-concentrated in the dielectric rods. This behavior is favorable for lasing, for it increases the mode overlap with the gain medium (which occupies the dielectric regions). The connected structure, Fig. 2.11(b), exhibits similar behavior, though the concentration is less apparent.

To quantify the mode concentration, we calculate the concentration factor $\mathcal{C}$, defined as

$$\mathcal{C} \equiv \frac{\int_{\epsilon=\epsilon_d} \epsilon_d |E_z(\vec{r})|^2 d^2r}{\int \epsilon(\vec{r}) |E_z(\vec{r})|^2 d^2r}. \quad (2.2)$$

Here, $\epsilon(\vec{r})$ denotes the dielectric function at position $\vec{r}$, and $\epsilon_d = (3.35)^2$ is the dielectric constant of the high-dielectric regions (rods and veins). The integral in the numerator is restricted only to the high-dielectric region, while the integral in the denominator is taken over all space. This figure-of-merit represents the proportion of electric field energy occupying the high-dielectric regions. The limit where the modes are entirely concentrated in the high-dielectric regions corresponds to $\mathcal{C} \rightarrow 1$.

Table 2.1 shows the concentration factors calculated from FDTD simulations.

Figure 2.11: Field patterns for the out-of-plane electric field (E_z), in the (a) unconnected and (b) connected structures. The modes are excited by five Gaussian sources at positions $[0, 0]$, $[\pm 14.6a, 0]$, and $[0, \pm 14.6a]$; all the sources have frequency center $f_0 = 0.21c/a$ and frequency width $\Delta f = 0.055c/a$. The field snapshot is taken at time $1.54 \times 10^3/f_0$ after the sources end.

Vein width w	Low-frequency	Mid-frequency	High-frequency
0	0.897 ± 0.002	0.961 ± 0.002	0.710 ± 0.008
$0.5r$	0.913 ± 0.002	0.952 ± 0.013	0.888 ± 0.002
$0.9r$	0.936 ± 0.003	0.899 ± 0.017	0.927 ± 0.001

Table 2.1: Concentration factor $\mathcal{C}$, as defined in Eq. (2.2), for the modes excited by Gaussian sources with different excitation frequencies. The sources are located at the same positions as in Fig. 2.11. Their center frequencies are $f_0 = 0.16c/a$ (low frequency, below the DOS dip), $f_0 = 0.21c/a$ (mid frequency, near the DOS dip), and $f_0 = 0.267c/a$ (high frequency, above the DOS dip). All sources have frequency width $\Delta f = 0.055c/a$. The results are averaged over 25 disorder realizations.

The simulations are run until long after the exciting Gaussian sources are turned off, in order for low- Q modes to decay away. For each simulation, the concentration factors are computed using the mean of 18 successive “snapshots” (to average over the oscillation period), and the results are further averaged over 25 disorder realizations.

From these results, we see that for $w = 0$, modes are highly concentrated in the dielectric rods in the “mid-frequency” region, where the Q -factors are strongly enhanced. The concentration is less prominent at other frequencies. A similar trend is observed for $w = 0.5r$. However, for $w = 0.9r$, we find that $\mathcal{C} \gtrsim 0.9$ in all three frequency regions. This is beneficial for lasing, since most of the electric field energy is concentrated in the dielectric region where the gain resides.

2.5 Discussion and Conclusion

In this chapter, I have demonstrated using simulations that an amorphous lattice of dielectric rods connected by relatively wide dielectric veins can support TM modes with high Q -factors. This is a promising design for electrically-pumped amorphous quantum cascade lasers (QCLs) operating in the infrared to terahertz frequency range. By contrast, the random QCL previously reported in [54], by Liang *et al.* consisted of a dielectric slab with random air holes. As discussed in

Section 2.1.2, even in the periodic (ordered) case, that class of lattice lacks any DOS gap. Hence, it does not exhibit any short-range order induced enhancement in the TM Q -factors.

Because the connectivity of the structure is important for electrical pumping, it is noteworthy that an enhancement of two orders of magnitude in the TM mode Q -factors can be obtained for relatively wide veins, with $w = 0.9r$ and area filling fraction of ≈ 0.42 . Whether this provides sufficient electrical contact for a practical QCL shall have to be determined empirically. If so, the relatively high concentration factors (with $\sim 90\%$ mode overlap with the high-dielectric region) implies that the resulting modes should be favorable for low-threshold lasing.

Our numerical study was based on 2D simulations, similar to previous numerical studies of disordered slab structures [25, 56, 62, 63]. These simulations neglect vertical (out-of-plane) scattering and emission, which will in practice reduce the Q -factors of the modes. However, these vertical scattering processes should be relatively independent of the DOS dip that arises from in-plane scattering. Hence, in the full 3D structures we should still expect a substantial Q -factor enhancement near the DOS dip, *relative to the other modes*. In Chapter 4, I will discuss a numerical method that was developed to try to address this class of problems.

Finally, we would like to comment on the relationship between our work and that of Steinhardt and co-workers [27, 28, 30], who have performed extensive studies of similar structures (rods connected by veins). Those authors were mainly concerned with optimizing the (TE and TM) bandgaps, and introduced veins in order to help open the TE gaps. For this purpose, relatively narrow veins of width $w \approx 0.15r$ were sufficient [27]. In our case, only the TM modes are of interest, and we are not necessarily interested in deep TM gaps. Hence, we assumed significantly wider veins $w \approx 0.9r$, giving rise to a TM DOS dip rather than a gap, which turns out sufficient to produce large Q -factor enhancements.

Chapter 3

Robust Edge States in Amorphous Gyromagnetic Photonic Lattices

Part of the material in this chapter is available as a preprint manuscript, and is currently under review [40].

3.1 Introduction

3.1.1 Overview of Photonic Topological Insulators

Photonic Topological Insulators (PTIs) are photonic crystal based structures that support edge states due to the properties of their underlying band structures. The first PTI was proposed in 2005 by Raghu and Haldane [34], who theoretically predicted the existence of edge states in TE (transverse electric) modes of gyroelectric photonic crystals (PhC). In gyroelectric materials, an external DC magnetic field alters the permittivity tensor, breaking the time-reversal ($\mathcal{T}$) symmetry of

Maxwell’s equations. Subsequently, it was shown in the theoretical work of Wang *et al.* [37] that a PTI could be realized in an experimentally realistic microwave-scale PhC with gyromagnetic elements, which break $\mathcal{T}$ through the permeability tensor rather than the permittivity tensor, using TM (transverse magnetic) modes. The same group reported the first experimental realization [38] of PTIs in the microwave frequency range. A number of works on PTIs followed [65–68], including the first PTI operating at optical frequencies, which was reported by Rechtsman *et al.* [69]. In that work, $\mathcal{T}$ symmetry was broken using effective time-modulation (based on the Floquet topological insulator concept).

It has also recently been shown that topological insulator-like behavior can be realized in photonic quasicrystals [70], which have no “well-defined” unit cells but possess hidden long-range order.

A common feature of all the PTIs discussed above is that they possess some form of long-range order and crystalline symmetry. It is natural to ask whether topological insulator-like behavior can be realized in systems having only short-range order, and no long-range order. This issue has been recently studied theoretically by Agarwala *et al.* [71], in the context of condensed-matter systems in the tight-binding limit. They showed that even in *random* lattices, it is possible to observe some remnant of topological insulator behavior (including for “class A” topological insulators, or Chern insulators, which are the class that I will be interested in). In this chapter, I will design and study amorphous photonic lattices, which possess only short-range and no long-range order, but nonetheless exhibit edge states similar to the characteristic topological edge states of PTIs. The finite element solver COMSOL Multiphysics was used for all the calculations shown in this chapter.

Figure 3.1: (a) TE and TM band structure of an ordered hexagonal lattice of dielectric cylinders with $\varepsilon = 14$ embedded in a background medium with $\varepsilon = 1$; a is the lattice constant and filling fraction of rods $f = 0.431$. A “Dirac point” degeneracy is observed for the TE mode at symmetry point J . This degeneracy is lifted if anisotropic ε is introduced, and then a band gap opens up where one-way edge modes reside. (b) Schematic showing the photonic crystals slab (blue rods) surrounded by metal on the top edge and microwave foam on the other three sides. The system is sandwiched between two copper plates for in-plane confinement of the electric field. The system is excited with an antenna A and the field is probed at antenna B. A metal obstacle of variable length l is introduced to study robustness of edge states, DC magnetic field (in z direction) is applied to break time-reversal symmetry. (c) Projected band structure of the system shown in (b); the red curve between 4 GHz and 5 GHz corresponds to topological edge states; the bands have Chern numbers 0, 1, -2 , 1 (from left to right). (d) Forward and backward transmissions measured for the system in (b) around 4.5 GHz showing that forward transmission is much higher than the backward, indicating one-way transport via edge states. Fig. 3.1(a) reproduced from Ref. [34]. Figs. 3.1(b)–(d) reproduced from Ref. [38].

3.1.2 Time reversal ($\mathcal{T}$) symmetry

Time reversal symmetry $\mathcal{T}$ is the symmetry transformation under which the time coordinate (t) is reversed:

$$t \longmapsto -t \quad (3.1)$$

Let us consider Maxwell's equations in the frequency domain:

$$\nabla \cdot \mathbf{D} = \rho \quad (3.2)$$

$$\nabla \cdot \mathbf{H} = 0 \quad (3.3)$$

$$\nabla \times \mathbf{E} = -i\omega\mu\mathbf{H} \quad (3.4)$$

$$\nabla \times \mathbf{H} = \mathbf{J} - i\omega\varepsilon\mathbf{E}. \quad (3.5)$$

$$\mathbf{D} = \varepsilon\mathbf{E}, \quad \mathbf{B} = \mu\mathbf{H}. \quad (3.6)$$

In the simplest case where μ and ε are real scalars, these equations are $\mathcal{T}$ -invariant.

In the frequency domain, the time-reversal operation acts as follows:

$$\begin{aligned} \mathcal{T} \mathbf{E} &\longmapsto \mathbf{E}^* \\ \mathcal{T} \mathbf{D} &\longmapsto \mathbf{D}^* \\ \mathcal{T} \mathbf{B} &\longmapsto -\mathbf{B}^* \\ \mathcal{T} \mathbf{H} &\longmapsto -\mathbf{H}^* \\ \mathcal{T} \rho &\longmapsto \rho^* \\ \mathcal{T} \mathbf{J} &\longmapsto -\mathbf{J}^*. \end{aligned} \quad (3.7)$$

Note that the magnetic fields and currents acquire extra negative signs under time reversal symmetry, because they are pseudovectors. To verify (3.7), observe that if

the time dependence of the various fields has the form $\exp(-i\omega t)$, and

$$\{\mathbf{E}(t), \mathbf{D}(t), \mathbf{B}(t), \mathbf{H}(t), \rho(t), \mathbf{J}(t)\}$$

is a solution to Maxwell's equations, then

$$\{\mathbf{E}(-t), \mathbf{D}(-t), -\mathbf{B}(-t), \mathbf{H}(-t), \rho(-t), \mathbf{J}(-t)\}$$

is also a solution. When translated back to the frequency domain, the time-reversed solution is

$$\{\mathbf{E}^*, \mathbf{D}^*, -\mathbf{B}^*, -\mathbf{H}^*, \rho^*, -\mathbf{J}^*\}. \quad (3.8)$$

More generally, ε and μ need not be real scalars; they can be Hermitian tensors (if they are not Hermitian, energy conservation is violated). When ε and μ are non-real, then $\mathcal{T}$ symmetry is broken. This can be achieved without violating Hermiticity by having imaginary off-diagonal tensor components. In gyroelectric materials, $\mathcal{T}$ can be broken by having a permittivity tensor of the form

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 & i\alpha & 0 \\ -i\alpha & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_2 \end{bmatrix} \quad (3.9)$$

where ε_1 , α , and ε_2 are real numbers. This corresponds to a gyroelectric material biased by a magnetic field pointing in the z direction. Similarly, $\mathcal{T}$ can be broken in gyromagnetic materials via the permeability tensor. For a magnetic bias in the

z direction, the permeability tensor has the form

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 & i\kappa & 0 \\ -i\kappa & \mu_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (3.10)$$

where μ_1 and κ are real.

3.1.3 Non reciprocal photonic crystals

In PhCs with broken $\mathcal{T}$ symmetry, electromagnetic wave propagation is “non-reciprocal”. This means that it is possible to have a wave traveling in one direction, with wave-vector $\mathbf{k}$, without the existence of another wave with wave-vector $-\mathbf{k}$. In particular, it is possible to have modes that travel unidirectionally along an edge of the crystal, as occurs in “photonic topological insulators” (PTIs). The theory of topological insulators in PhCs was introduced in Refs. [34, 35], based on TE (transverse electric) modes in a gyroelectric PhC. Fig. 3.1(a) shows the band structure of an ordered hexagonal lattice [34, 35]. For isotropic permittivity $\varepsilon = 14$, the TE band shows “Dirac-point” degeneracy; this degeneracy is lifted upon the introduction of an anisotropic ε , opening up a band gap where one-way edge modes reside.

However, it is difficult to realize the PhC proposed in Refs. [34, 35], because actual gyroelectric materials have very weak gyromagnetic ratios (in terms of Eq. (3.9), $|\alpha| \ll \varepsilon_1$). This means that the frequency width of the topological band gap, in which the unidirectional modes reside, is extremely small relative to the operating frequency. Therefore, the edge states are too weakly-confined to be observable in a lattice of realistic dimensions.

The first experimental realization of a PTI was achieved using TM (transverse magnetic) modes of a gyromagnetic PhC. The system is sandwiched between metal

plates, as shown in Fig. 3.1(b), so that the fields are effectively 2D. At microwave frequencies, gyromagnetic materials such as yttrium iron garnet (YIG) have high gyromagnetic ratios under reasonable magnetic field strengths [38, 65]. In the absence of a magnetic field (unbroken $\mathcal{T}$ symmetry), the PhC is designed so that there is a degeneracy (or “band crossing point”) somewhere in the band structure [37, 38]. As soon as the external magnetic field is applied (breaking $\mathcal{T}$ symmetry), the band degeneracy can be lifted, opening a topologically nontrivial band gap.

Each photonic band in a 2D crystal is characterized by a topological invariant called the Chern number [34, 37]. The Chern number of the n -th photonic band is defined as [37]

$$\begin{aligned} \mathcal{C}_n &= \frac{1}{2\pi i} \int_{BZ} d^2k \left(\frac{\partial \mathcal{A}_y^{nn}}{\partial k_x} - \frac{\partial \mathcal{A}_x^{nn}}{\partial k_y} \right) \\ &= \frac{1}{2\pi i} \int_{BZ} d^2k (\nabla_k \times \vec{\mathcal{A}}^{nn}(k)) \cdot \hat{z}. \end{aligned} \quad (3.11)$$

Here, the integral is taken over the 2D Brillouin zone, and the vector $\vec{\mathcal{A}}^{nn'}(k)$, known as Berry connection, is given by

$$\begin{aligned} \vec{\mathcal{A}}^{nn'}(k) &\equiv \langle \psi_{nk} | \nabla_k | \psi_{n'k} \rangle \\ &= \int_{\Omega} d^2r \psi_{nk}^* \nabla_k \psi_{n'k}. \end{aligned} \quad (3.12)$$

Here, $|\psi_{nk}\rangle$ denotes the Bloch wavefunction for band n and wavevector k , and ∇_k denotes the k -space derivative. The integral on the last line is taken over the real-space unit cell Ω .

For a $\mathcal{T}$ symmetric photonic crystal, all the bands have trivial Chern number: $\mathcal{C}_n = 0$. However, if $\mathcal{T}$ is broken, the bands may acquire non-zero Chern numbers. Such bands are said to be “topologically nontrivial”. In the presence of topologically nontrivial bands, the “bulk-edge correspondence principle” [37] states that a finite lattice (i.e., a lattice containing edges) will exhibit “topological edge states”

Figure 3.2: Electric field (E_z) distribution, with red/blue corresponding to positive/negative colors. Each structure consists of gyromagnetic rods arranged in a square lattice, with a PEC edge on the top and surrounded on other three sides by perfectly-matched layers (PMLs). The rods have dielectric constant $\epsilon = 15$, radius $r = 3.9$ mm, and lattice constant $a = 40$ mm. (a)–(b) $\mathcal{T}$ symmetric case, with isotropic permeability $\mu = 1$. A steady state point TM source (star), emitting at frequency $f = 4.5$ GHz, is placed at position $\mathbf{A}$ in (a), and a symmetric point $-\mathbf{A}$ in (b). (c)–(d) $\mathcal{T}$ -broken case, with anisotropic permeability $[\mu_1 = 14, \kappa = 12.4]$; see Eq. (3.10)]. In both cases, the waves emitted by the point sources are confined to the edge, and travel unidirectionally from left to right.

(TESs) within certain band gaps. More precisely, we can characterize each band gap by an integer $\Delta\mathcal{C}$, the sum of the Chern numbers for the bands below the gap. Then $\Delta\mathcal{C}$ is equal to the net number (right-moving minus left-moving) of topological edge states in that gap.

Fig. 3.1(c) shows the projected band structure of the system of gyromagnetic rods in square crystal array. It can be observed that there are topological edge states (red curve) between 4 GHz and 5 GHz [38]. Moreover, some of the bands have non-zero Chern numbers $\mathcal{C}$. The experimentally-obtained forward and backward transmission measurements reveal a huge suppression of the backward transmission, implying the presence of the one-way edge states around 4.5 GHz, as shown in Fig. 3.1(d).

Fig. 3.2 shows simulation results illustrating the behavior of TESs in a gyromagnetic PhC. Here, the electric field (E_z) distribution is plotted in red and blue colors. The PhC consists of gyromagnetic rods arranged in a square lattice, surrounded by air, similar to Refs. [37, 38]. The upper edge of the lattice is a perfect electric conductor (PEC), and the other three boundaries have perfectly matched layers (PML) to absorb the impinging waves. The parameters are chosen according to the literature [37, 38], with rod radius $r = 3.9$ mm, lattice constant $a = 40$ mm, and dielectric constant $\varepsilon = 15$. Fig. 3.2 (a)–(b) shows the case of unbroken $\mathcal{T}$ symmetry, with isotropic permeability $\mu = 1$. Steady state TM point sources emit at frequency 4.5 GHz, at the position $\mathbf{A}$ in 3.2(a), and position $-\mathbf{A}$ in Fig. 3.2(b). Evidently, waves are emitted in both directions.

Fig. 3.2(c)–(d) shows the case where the gyromagnetic rods are biased by a magnetic field, so that the permeability becomes anisotropic (hence, $\mathcal{T}$ is broken). In the parameterization of Eq. (3.10), we take $\mu_1 = 14$ and $\kappa = 12.4$. We find that the wave emitted by the point sources only travel from left to right, and are confined to the edge. This is evidence for the existence of a TES in the $\mathcal{T}$ -broken

Figure 3.3: Robustness of edge states against localized defects. The PhC consists of a square lattice of $\mathcal{T}$ -broken gyromagnetic rods, with parameters the same as in Fig. 3.2(c)–(d). (a) Edge state propagation with localized defects, consisting of two rods removed along the PEC edge (denoted by dashed green circles). The boundary conditions are the same as in Fig. 3.2, with PEC on top and PMLs on other three sides. A point source at **A** (star), emitting at 4.5 GHz, produces a TES that bypasses the defects without backscattering. (b) A defect is introduced in the form of a slab (grey rectangle) of perfectly conducting material, with dimension $0.4a \times 3a$, where a is the lattice constant. The TES again bypasses the defect without backscattering.

PhC.

Because they originate from a topological property of the underlying bandstructure, TESs are highly robust to isolated disorder and defects [34, 35, 37, 38, 67, 69]. Fig. 3.3(a) shows an example of a PTI (based on square lattice of $\mathcal{T}$ -broken gyromagnetic rods, with the same parameters as above), in which a localized defect is introduced by removing two rods along the PEC edge. The TES, emitted by a 4.5 GHz point source at point **A**, bypasses the defects without any backscattering whatsoever. Even when we insert a large obstacle in the form of a conducting slab, as shown in Fig. 3.3(b), the edge states travel around the obstacle and continue moving left-to-right along the edge. Other works have shown how TESs can guide light around arbitrarily-shaped patches, including zig-zag edges [72].

However, the robustness of these photonic TESs have all been tested only in the case where the underlying lattice is an ordered PhC. In this chapter, I present a theoretical investigation into the case where the underlying lattice has

an amorphous character, having some short-range order but lacking long-range order. In particular, we wish to know if the TES phenomenon survives into the amorphous regime, with the same properties as in the crystalline case. As discussed in Chapters 1 and 2, there have been multiple studies of amorphous $\mathcal{T}$ -symmetric photonic lattices; it has been shown that band gaps can persist into the amorphous regime, resulting in observable phenomena such as Q -factor enhancements [25, 26, 33, 62]. However, this has not previously been observed for “topologically nontrivial” photonic band gaps, which occur in $\mathcal{T}$ -broken lattices. I will work with a lattice of gyromagnetic rods, very similar to the design used in Refs. [37, 38, 65, 66]. Similar to Chapter 2, I use molecular dynamics simulations to assign the rod positions, so that the level of short-range order can be controlled by the parameters of the placement algorithm. I will then investigate the existence of TESs in the amorphous lattices, and study their various properties, including the isolation ratio, group velocity, and confinement factor.

3.2 Band structure of a gyromagnetic triangular photonic crystal

Our 2D amorphous photonic lattices are based on gyromagnetic rods arranged in the x - y plane, surrounded by air. As mentioned above, the structure is assumed to be sandwiched between parallel metal plates, so that within the operating frequency region there are only 2D TM modes, with out-of-plane electric field (E_z) and magnetic field parallel to the x - y plane [37, 38, 65]. Because the amorphous lattice sites are to be generated by a packing algorithm (see below), let us first study the case of perfect packing, which corresponds to a triangular lattice.

Consider a triangular lattice with lattice constant $a = 30.91$ mm, rod radius $r = 0.11a$, and dielectric constant $\varepsilon = 15$. These parameters are deliberately chosen to

Figure 3.4: (a) Transverse Magnetic (TM) band structure of a triangular PhC (inset), consisting of gyromagnetic rods with radius $r = 3.4$ mm, nearest-neighbor spacing $a = 30.91$ mm, permittivity $\epsilon = 15$, and anisotropic isotropic permeability $\mu = 1$. (b) Band structure of the same lattice, with anisotropic permeability $\mu_{xx} = \mu_{yy} = 14$, $\mu_{zz} = 1$, $\mu_{xy} = -\mu_{yx} = 10i$. Topological band gaps are highlighted in green. The Chern number $\mathcal{C}$ for each band is indicated.

be similar to previous experiments on YIG PhCs [37, 38, 65] (except that those used square and honeycomb lattices, rather than a triangular lattice). Fig. 3.4(a) shows the bandstructure in the $\mathcal{T}$ -symmetric case where the permeability is isotropic ($\mu = 1$). Observe that the second and third bands have Dirac point degeneracies at the K and K' points (the corners of the hexagonal Brillouin zone), while the third and the fourth bands have quadratic and Dirac band crossing at Γ (the center of the Brillouin zone) as well as along the zone boundaries.

The degeneracy of the bands is now lifted by making the permeability tensor $\boldsymbol{\mu}$ anisotropic. In the parameterization of Eq. (3.10), we take $\mu_1 = 14$ and $\kappa = 10$ (this matches actual materials such as YIG, at microwave frequencies with a magnetic bias of ~ 0.1 T). The resulting bandstructure is shown in Fig. 3.4(b). Note that the band degeneracies between bands 2, 3, and 4 are lifted, producing bandgaps at $4.382 \text{ GHz} \leq f \leq 4.536 \text{ GHz}$ and $4.611 \text{ GHz} \leq f \leq 4.672 \text{ GHz}$.

By computing the Chern numbers of the photonic bands [37, 73], we find that

the lowest bands have Chern numbers of $\mathcal{C} = \{0, 1, -2, 1\}$. Hence, according to the discussion in Section 3.1.3, the lowest band gap is trivial ($\Delta\mathcal{C} = 0$), while the next two higher-order gaps are nontrivial ($\Delta\mathcal{C} = 1$ and $\Delta\mathcal{C} = -1$ respectively).

3.3 Generating the amorphous lattices

The amorphous structures are generated using molecular dynamics simulations [25], similar to the method used in Chapter 2. The procedure is illustrated in Fig. 3.5. We start with a random distribution of 400 disks in a circular region. The disks are bidisperse, with radius ratio 1:1.2 with 50:50 distribution. At first the disks are assigned small radius and hence a small value of filling fraction. We then run the molecular dynamics simulation, in which the disks are slowly inflated (i.e. radius is increased), resulting in a jam-packing of the disks. The simulation continues running until a target filling fraction Φ is reached.

After achieving the desired Φ , the actual gyromagnetic rods are placed at the centers of the disks. We then choose the length scale and rod radius so that (i) the amorphous lattice has the same average filling fraction as the equivalent triangular lattice described in Section 3.2, and (ii) the rod radius r is the same as in the equivalent triangular lattice. Finally, the lattice is truncated to the desired shape.

The results are shown in Fig. 3.5. Higher values of Φ , which we call the “packing parameter”, correspond to a lattice that is more ordered. But even in the relatively ordered case shown in Fig. 3.5(a), corresponding to $\Phi = 0.7$, there is no long-range periodicity.

To quantify the level of short-range order, we compute the correlation function $C(\Delta r)$, which is defined as

$$C(\Delta r) = \frac{\langle \Theta(\mathbf{r} + \Delta \mathbf{r}) \Theta(\mathbf{r}) \rangle}{\langle \Theta(\mathbf{r}) \rangle^2} - 1. \quad (3.13)$$

Figure 3.5: Procedure for generating the amorphous lattice. (a) Start with a random configuration of 400 bidisperse disks with radius ratio 1.2 (50:50 distribution). The radius of the disks is assigned a small value (maintaining 1.2 ratio), so that the filling fraction is small. The disks are then packed by running a molecular dynamics simulation in which the radius of all the disks slowly increases, until they reach a target filling fraction Φ . We call Φ the “packing parameter”. In the final step, we place gyromagnetic rods at center of the disks, and assign rod radius and the length scale so that the rod radius and average filling fraction are the same as in the ordered triangular lattice. Here, we show the results for $\Phi = 0.7$. (b)–(c) show configurations with $\Phi = 0.4$ and 0.1. Higher value of Φ correspond to higher levels of short-range order.

Figure 3.6: (a) Spatial correlation function $C(\Delta r)$ for different values of Φ , ensemble averaged over 100 different samples for each value of Φ . Inset: close-up for the peak of $C(\Delta r)$ corresponding to the nearest neighbor. (b) Ensemble averaged (over 100 different samples) correlation function for different values of rod radius, with fixed packing parameter $\Phi = 0.7$. Inset: close-up of the peak of $C(\Delta r)$ corresponding to nearest neighbor.

Here, $\Theta = 1$ inside the rods and $\Theta = 0$ outside the rods. Fig. 3.6(a) plots the correlation function for different values of Φ from 0.1 to 0.7. For each Φ , $C(\Delta r)$ is averaged over 100 different samples, and $\mathbf{r}$ is 450 different sampling points within each sample. For higher values of Φ , the first order correlation peak can be observed around $\Delta r \approx a$, which is typically of the order of nearest neighbor distance in the ordered lattice. With increase in Δr the correlation function decreases indicating the absence of long-range order and presence of short-range order. For $\Phi = 0.1$, the first order peak almost disappears indicating the presence of very weak short-range order and high positional disorder.

In Fig. 3.6(a), we also observe that for higher values of Φ , $C(\Delta r) \approx -1$ to the left of the first-order peak. This can be understood from the definition of the correlation function in Eq. (3.13). For our choice of rod radius r , the average distance between rods (determined by the radii of the discs during the packing simulation) is significantly larger than r (see Fig. 3.5). Therefore, as we move away from the center of each rod, there tends to be on average no other rod up to a distance of $\sim a$. In other words, the short-range order gives rise to an effective short-range repulsion between the rods. If we increase the rod radius relative to a , that tends to smear out the correlation function, as shown in Fig. 3.6 (b). Note that changing the rod radius does not shift the position of the first-order correlation peaks.

3.4 Bulk states and Edge states

3.4.1 Calculation of the spectral weight

In order to study the topologically trivial and nontrivial band gaps in the amorphous lattices, we calculate the “spectral weight” of the TM electromagnetic modes. The setup for the calculation is shown in Fig. 3.7(a). We take a square section of

Figure 3.7: (a) Schematic for calculation of spectral weight: a square section of amorphous lattice is surrounded by air, with a circular perfectly-matched layer (PML) boundary. The structure is excited by a TM point source, of fixed current amplitude, at the center of the lattice (star). The resulting field intensity $|E_z|^2$ is averaged over the lattice (square) region. (b) Schematic for the calculation of isolation ratio. The upper edge has perfect electric conductor (PEC) as boundary and the other three sides are surrounded by PML. The structure is excited by a TM point source at A (star) and electric field intensity is measured at point B (blue circle). In both subplots, we also plot the real electric field E_z (with red/blue colors corresponding to positive/negative values) produced by the source at frequency 4.448 GHz; the amorphous lattice in this case has packing parameter $\Phi = 0.7$.

the amorphous lattice of size, L^2 (where $L = 48.49$ cm), surrounded by air, with a circular perfectly-matched layer (PML) to serve as a perfect absorber. The electromagnetic modes of the structure are excited using a steady-state TM point source (i.e., a wire pointing in the out-of-plane direction), with a fixed current amplitude. Our estimate for the spectral weight consists of the mean of the field intensity $|E_z|^2$, taken over the lattice area. This is then further averaged over 10 independently-generated samples of the amorphous lattice (with the same Φ).

Fig. 3.8(a) plots the resulting mean spectral weight versus frequency, for different values of Φ . Three dips can be observed, which roughly coincide with the band gaps of the triangular photonic crystal shown in Fig. 3.4(b). The dips are more prominent for higher values of Φ (i.e., more short-range order).

These observations are consistent with the previous studies [25, 26, 33] on $\mathcal{T}$ -symmetric lattices, where dips in the photonic density of states were observed to coincide band gaps of the equivalent ordered lattices. In this case, however, we observe dips that correspond not only to the first (primary) band gap, but also two higher-order band gaps, which are known to be topologically nontrivial.

3.4.2 Calculation of isolation ratio

Next, we seek to determine whether the dips in the spectral density coincide with unidirectional edge states. To do this, we use the setup shown in Fig. 3.7(b). A square section of the amorphous lattice (consisting on average of 266 rods) is bounded on the top edge by a perfect electric conductor (PEC), while the other three sides have PMLs to absorb impinging waves. A steady-state TM point source is placed at point A , near the PEC edge; the field intensity $I_{AB} = |E_z|^2$ is measured using a point probe at B , some distance away along the edge. We then repeat the simulation, switching the positions of the source and probe; the intensity measured at A is denoted by I_{BA} .

Figure 3.8: (a) Spectral weight versus frequency, averaged over 10 configurations for each value of packing parameter Φ . For $\Phi = 0.7$, three prominent spectral dips are observed, which diminish with greater disorder (smaller Φ). (b) Isolation ratio ($\mathcal{I}_R$) versus frequency. It can be observed that $\mathcal{I}_R$ is near-unity in the trivial band gap region, but peaked in the frequency ranges corresponding to the topologically nontrivial band gaps. (c)–(d) Close-ups of (a) and (b) in this frequency range.

The isolation ratio $\mathcal{I}_R$ is then defined as

$$\mathcal{I}_R = \frac{I_{AB}}{I_{BA}}. \quad (3.14)$$

If $\mathcal{T}$ symmetry is unbroken, it follows from optical reciprocity that $\mathcal{I}_R = 1$. On the other hand, we expect $\mathcal{I}_R$ to depart significantly from unity if the system hosts unidirectional (or strongly-directional) edge states.

The isolation ratio is calculated for the same frequency range over which we calculated the spectral weight. The results are averaged over 10 independent samples, for each value of Φ . In the results plotted in Fig. 3.8(b), we observe that $\mathcal{I}_R \approx 1$ throughout the spectral dip corresponding to the primary photonic band gap. This is consistent with theoretical predictions that the primary gap is topologically nontrivial (see Section 3.2). But at the frequencies of the higher-order dips, we observe prominent peaks in the isolation ratio. The existence of these peaks, as well as their different directions, is consistent with the fact that the corresponding photonic band gaps are topologically nontrivial, with opposite signs of $\Delta\mathcal{C}$, as shown in Fig. 3.4(b).

Fig. 3.8(c)–(d) show magnified views of the spectral weight and isolation ratio, in the frequency region corresponding to the “topologically nontrivial” spectral dips. We can see that with decreasing Φ (decreasing short-range order), the spectral dip becomes less prominent, and practically disappears for $\Phi = 0.1$. However, even when there is no discernable spectral dip, we can still observe a substantial enhancement in $\mathcal{I}_R$. This interesting result appears to be consistent with a theoretical principle, originating in theoretical studies of the quantum Hall effect, that robust edge states require only a mobility gap, not a spectral gap [74]. It is also reminiscent of the earlier findings, in $\mathcal{T}$ -symmetric amorphous structures, that even after a gap appears to close due to disorder, remnant effects such as

Figure 3.9: Field distribution of the edge states for two different lattice shapes. The steady-state real electric field E_z is plotted (with red/blue colors corresponding to positive/negative values). Point TM sources are placed at positions indicated by stars, and operate at 4.448 GHz (within the first topological gap). The lattices are generated with packing parameter $\Phi = 0.5$, and are surrounded by PEC on all edges.

Q-factor enhancements persist near the gap frequency [25, 26, 33, 62].

From the field distributions, we can verify that the enhanced transmission near the “topologically nontrivial” spectral dips occurs primarily along the edges. An example of this is shown in Fig. 3.7(b). In Fig. 3.9, we also plot the field distributions for circular and triangular boundaries, demonstrating that the propagation follows curved edges and sharp corners.

3.5 Group velocity and penetration depth

A more rigorous way to establish the presence of the edge states is to calculate the group velocity v_g . The ballistic nature of photonic topological edge states has previously been demonstrated using a perfectly-ordered bulk lattice with a deformed edge [72]. Here, we seek to perform a similar investigation for our amorphous system. The setup is similar to Fig. 3.7(b), except that we use a single source and multiple equally-spaced probes which are placed along the edge near the PEC boundary. At each of the probes, the phase φ is measured (by recording the real and imaginary parts of the electric field E_z) as a function of the

angular frequency $\omega = 2\pi f$. We perform this measurement at 21 equally-spaced frequencies in the range $4.4292 \text{ GHz} \leq f \leq 4.4677 \text{ GHz}$. This frequency range lies in the first non-trivial gap, and coincides with the first peak of the isolation ratio $\mathcal{I}_R$ (see Section 3.4.2).

To calculate the group velocity, for a given sample we calculate the dwell time $d\varphi/d\omega$. This is done at each probe (as a function of ω), and then averaged over all the probes, and further averaged over 10 different samples for each value of disorder parameter Φ .

Fig. 3.10(a) shows the dwell time vs path length (s) plots for different values of Φ . The group velocity v_g is calculated as the inverse of the slope; the linear fits have coefficient of determination $R^2 > 0.9$ for all the different amorphous systems with $0.1 \leq \Phi \leq 0.7$. For higher values of Φ , the value of v_g is quite close to the value obtained for the equivalent ordered lattice. However with increasing disorder (decreasing Φ), v_g becomes smaller. The linear scaling of $d\varphi/d\omega$ with path length s is a signature of ballistic transport, and supports the conclusion that these modes of the amorphous lattice are qualitatively similar to the TESs of the ordered PTI.

To verify that the group velocity calculations are correct, we perform a band structure calculation for a 1D supercell consisting of 13 unit cells of the gyromagnetic ordered triangular lattice; the results are shown in the inset of Fig. 3.10(b). We then estimate the TES group velocity by taking the slope $d\omega/dk$ of the dispersion curve in the same frequency range (4.4292 to 4.4677 GHz). The result is $v_g = 0.045c$, close to the value obtained from the dwell time calculation.

Finally, we verify in Fig. 3.11 that the propagating waves are exponentially localized to the edge. Here, we use a setup similar to Fig. 3.7(b), but with multiple probes placed in a grid (with x -spacing $1.1a$ and y -spacing $0.75a$, and 11 probes for each y). The normalized intensity $I = |E_z|^2$ is then averaged over the probes, over 21 equally-spaced frequencies in $4.4292 \text{ GHz} \leq f \leq 4.4677 \text{ GHz}$, and over 10

Figure 3.10: (a) Dwell time $d\phi/d\omega$ versus path length s , plot for different values of packing parameter Φ , ensemble averaged over 10 samples for each Φ (calculation procedure has been described in text) in the frequency range $4.4292 \text{ GHz} \leq f \leq 4.4677 \text{ GHz}$. Also shown is the plot for the “equivalent” ordered triangular lattice. The error bars are the standard deviations and the linear fits give group velocity v_g , with c as the speed of light. (b) Bandstructure for a strip of the triangular lattice. This is calculated using a supercell (shown inset) of 13 unit cells, with PEC boundaries in the x directions and Bloch-Floquet boundary conditions at the upper and lower edges (the y direction). The group velocity for supercell is measured by calculating the slope $d\omega/dk_y$ (where $\omega = 2\pi f$) in the frequency range $4.4292 \text{ GHz} \leq f \leq 4.4677 \text{ GHz}$, bounded by the red broken lines.

Figure 3.11: Semi-logarithmic plot of the intensity I versus the distance from the edge y . As explained in the text, I is the value of $|E_z|^2$ averaged over probe positions in grid formation (overlaid on the amorphous structure), then further averaged over a frequency band and 10 independent lattice samples. The results demonstrate that the emitted waves are exponentially localized to the edge, $I \propto \exp(-\beta y)$. Inset: plot of the fitted values of β versus Φ (this includes values of Φ which were not shown in the main plot for clarity of presentation).

independent lattice realizations for each Φ . Using these results, we perform a fit $I \propto \exp(-\beta y)$ to extract the inverse penetration depth β , which is found to increase with Φ (i.e., more ordered lattices exhibit stronger confinement). The result shows that the modes are clearly exponentially localized to the edge. The result, shown in the inset to Fig. 3.11, shows that β is larger (i.e., the edge modes are more strongly confined) for more ordered lattices.

3.6 Conclusion

The results in this chapter show that the topological edge states of photonic topological insulators persist into the disordered regime. This study was based on amorphous lattices, generated using a packing algorithm that allowed us to control the level of short-range order [25, 75]. For strong short-range order, the lattices exhibit spectral dips that are obvious counterparts of the ordered lattice’s photonic band gaps—not just the topologically trivial primary gap, but also the topologically nontrivial higher-order gaps. Strongly non-reciprocal, ballistic, edge-localized transmission is observed at frequencies corresponding to the topologically nontrivial gaps. This confirms the principle that topological edge states should be protected against disorder; in the photonic context, this protection had previously been probed using localized defects or edge deformations “overlaid” on an ordered bulk [37, 38, 72].

Edge state dominated transmission was observed even when the short-range order is so weak that the spectral dips are not discernable, which appears to be consistent with theoretical arguments that edge states in disordered systems rely on the existence of a mobility gap, not a spectral gap [74]. The evidence is not conclusive, however, because our sample sizes are too small to distinguish between localized and extended bulk states (and hence to locate the mobility gaps). Larger-

scale numerical studies might be able to identify the percolating bulk states, and probe their relationship with the edge states.

The lattice parameters that I have chosen are consistent with previously-reported experiments [38, 65, 66]. Hence, these amorphous photonic lattices may be a fruitful experimental photonic platform for studying various effects involving topological band structures and disorder, such as topological Anderson insulators [76, 77] and the floating or annihilation of extended states [78–81].

Chapter 4

The FLAME-slab Method for Electromagnetic Wave Scattering in Slab Structures

This work was done in collaboration with Prof. Igor Tsukerman from the University of Akron.

4.1 Introduction

4.1.1 Electromagnetic wave scattering in slab structures

The scattering of electromagnetic waves in a structured photonic slab is an important but challenging class of problems in computational electromagnetics. Typically, such a structure consists of one or more layers of finite thickness, stacked along the “vertical” axis (z), whereas along the other two “horizontal” directions (the x - y plane) the slab is effectively infinite in extent but spatially non-uniform [7]. For the case of photonic crystal slabs, the horizontal modulations are periodic.

Slab structures encompass a wide range of important photonic devices, including photonic crystal slab lasers and metasurfaces.

The wave scattering problem is commonly tackled using standard finite element (FE) and finite difference (FD) discretization schemes, with absorbing conditions or perfectly matched layers (PMLs) to simulate the infinite free space region outside the slab. When dealing with photonic crystal slabs, however, there are two alternative computational methods that are more suitable to use, being specially formulated for periodic slab geometries. These are Rigorous Coupled Wave Analysis (RCWA) [43, 44] and the Vertical Mode Expansion Method (VMEM) [82]. In RCWA, 2D Fourier transforms are performed within each horizontal layer, and the solutions are matched along the layer boundaries. In VMEM, a mode expansion is performed on a set of vertical boundaries (e.g., cylinder or hole surfaces) in each unit cell, and boundary integral equations are used to match the expansions between adjacent cells.

All of these methods are fairly efficient when dealing with photonic crystal slabs, where the periodicity can be exploited so that the effective computational domain consists of just one horizontal unit cell. The problem becomes significantly more severe when there is no horizontal periodicity, such as for random or amorphous patterned slabs [26, 27, 33, 54, 62, 83, 84]. To simulate a non-periodic slab, it is generally necessary to take a horizontal supercell, which in turn requires a large mesh (for FE and FD methods) or a high-order series expansion (for RCWA and VMEM).

We will explore a computational method, which we call FLAME-slab, that is adapted to solving the wave scattering problem in *amorphous* slab structures, in which the horizontal patterning exhibits short-range order but no long-range periodicity. Amorphous photonic slabs have been studied in many theoretical and experimental works [26, 27, 33, 54, 62, 83, 84]. Among other interesting

features, such structures are able to exhibit spectral gaps similar to the band gaps of photonic crystals; but unlike the photonic crystal case, these gaps are highly isotropic, because they are produced by short-range order without the existence of special crystalline axes.

The method is based on the use of Trefftz approximations—that is, approximations generated using *local* basis functions that satisfy the underlying differential equations (Maxwell’s equations) locally. Previously, Trefftz approximations have been successfully used in classical variational contexts (FE-Trefftz methods), in Discontinuous Galerkin methods, and in a nonstandard FD scheme known as FLAME (the Flexible Local Approximation Method) [41, 42]. Our FLAME-slab approach uses small-scale RCWA simulations to calculate a set of local basis functions, which are then fed into FLAME to generate the FD scheme for the entire supercell. Due to the short-range order of the amorphous structure, we only need a small number of RCWA simulations, carried out over “representative unit cells” much smaller than the supercell representing the full amorphous lattice. When the FLAME algorithm uses these basis functions to generate the FD scheme, it makes the appropriate adjustments to account for the differences between the representative unit cells and the actual local structure. The basis functions can be precomputed and re-used, which is very helpful for studies that involve ensemble averages over multiple independent amorphous lattice realizations. The FLAME scheme is supplemented by radiation boundary conditions, computed via Fast Fourier Transforms (FFT). The supercell calculations are tractable because the FD mesh can be very coarse, with as few as three grid layers across the thickness of the slab.

Figure 4.1: Schematic for a typical RCWA calculation. The structure consists of a photonic crystal with a square hole (black) in the center of each unit cell. The unit cell is divided into different layers, which can have different dielectric constants. A plane wave is incident from the $-z$ side, with wave vector $\mathbf{k}_{\text{in}}$, which has in-plane projection k . In a given layer n , α_n and β_n denote the forward and backward propagation coefficients.

4.1.2 Rigorous Coupled Wave Analysis (RCWA)

In this section, we briefly review how the Rigorous Coupled Wave Analysis (RCWA) method solves the electromagnetic wave scattering problem in slab structures [43, 44]. We closely follow the RCWA formulation used by the S^4 (Stanford Stratified Structure Solver) program [44], which is employed as a subroutine of our FLAME-slab solver.

The slab is assumed to be periodic in the horizontal (in-plane) directions, and divided into layers that are stacked in the vertical (z) direction. Within each layer, the dielectric function ε is assumed to be z -independent. The electric field $\mathbf{E}$ and magnetic field $\mathbf{H}$ obey the frequency-domain Maxwell equations

$$\nabla \times \mathbf{E} = i\omega\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}, \quad (4.1)$$

where ω is the frequency. We employ computational units, and take the magnetic

permeability to be unity ($\mathbf{B} = \mathbf{H}$). As shown in Fig. 4.1, a plane wave is incident from the $-z$ direction, with wave vector $\mathbf{k}_{\text{in}}$. We denote its projection onto the horizontal plane by $\mathbf{k}$. The scattered field, to be determined, is purely outgoing at infinity.

Due to the in-plane periodicity, we can perform a 2D in-plane Fourier decomposition of the electromagnetic field in each layer [85]. The $\mathbf{H}$ field expansion has the form

$$\mathbf{H}(\mathbf{r}, z) = \sum_{\mathbf{G}} \tilde{\mathbf{H}}_{\mathbf{G}}(z) \exp[i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}], \quad (4.2)$$

where $\mathbf{r} = (x, y)$ denotes in-plane coordinates, $\{\mathbf{G}\}$ is the set of reciprocal lattice vectors, and $\tilde{\mathbf{H}}_{\mathbf{G}}(z)$ is the Fourier expansion coefficient. The series expansion is circularly truncated: i.e., an upper bound for $|\mathbf{G}|$ is specified, and only reciprocal lattice vectors within that bound are included in the series. The coefficients are then assembled into a finite complex vector

$$h_j(z) = \begin{pmatrix} \tilde{H}_{G_1}^j(z) \\ \tilde{H}_{G_2}^j(z) \\ \vdots \end{pmatrix}, \quad j \in \{x, y, z\}. \quad (4.3)$$

The electric field $\mathbf{E}$, electric displacement field $\mathbf{D}$, and dielectric function ε are expanded in a similar way. For the electric field, we define the vector $\mathbf{e}(z)$ in a manner similar to Eqs. (4.2)–(4.3). For the dielectric function, we take

$$\varepsilon(r, z) = \sum_{\mathbf{G}} \tilde{\varepsilon}_{\mathbf{G}}(z) \exp(i\mathbf{G} \cdot \mathbf{r}). \quad (4.4)$$

For simplicity, we take ε to be a scalar; the tensor case can be handled with only a few complications [85]. In the above equation,

$$\tilde{\varepsilon}_{\mathbf{G}}(z) = \frac{1}{A} \int \varepsilon(r) \exp(-i\mathbf{G} \cdot \mathbf{r}) d^2r, \quad (4.5)$$

where the integral is taken over the unit cell, and A is area of the unit cell. From the constituent relation $\mathbf{D} = \varepsilon \mathbf{E}$, we then obtain

$$\tilde{\mathbf{D}}_{\mathbf{G}}(z) = \sum_{\mathbf{G}'} \tilde{\varepsilon}_{\mathbf{G}-\mathbf{G}'}(z) \tilde{\mathbf{E}}_{\mathbf{G}'}(z), \quad (4.6)$$

where $\tilde{\mathbf{D}}_{\mathbf{G}}(z)$ and $\tilde{\mathbf{E}}_{\mathbf{G}}(z)$ are the Fourier components of $\mathbf{D}$ and $\mathbf{E}$, defined similarly to Eq. (4.2). After assembly into vector form similar to Eq. (4.3), the constituent relation (4.6) takes the form

$$d_j(z) = \hat{\varepsilon}(z) e_j(z), \quad (4.7)$$

where $\hat{\varepsilon}(z)$ is a matrix whose components are the various values of $\tilde{\varepsilon}_{\mathbf{G}-\mathbf{G}'}(z)$.

The Maxwell equations (4.1) can then be written as [44]:

$$i\hat{k}_y h_z(z) - \frac{\partial h_y(z)}{\partial z} = -i\omega d_x(z) \quad (4.8)$$

$$\frac{\partial h_x(z)}{\partial z} - i\hat{k}_x h_z(z) = -i\omega d_y(z) \quad (4.9)$$

$$i\hat{k}_x h_y(z) - i\hat{k}_y h_x(z) = -i\omega d_z(z) \quad (4.10)$$

$$i\hat{k}_y e_z(z) - \frac{\partial e_y(z)}{\partial z} = i\omega h_x(z) \quad (4.11)$$

$$\frac{\partial e_x(z)}{\partial z} - i\hat{k}_x e_z(z) = i\omega h_y(z) \quad (4.12)$$

$$i\hat{k}_x e_y(z) - i\hat{k}_y e_x(z) = i\omega h_z(z). \quad (4.13)$$

Here, the $\hat{k}_j$'s denote the diagonal matrix

$$\hat{k}_j = \begin{pmatrix} k_j + G_{1j} & 0 & 0 & \dots \\ 0 & k_j + G_{2j} & 0 & \dots \\ \vdots & \vdots & \ddots & \end{pmatrix}. \quad (4.14)$$

Using Eq. (4.7), (4.10) and (4.13), we get

$$e_z(z) = \frac{1}{\omega} \hat{\varepsilon}^{-1} \left(-\hat{k}_x h_y(z) + \hat{k}_y h_x(z) \right) \quad (4.15)$$

$$h_z(z) = \frac{1}{\omega} \left(\hat{k}_x e_y(z) - \hat{k}_y e_x(z) \right), \quad (4.16)$$

which can be used to eliminate e_z and h_z from the other four equations. First, using Eq. (4.15) on Eqs. (4.11) and (4.12) gives

$$\left[\omega^2 \mathcal{I} - \begin{pmatrix} \hat{k}_y \hat{\varepsilon}^{-1} \hat{k}_y & -\hat{k}_y \hat{\varepsilon}^{-1} \hat{k}_x \\ -\hat{k}_x \hat{\varepsilon}^{-1} \hat{k}_y & \hat{k}_x \hat{\varepsilon}^{-1} \hat{k}_x \end{pmatrix} \right] \begin{pmatrix} h_x(z) \\ h_y(z) \end{pmatrix} = -i\omega \partial_z \begin{pmatrix} -e_y(z) \\ e_x(z) \end{pmatrix}, \quad (4.17)$$

where $\mathcal{I}$ denotes an identity matrix. Second, using Eq. (4.16) on Eqs. (4.8) and (4.9) gives

$$\left[\omega^2 \begin{pmatrix} \hat{\varepsilon} & 0 \\ 0 & \hat{\varepsilon} \end{pmatrix} - \begin{pmatrix} \hat{k}_x \hat{k}_x & \hat{k}_x \hat{k}_y \\ \hat{k}_y \hat{k}_x & \hat{k}_y \hat{k}_y \end{pmatrix} \right] \begin{pmatrix} -e_y(z) \\ e_x(z) \end{pmatrix} = -i\omega \partial_z \begin{pmatrix} h_x(z) \\ h_y(z) \end{pmatrix}. \quad (4.18)$$

It is convenient to define

$$\begin{aligned} \Lambda_e(z) &\equiv \begin{bmatrix} -e_y(z) \\ e_x(z) \end{bmatrix}, \quad \Lambda_h(z) \equiv \begin{bmatrix} h_x(z) \\ h_y(z) \end{bmatrix}, \\ \mathcal{K}_1 &\equiv \begin{bmatrix} \hat{k}_y \hat{\varepsilon}^{-1} \hat{k}_y & -\hat{k}_y \hat{\varepsilon}^{-1} \hat{k}_x \\ -\hat{k}_x \hat{\varepsilon}^{-1} \hat{k}_y & \hat{k}_x \hat{\varepsilon}^{-1} \hat{k}_x \end{bmatrix} \\ \mathcal{K}_2 &\equiv \begin{bmatrix} \hat{k}_x \hat{k}_x & \hat{k}_x \hat{k}_y \\ \hat{k}_y \hat{k}_x & \hat{k}_y \hat{k}_y \end{bmatrix} \\ \mathcal{E} &= \begin{pmatrix} \hat{\varepsilon} & 0 \\ 0 & \hat{\varepsilon} \end{pmatrix}. \end{aligned} \quad (4.19)$$

Then Eqs. (4.17) and (4.18) can be written more compactly as

$$\left(\omega^2 \mathcal{I} - \mathcal{K}_1\right) \Lambda_h(z) = -i\omega \partial_z \Lambda_e(z), \quad (4.20)$$

$$\left(\omega^2 \mathcal{E} - \mathcal{K}_2\right) \Lambda_e(z) = -i\omega \partial_z \Lambda_h(z). \quad (4.21)$$

To proceed, we consider values of z lying within a single layer, and particular solutions such that the z -dependence goes as $\exp(i\gamma z)$ for some $\gamma \in \mathbb{C}$. For instance, in the $\mathbf{H}$ -field expansion (4.2), we let

$$\mathbf{H}_{\mathbf{G}} = \begin{pmatrix} \psi_{\mathbf{G},x} \\ \psi_{\mathbf{G},y} \\ \psi_{\mathbf{G},z} \end{pmatrix} \exp(i\gamma z) \quad (4.22)$$

for some $\psi_{\mathbf{G},x}$, $\psi_{\mathbf{G},y}$, and $\psi_{\mathbf{G},z}$. Then we can replace ∂_z with $i\gamma$ in Eqs. (4.20) and (4.21), and combine the two equations to yield

$$\left(\omega^2 \mathcal{E} - \mathcal{K}_2\right) \left(\omega^2 \mathcal{I} - \mathcal{K}_1\right) \Psi_h = \omega^2 \gamma^2 \Psi_h, \quad (4.23)$$

where

$$\Psi_h = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix}, \quad \psi_j = \begin{pmatrix} \psi_{G_1}^j(z) \\ \psi_{G_2}^j(z) \\ \vdots \end{pmatrix}. \quad (4.24)$$

Using (4.23), along with the fact that $\mathcal{K}_2 \mathcal{K}_1 = 0$ [which can be verified using (4.19); note that the $\hat{k}_j$ matrices are diagonal], we find that γ^2 is an eigenvalue of the matrix

$$\mathcal{A}(\omega) = \omega^2 \mathcal{E} - \mathcal{E} \mathcal{K}_1 - \mathcal{K}_2. \quad (4.25)$$

The eigenvectors of this matrix are used as a basis for expanding the field coeffi-

Figure 4.2: Run time vs N_G for the S^4 RCWA solver, plotted with (a) linear scales, and (b) logarithmic scales with a best-fit plot (slope 2.7235).

cients in the layer:

$$h_j(z) = \sum_m \psi_m^j \left(\alpha_m \exp(i\gamma_m z_n) + \beta_m \exp[i\gamma_m(d_n - z)] \right), \quad (4.26)$$

where $\{\gamma_m, \psi_m^j\}$ are obtained from the m -th eigensolution, and α_m and β_m are forward and backward scattering coefficients at $z = z_n$ and $z = z_n + d_n$, respectively. These scattering coefficients can then be worked out by the scattering matrix method [86], which relates the amplitudes of the forward and backward travelling waves, α_n and $\beta_{n'}$ in two different layers by the equation:

$$\begin{pmatrix} \alpha_n \\ \beta_{n'} \end{pmatrix} = \mathbf{S}(n', n) \begin{pmatrix} \alpha_{n'} \\ \beta_n \end{pmatrix}, \quad (4.27)$$

where $\mathbf{S}(n', n)$ is the scattering matrix. By repeated application of Eq. (4.27), we can match the fields to the incoming wave at the outmost layer, and hence calculate the reflection and transmission coefficients, and hence all other quantities of interest [44].

The runtime of the RCWA calculation is determined by the integer N_G , the number of reciprocal lattice vectors $\mathbf{G}$ included in the vectors $h_j(z)$, $e_j(z)$, etc. The

method involves running an eigensolver on the matrix $\mathcal{A}(\omega)$ defined in Eq. (4.25), which has $O(N_G)$ rows/columns and is non-sparse [see (4.17)]. Moreover, assembling the matrix requires the calculation of the $\hat{\varepsilon}$ matrix, which has $O(N_G)$ rows/columns and is non-sparse. Hence, the runtime scaling is

$$t_{\text{RCWA}} \sim O(N_G^3). \quad (4.28)$$

Fig. 4.2 shows the runtime vs N_G for actual calls to the S^4 RCWA solver (the solver is run on the structure described in Section 4.4, which will be the basis of our numerical tests). A linear fit of $\log(\text{runtime})$ versus $\log(N_G)$ gives a slope of ≈ 2.7325 , consistent with Eq. (4.28).

4.1.3 The FLAME approach

Here, we review the numerical method known as FLAME (the Flexible Local Approximation MEthod) [41, 42], which is the basis of our FLAME-slab scheme. In FLAME, the computational domain is divided into overlapping patches, and the underlying differential equations are solved within each patch (either analytically or numerically) to obtain a set of *local* basis functions. The basis functions are then used to generate a finite-difference (FD) equation for the entire domain. If done correctly, the resulting FD scheme can give very accurate results, even for a coarsely discretized grid. As discussed in Section 4.1.1, this is an especially attractive feature when dealing with amorphous photonic structures.

The essentials of FLAME can be demonstrated using a simple example, involving Laplace's equation in 1D [41]:

$$\frac{d^2}{dx^2} \psi = 0. \quad (4.29)$$

As shown in Fig. 4.3(a), the 1D space is discretized into M equally-spaced nodes (in this case $M = 7$), indexed by $n = 0, 1, 2, \dots$. Each set of three adjacent nodes constitutes a “patch”, as shown in Fig. 4.3(b). Each of the overlapping patches can be indexed by the node at its center.

In the vicinity of any given node n , the solution can be written in the form

$$\psi(x) = \alpha_1 \varphi_1(x) + \alpha_2 \varphi_2(x), \quad (4.30)$$

where $\varphi_1(x)$ and $\varphi_2(x)$ are basis functions that satisfy Eq. (4.29), while α_1 and α_2 are constants. We are free to pick convenient basis functions, and take $\varphi_1(x) = 1$, $\varphi_2(x) = x$. Therefore, the solution at the three grid points centered around n has the form

$$\psi(x_\gamma) = \alpha_1 \varphi_1(x_\gamma) + \alpha_2 \varphi_2(x_\gamma), \quad \gamma \in \{n-1, n, n+1\}. \quad (4.31)$$

This can be written in matrix form as

$$\boldsymbol{\psi} = \mathbf{N} \boldsymbol{\alpha}, \quad (4.32)$$

where

$$\boldsymbol{\psi} = \begin{pmatrix} \psi(x_{n-1}) \\ \psi(x_n) \\ \psi(x_{n+1}) \end{pmatrix}, \quad \mathbf{N} = \begin{pmatrix} 1 & x_{n-1} \\ 1 & x_n \\ 1 & x_{n+1} \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}. \quad (4.33)$$

We seek an equation of the form

$$\mathbf{s}^T \boldsymbol{\psi} = 0, \quad (4.34)$$

where $\mathbf{s}$ is a vector of “stencil coefficients” to be determined. (This equation will constitute one line of the FD matrix equation describing the entire system.)

Figure 4.3: Schematic for 1D FLAME calculation: (a) Discretization of the 1D space into nodes x_n ($n = 0, 1, 2, \dots$). (b) Construction of stencil patches for nodes in (a), each patch contains three nodes and overlap with neighboring patch; β denotes the patch number.

Combining this with Eq. (4.32) gives

$$\mathbf{s}^T \mathbf{N} \boldsymbol{\alpha} = 0, \quad (4.35)$$

Since $\boldsymbol{\alpha}$ is an arbitrary vector, it follows that $\mathbf{s}^T \mathbf{N} = 0$. Hence, we can pick $\mathbf{s}$ to be any vector in the null space of $\mathbf{N}^T$:

$$\mathbf{s} \in \text{null}(\mathbf{N}^T). \quad (4.36)$$

By repeating this procedure for all n , we can assemble a FD matrix equation for the entire problem.

Another simple example is the 1D Helmholtz equation [41],

$$\left(\frac{d^2}{dx^2} + k^2 \right) \psi(x) = 0. \quad (4.37)$$

Consider, for simplicity, a patch with three equally-spaced nodes at $x = [-h, 0, h]$. We choose the basis function $\varphi_1 = \exp(ikx)$ and $\varphi_2 = \exp(-ikx)$, which satisfy

Eq. (4.37). Then, following the same steps as Eqs. (4.31)–(4.33) gives

$$\mathbf{N}^T = \begin{pmatrix} \exp(-ikh) & 1 & \exp(ikh) \\ \exp(ikh) & 1 & \exp(-ikh) \end{pmatrix}. \quad (4.38)$$

Hence, we can choose

$$\mathbf{s} = \begin{pmatrix} 1 \\ -2 \cos(kh) \\ 1 \end{pmatrix} \in \text{null}(\mathbf{N}^T). \quad (4.39)$$

Note that if we Taylor expand $\cos(kh)$ to order $(kh)^2$, this result is equivalent to the usual FD scheme based on the three-point discretization rule.

4.2 Finite-difference scheme for slab geometry

We will apply the ideas of FLAME to a slab structure. As a proof of concept, we restrict ourselves to a slab that is modulated in only one horizontal direction, x , and uniform along y . Hence, the system is effectively 2D. However, the method presented here is generalizable to fully 3D problems.

4.2.1 Grid layout

The setup is shown in Fig. 4.4. We restrict our attention to transverse magnetic (TM) polarization, or s -polarization, for which the electric field points along y while the magnetic field lies in the x - z plane. A TM-polarized plane wave is incident from the $-z$ (“top”) side of the slab. Our goal is to obtain the scattered electric and magnetic fields.

The computational domain consists of a horizontal supercell of length L_x with

Figure 4.4: Orientation of the slab structure (light blue colored structure) and the discretization grid. Each grid column m contains three layers of grid points. Each patch is defined by a 9-point stencil centered on one column. The field variables are the y component of the electric field, E_m^μ , defined at all grid points, and the x -component of the magnetic field, $H_m^\pm$, defined only along the two outer layers. Hence, each patch contains 15 variables. The overall grid has periodicity L_x along the x direction.

column indices $m = 0, 1, 2, \dots, N - 1$ (using periodic boundary conditions, so that column N is equivalent to column 0). For each m , there are three grid points in the z direction, denoted by $\mu \in \{+, 0, -\}$ for the top, middle, and bottom layers. The two outer grid layers must lie in the external, “free space”, region (see Section 4.2.3). Our computational variables are (i) the y -polarized electric fields in the three layers, denoted E_m^μ , and (ii) the x -component of the magnetic field, denoted $H_m^\pm$. As discussed below, we need not include the magnetic field in the middle layer, or the z -component of the magnetic field, in our calculation; these variables can be extracted from the solution. These field variables refer to the *total* fields; the decomposition into incident and scattered fields is discussed later in Section 4.2.2.

For each m , we define a 9-point patch centered around that column, as shown in Fig. 4.4. Each patch thus supports 15 field variables: 9 electric field variables defined on all layers, and 6 magnetic field variables on the top and bottom layers.

The system contains N columns, with periodic boundary conditions along the x direction:

$$E_0^\mu = E_N^\mu, \quad \mu \in \{+, 0, -\}, \quad \text{and} \quad H_0^\pm = H_N^\pm. \quad (4.40)$$

Hence, there are $15N$ field variables in total.

4.2.2 Organization of stencil coefficients

We now consider each 9-point patch individually. From each patch, we will derive 3 equations using FLAME. Repeated over all patches, this will yield a total of $3N$ equations in total; the remaining $2N$ equations needed to invert the FD problem come from the scattering conditions, described in Section 4.2.3.

The stencil coefficients are derived in the following way. Let the patch index be m , and denote the columns *within the current patch* by $n \in \{-1, 0, 1\}$. The patch is divided into three non-distinct subsets, as shown in Fig. 4.5; each sub-patch will yield one equation.

The first sub-patch, shown in Fig. 4.5(a), consists of the E field variables only,

Figure 4.5: Breakdown of patch S_2 into three parts.: Each patch is broken down into three subpatches. An example of three subpatches of patch S_2 in Fig.4.4. (a) Subpatch 1: with 9 point nodes having single DOF. (b) Subpatch 2: 6 node patch with three nodes having double DOF in upper layer. (c) Subpatch 3: 6 node patch with double DOF in the lower layer.

defined at all 9 nodal points. It produces a FD equation of the form

$$\sum_{n=-1}^1 (s_{m+n}^{00} E_{m+n}^+ + s_{m+n}^{01} E_{m+n}^0 + s_{m+n}^{02} E_{m+n}^-) = 0. \quad (4.41)$$

The second sub-patch, shown in Fig. 4.5(b), consists of two layers of grid points only, but includes both the electric and magnetic fields. The FD equation has the form

$$\sum_{n=-1}^1 (s_{m+n}^{10} E_{m+n}^+ + s_{m+n}^{11} E_{m+n}^0 + s_{m+n}^{13} H_{m+n}^+) = 0. \quad (4.42)$$

The final sub-patch is shown in Fig. 4.5(c), and produces the FD equation

$$\sum_{n=-1}^1 (s_{m+n}^{21} E_{m+n}^0 + s_{m+n}^{22} E_{m+n}^- + s_{m+n}^{24} H_{m+n}^-) = 0. \quad (4.43)$$

These three equations can be combined into

$$\mathbf{A}^{(m)} \boldsymbol{\psi}^{(m)} = 0, \quad (4.44)$$

where $\mathbf{A}^{(m)}$ is a 3×15 matrix containing the coefficients s_{m+n}^{pq} (where p, q are whole numbers) and $\boldsymbol{\psi}^{(m)}$ is a vector containing the 15 field variables in patch m .

In order to formulate the wave scattering problem, we seek an *inhomogenous* equation. This is done by splitting each of the field variables into incident and scattered parts:

$$\begin{aligned} E &= E_{\text{in}} + E_s \\ H &= H_{\text{in}} + H_s. \end{aligned} \quad (4.45)$$

This decomposition is applied to each of Eqs. (4.41)–(4.43). For Eq. (4.41), we

obtain

$$\sum_{n=-1}^1 (s_{m+n}^{00} E_{m+n,s}^+ + s_{m+n}^{01} E_{m+n,s}^0 + s_{m+n}^{02} E_{m+n,s}^-) = b_0,$$

$$\text{where } b_0 = - \sum_{n=-1}^1 (s_{m+n}^{00} E_{m+n,\text{in}}^+ + s_{m+n}^{01} E_{m+n,\text{in}}^0 + s_{m+n}^{02} E_{m+n,\text{in}}^-), \quad (4.46)$$

and similarly for Eqs. (4.42) and (4.43). This yields

$$\mathbf{A}^{(m)} \boldsymbol{\psi}_s^{(m)} = \mathbf{b}^{(m)}, \quad \mathbf{b}^{(m)} = -\mathbf{A}^{(m)} \boldsymbol{\psi}_{\text{in}}^{(m)}, \quad (4.47)$$

where $\mathbf{A}^{(m)}$ is the matrix of stencil coefficients from Eq. (4.44), while $\boldsymbol{\psi}_{\text{in}}^{(m)}$ and $\boldsymbol{\psi}_s^{(m)}$ are the incident and scattered parts of the field variables within patch m .

4.2.3 Implementation of scattering boundaries

The remaining $2N$ equations impose the condition that the scattered electromagnetic fields must be purely outgoing. There are N equations for the top layer and N for the bottom layer, each consisting of relations between the scattered electric field E_s and scattered magnetic field H_s .

As noted in Section 4.2.1, the two outer layers of grid points all reside in the external regions, which have $\varepsilon = 1$ extending to infinity. We seek to relate the electric and magnetic field variables at different points within each of these two layers. According to Maxwell's equations (4.1), for TM modes we can relate $H_s(x, z)$ (the x -component of the magnetic field) to $E_s(x, z)$ (the y -component of the electric field) by

$$H_s(x, z) = \frac{i}{\omega} \frac{\partial E_s}{\partial z}. \quad (4.48)$$

Using the fact that the structure has periodicity L_x in the x direction, we can

expand the electric field in the free space regions by

$$E_s(x, z) = \sum_n c_n \exp [i(k_{nz}z + k_{nx}x)] \quad (4.49)$$

where n is summed over integer values and the horizontal wavenumbers k_{nx} have spacing

$$\Delta k_{nx} = 2\pi/L_x. \quad (4.50)$$

Combining Eq. (4.48) and Eq. (4.49) gives

$$H_s(x, z) = -\frac{1}{\omega} \sum_n c_n k_{nz} \exp [i(k_{nx}x + k_{nz}z)]. \quad (4.51)$$

From the dispersion relation in free space, k_{nx} and k_{nz} are related by

$$k_{nz} = \pm \sqrt{\omega^2 - k_{nx}^2}. \quad (4.52)$$

The choice of $\pm$ sign depends on which layer we are interested in. Referring to the grid layout shown in Fig. 4.4, we choose $+$ for the $z = z_+$ layer (on the $-z$ side of the slab), and $-$ for the $z = z_-$ layer (on the $+z$ side of the slab). These choices impose the condition that the scattered waves are *outgoing*, i.e., flowing away from the slab in either direction, towards infinity.

Let us now evaluate (4.49) and (4.51) along the z_+ layer of grid points (the discussion for the z_- layer is almost identical). In the layer, there are N distinct equally-spaced points at

$$x_m = L_x \left(\frac{-1}{2} + \frac{m}{N} \right), \quad m = 0, 1, \dots, N-1. \quad (4.53)$$

Due to the spatial discretization, we can perform the sums over n in Eqs. (4.49) and (4.51) over a finite range of n . In order to sample both positive and negative

wavenumbers, we choose N to be an odd integer and define k_{nx} as

$$k_{nx} = \frac{2\pi}{L_x} \left(n - \frac{N-1}{2} \right), \quad n = 0, 1, \dots, N-1. \quad (4.54)$$

Substitution into Eq. (4.49) gives

$$\begin{aligned} E_s(x_m, z_+) &= \sum_{n=0}^{N-1} c_n e^{ik_{nz}z_+} e^{2\pi i m n / N} e^{-in\pi} e^{i\pi(\frac{1}{2} - \frac{m}{N})(N-1)} \\ &= N \cdot \text{IFT} \left\{ c_n e^{-in\pi} e^{ik_{nz}z_+} \right\}_m e^{-im\pi(1-\frac{1}{N})} e^{\frac{i\pi}{2}(N-1)}, \end{aligned} \quad (4.55)$$

where $\text{IFT}(\dots)$ denotes the inverse discrete Fourier transform. Hence,

$$c_n e^{-in\pi} e^{ik_{nz}z_+} = \frac{1}{N} e^{-\frac{i\pi}{2}(N-1)} \text{FT} \left\{ E_s(x_m, z_+) e^{im\pi(1-\frac{1}{N})} \right\}_n, \quad (4.56)$$

where $\text{FT}(\dots)$ denotes the discrete Fourier transform. Applying this to Eq. (4.51), we obtain

$$\begin{aligned} H_s(x_m, z_+) &= -\frac{N}{\omega} \cdot \text{IFT} \left\{ c_n k_{nz} e^{-in\pi} e^{ik_{nz}z_+} \right\}_m e^{-im\pi(1-\frac{1}{N})} e^{\frac{i\pi}{2}(N-1)} \\ &= -\frac{1}{\omega} e^{-im\pi(1-\frac{1}{N})} \text{FT} \left\{ k_{nz} \text{FT} \left\{ E_s(x_{m'}, z_+) e^{im'\pi(1-\frac{1}{N})} \right\}_n \right\}_m. \end{aligned} \quad (4.57)$$

Here, k_{nz} is given by Eq. (4.52) with the $+$ sign. The result for the z_- layer is identical, except that Eq. (4.52) is used with the $-$ sign.

For each boundary layer, Eq. (4.57) contributes N distinct equations, one for each value of m . Thus, the scattering boundary conditions contribute $2N$ equations in total.

4.2.4 Assembling the finite-difference matrix equation

Based on the discussion in Sections 4.2.2–4.2.3, we have $5N$ distinct equations for the $5N$ field variables in the system. The equations have the form

$$\mathbf{A}\boldsymbol{\psi}_s = \mathbf{b}, \quad (4.58)$$

where $\boldsymbol{\psi}_s$ is a $5N$ -component vector of scattered field variables, of the form

$$\boldsymbol{\psi}_s = \begin{pmatrix} \mathbf{E}^+ \\ \mathbf{E}_s^0 \\ \mathbf{E}_s^- \\ \mathbf{H}_s^+ \\ \mathbf{H}_s^- \end{pmatrix}. \quad (4.59)$$

$\mathbf{A}$ is a $5N \times 5N$ matrix of the form

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{\text{FLAME}} \\ \mathbf{A}_{\text{BC}} \end{pmatrix}. \quad (4.60)$$

Here, $\mathbf{A}_{\text{FLAME}}$ is a $3N \times 5N$ sparse sub-matrix containing the FD stencil coefficients; these coefficients will be generated via FLAME, as discussed in Section 4.3. The vector on the right-hand side in (4.58), has the form

$$\mathbf{b} = \begin{pmatrix} -\mathbf{A}_{\text{FLAME}}\boldsymbol{\psi}_{\text{in}} \\ \mathbf{0} \end{pmatrix}, \quad (4.61)$$

where $\boldsymbol{\psi}_{\text{in}}$ is defined similarly to (4.59) but using the field variables for the incident wave, and $\mathbf{0}$ is a vector of $2N$ zeros.

In Eq. (4.60), $\mathbf{A}_{\text{BC}}$ is a $2N \times 5N$ sub-matrix which can be derived from (4.57).

It contains the coefficients of the linear expression

$$H_s(x_m, z_{\pm}) + \frac{1}{\omega} e^{-im\pi(1-\frac{1}{N})} \text{FT} \left\{ k_{nz}^{(\pm)} \text{FT} \{ E_s(x_{m'}, z_{\pm}) e^{im'\pi(1-\frac{1}{N})} \}_n \right\}_m, \quad (4.62)$$

computed for each m and each of the two outer layers ($\pm$). This sub-matrix is non-sparse, so if we explicitly construct it and use it to solve Eq. (4.58), the overall runtime is $O(N^3)$.

A speedup can be achieved if we avoid computing $\mathbf{A}_{\text{BC}}$ directly, and instead solve Eq. (4.58) using an iterative solver such as GMRES (the Generalized Minimum Residual Method). Each step of the iterative solver calls a subroutine to evaluate the matrix-vector product $\mathbf{A}\psi$ for some trial solution ψ . The first $3N$ components are evaluated using the sparse stencil matrix $\mathbf{A}_{\text{FLAME}}$, as discussed above; the remaining $2N$ components are computed from Eq. (4.62) using the Fast Fourier Transform (FFT) algorithm. For a non-sparse matrix, the runtime to compute a matrix-vector product scales as $O(N^2)$; by using the FFT, the runtime scaling is $O(N \log N)$. Hence, if GMRES finds the solution with efficiency comparable to an eigensolver, the overall problem will be solvable in $O(N^2 \log N)$ time.

4.3 Generation of FLAME stencil coefficients

In this section, we describe how FLAME is used to generate the $\mathbf{A}_{\text{FLAME}}$ matrix defined in Section 4.2.4.

The procedure is shown schematically in Fig. 4.6. We assume that the slab consists of rods of height d , placed on a substrate of thickness d . The rods need not be equally-spaced. The rods and substrate have the same dielectric constant ϵ , and are surrounded by air. The computational domain has length L_x in the x direction, divided into N equally-spaced columns.

Figure 4.6: (a) Schematic of a slab consisting of dielectric rods placed randomly on a flat dielectric substrate, surrounded by air. The rods have height $d = 0.25$ and width $w = 0.2$, and the substrate has height $d = 0.25$. Both rods and substrate have dielectric constant $\varepsilon = 12$. The overall structure has length $L_x = 14$, with periodic boundary conditions. Light is incident normally on the structure from the top. (b) The structure is discretized into N_x points along the x direction. On a given column x_m , we define a patch containing a 9-point stencil of grid points. A “local lattice” is defined by locating the rod closest to x_m (say at position x'), and generating a photonic crystal with a rod at x' and periodicity L or $2L$. (c)–(d) Schematic of one unit cell of a local lattice. For each unit cell, we use an RCWA solver subroutine to compute 4 basis functions, corresponding to different input waves with incidence angles $\{\theta_1, \dots, \theta_4\}$.

Consider a 9-point patch centered on an arbitrary column at $x = x_m$. As discussed in Section 4.2.2, we seek stencil equations of the form (4.41), (4.42), and (4.43). Each stencil equation involves 9 field variables (a subset of the 15 field variables within the patch); according to the FLAME procedure outlined in Section 4.1.3, we need 8 basis functions in order to define a 9×8 matrix $\mathbf{N}$, so that $\mathbf{N}^T$ has a one-dimensional null space that defines the 9 stencil coefficients. In other words, we need 8 independent solutions of Maxwell's equations that are valid in the vicinity of x_m .

To accomplish this, we locate the rod nearest to x_m ; let its position be x' . We define a “local lattice” consisting of rods at $x = x' + nL$, where $n \in \mathbb{Z}$ and $L \ll L_x$ is some chosen period. In other words, the local lattice has a period much smaller than the computational domain, but its dielectric function matches the actual structure in the immediate vicinity of x_m . We then call the S^4 program [44], which uses the RCWA method to solve the electromagnetic wave scattering problem for the local lattice. Independent solutions are obtained for four different incident wave angles $\{\theta_1, \dots, \theta_4\}$ (we emphasize that the RCWA solutions' boundary conditions at infinity do *not* need to match those of the actual scattering problem we want to solve). The procedure is repeated for a doubled local lattice period $2L$.

Using the 8 independent RCWA solutions, we apply the FLAME equation $s \in \text{null}(\mathbf{N}^T)$ to different combinations of the field variables, corresponding to Eqs. (4.41), (4.42), and (4.43). For instance, Eq. (4.41) involves only the 9 E -field variables, denoted by E_{m+n}^μ where $n \in \{-1, 0, 1\}$ and $\mu \in \{+, 0, -\}$. We denote the E -field variables in the 8 independent RCWA solutions ($p = 1, \dots, 8$) by $\mathcal{E}_{m+n}^{\mu,p}$. These are used as a basis for the actual E -field within the patch:

$$E_{m+n}^\mu = \sum_{p=1}^8 \alpha_p \mathcal{E}_{m+n}^{\mu,p} = \mathbf{N}\boldsymbol{\alpha}. \quad (4.63)$$

Here, $\mathbf{N}$ is a 9×8 matrix containing the RCWA-derived solutions $\mathcal{E}_{m+n}^{\mu,p}$ (the row index is an aggregate of μ and n , while the column index is p). We compute $\text{null}(\mathbf{N}^T)$, and the result is a set of stencil coefficients $\{s_n^{00}, s_{m+n}^{01}, s_{m+n}^{02}\}$ for Eq. (4.41). This process is repeated for (4.42) and (4.43).

For each m , we thus populate 3 rows in the stencil coefficients matrix $\mathbf{A}_{\text{FLAME}}$ defined in Eq. (4.60). The procedure is carried out for all m , giving us all $3N$ rows of $\mathbf{A}_{\text{FLAME}}$. At this point, we can also use Eq. (4.61) to compute the vector $\mathbf{b}$, which specifies the incident wave.

Many “amorphous” structures of interest, including those studied in previous works, are composed of locally identical elements arranged in a disordered pattern [26, 27, 33, 54, 62, 83, 84]. (The same is true of other kinds of complex structures, such as quasicrystals, which are constructed from a small number of standard “building blocks”.) When this sort of short-range similarity is present, we can use it to avoid calling the RCWA solver (S^4) many times. For the slab structure shown in Fig. 4.6, for instance, all the rods are geometrically identical; only their placement is random. Therefore, when performing fixed-frequency calculations on this kind of slab, we only need to call the RCWA solver 8 times, using the standard rod dimensions (and with different incidence angles and lattice periods, as described above). Each solution is calculated for a relatively large spatial resolution, and cached. Thereafter, when we need to construct the stencil coefficients for each patch m , with nearest rod distance $\Delta = |x_m - x'|$, we refer to the cached solution, shifting by Δ and interpolating to get the fields at the desired grid positions. With this approach, the RCWA solver typically occupies a negligible portion of the total runtime. Even more appealingly, when we need to calculate ensemble averages over multiple independent realizations of the amorphous slab, the cache can be re-used in all the calculations.

4.4 Results

In this section, we present the numerical results produced by our implementation of the FLAME-slab algorithm.

Our test system, shown in Fig. 4.6(a), consists of 10 dielectric rods placed randomly on a flat dielectric substrate. In computational units, the rods have height $d = 0.25$ and width $w = 0.2$, the substrate also has height $d = 0.25$, the dielectric constant of the rods and substrate is $\varepsilon = 12$, and the length of the computational domain (supercell period) is $L_x = 14$. The dielectric constant in the air regions is 1. The horizontal grid layers are placed at $z_+ = 0$, $z_0 = 0.26$, and $z_- = 0.5$. For the FLAME local lattices (Section 4.3), we take $\theta_1 = 36^\circ$, $\theta_2 = 72^\circ$, $\theta_3 = 108^\circ$, and $\theta_4 = 144^\circ$, in *anti-clockwise* direction from the horizontal x -axis.

4.4.1 Calculation of scattered electric and magnetic fields

As described in Section 4.2.1, each FLAME-slab calculation yields the scattered electric field $E_{y,s}$ along the three layers of grid points, which we denote by $\{E_s^+, E_s^0, E_s^-\}$, as well as the scattered magnetic field $H_{x,s}$ along the two outer layers, denoted by $\{H_s^+, H_s^-\}$.

The FLAME-slab solver uses the RCWA-based solver S^4 [44] as a subroutine for generating the FLAME basis functions (the subroutine is called 8 times during each calculation). As described in Section 4.1.2, the accuracy of the RCWA solutions depends on an integer N_G , which specifies the number of reciprocal lattice vectors included in the Fourier expansion. In Section 4.5, we will study how the accuracy of the FLAME-slab result depends on the choice of N_G in the RCWA subroutine. Here, we choose $N_G = 97$, and take $N_x = 101$ grid points in the x direction.

To check for correctness of the FLAME-slab solution, we compare it to a “target solution” obtained by applying S^4 to the entire structure. It is necessary to use a

Figure 4.7: Real parts of the scattered electric field $E_{y,s}$ and magnetic field $H_{x,s}$, calculated along the layers $z_+ = 0$, $z_0 = 0.26$, and $z_- = 0.5$. Blue dots show FLAME-slab results calculated using x -discretization $N_x = 101$ and $N_G = 97$ for the RCWA subroutine. Red lines show the “target solution” produced by running RCWA on the entire structure with $N_G = 1000$. The operating frequency is $f = 0.25$; other system parameters are given in the main text.

much larger value of N_G for the target solution, compared to when we are calling S^4 as a FLAME subroutine, because the entire structure is much larger than FLAME's "local lattice". Here, we use $N_G = 1000$.

The resulting electric and magnetic fields are plotted in Fig. 4.7. The input wave is normally incident, with frequency $f = 0.25$ (in computational units). The FLAME-slab and RCWA results are evidently in excellent agreement.

4.4.2 Calculation of reflectance

Two important quantities, the reflectance R and transmittance T , can be extracted from the FLAME-slab solution. These can be computed using the Poynting vector $\mathbf{S} = \text{Re}[\mathbf{E} \times \mathbf{H}^*]$. For TM (s -polarized) fields, the electric field points along y and the magnetic field points in the x - z plane. Hence, the z component of the Poynting vector is

$$S_z(x, z) = \text{Re} \left[E(x, z) H^*(x, z) \right], \quad (4.64)$$

where E_s is the y -component of the electric field and H_s is the x -component of the magnetic field (which are precisely the field variables used in FLAME-slab).

To obtain the reflectance R , we take the upper layer $z = z_+$, and find the average of S_z over the N_x grid points in that layer. In that calculation, we use only the scattered fields (since only the scattered fields are outgoing):

$$R = -\frac{1}{N_x} \sum_{m=0}^{N_x-1} \text{Re} \left[E_s(x_m, z_+) H_s^*(x_m, z_+) \right]. \quad (4.65)$$

To obtain the transmittance T , we average S_z over the N_x grid points in the lower layer $z = z_-$. In this case, however, both the incident field and the scattered

Figure 4.8: Reflectance R versus frequency for the slab structure shown in Fig. 4.6(a). Blue dots show FLAME-slab results, obtained using x -discretization $N_x = 101$ and using $N_G = 97$ for the RCWA subroutine. The red curve shows the results from direct RCWA calculations, using $N_G = 1000$.

field are outgoing, so we must use the *total* fields ($E = E_{\text{in}} + E_s$ and $H = H_{\text{in}} + H_s$):

$$T = \frac{1}{N_x} \sum_{m=0}^{N_x-1} \text{Re} \left[E(x_m, z_-) H^*(x_m, z_-) \right]. \quad (4.66)$$

Fig. 4.8 plots the reflectance R versus frequency f , for the test slab shown in Fig. 4.6(a). For frequencies $f \lesssim 0.5$, the FLAME-slab results are again in good agreement with the target solution produced by the RCWA solver S^4 . The transmittance is not shown here, but it satisfies the energy conservation condition $R + T = 1$ to high precision.

At higher frequencies, numerical errors are evident in Fig. 4.8. A similar frequency dependence of the numerical errors can also be observed in the field plots. In Fig. 4.7, we showed the results for $f = 0.25$; if this is increased to $f \gtrsim 0.6$, we find substantial deviations between the FLAME-slab and RCWA results. It is to be expected that higher frequencies require finer grid discretization and other parameter adjustments. In the next section, we will undertake an analysis of the

numerical errors in the FLAME-slab method.

4.5 Error Analysis

There are three main sources of error in FLAME-slab. First, the FLAME expansion uses a finite number of basis functions in each stencil (Section 4.1.3), which may not form a complete basis set for expanding the true solutions; intuitively, we expect this problem to be worse if the grid is more coarsely discretized. Second, the basis functions are calculated using the RCWA subroutine (Section 4.3), which itself has finite accuracy, as determined by the parameter N_G (Section 4.1.2). Third, the RCWA solutions are calculated on a discretized grid, and interpolation is used to convert the cached solutions into basis functions for each local stencil.

To help quantify these errors, we define a “consistency error” for the FLAME-slab solution. As described in Sections 4.2.2 and 4.2.4, the FLAME procedure

Figure 4.9: Consistency error ξ versus N_G , the number of reciprocal lattice vectors used in the RCWA subroutine of the FLAME-slab algorithm. The FLAME-slab calculations use the test structure shown in Fig. 4.6(a), with $N_x = 101$ discretization points in the x direction, and a normally incident plane wave of frequency $f = 0.25$. The target solution is obtained from a direct RCWA calculation using $N_G^{(\text{target})} = 1000$. The consistency error is defined in Eq. (4.68).

Figure 4.10: Consistency Error ξ versus N_x , the number of spatial discretization points in the x direction. The three curves correspond to different values of $N_G^{(\text{target})}$, the number of reciprocal lattice vectors used in the target solution obtained using a direct RCWA calculation. The FLAME-slab calculations use the test structure shown in Fig. 4.6(a), with a normally incident plane wave of frequency $f = 0.25$ and $N_G = 97$ for its RCWA subroutine.

generates a matrix $\mathbf{A}_{\text{FLAME}}$ which is intended to satisfy

$$\mathbf{A}_{\text{FLAME}}\boldsymbol{\psi} = 0, \quad (4.67)$$

where $\boldsymbol{\psi}$ is a vector of field variables describing the total (scattered plus incident) field. Therefore, if we know the exact solution $\boldsymbol{\psi}$, we can calculate $\mathbf{A}_{\text{FLAME}}\boldsymbol{\psi}$ and check whether it is indeed the zero vector. In the absence of an exactly-known analytic solution, we use instead a target solution, $\boldsymbol{\psi}_{\text{target}}$, computed using RCWA.

We then define the consistency error ξ as

$$\xi = \text{mean}\left(|\mathbf{A}_{\text{FLAME}}\boldsymbol{\psi}_{\text{target}}|\right), \quad (4.68)$$

where the mean is taken over all vector components. One complication that should be borne in mind is that the target solution is computed using a value of $N_G^{(\text{target})}$ that is large but finite, so it too has some deviation from the “true” solution.

In Fig. 4.9, we show how the consistency error varies with the value of N_G used in the RCWA subroutine. Here, we fix $N_x = 101$, frequency $f = 0.25$, and $N_G^{(\text{target})} = 1000$. As we increase the value of N_G in the RCWA subroutine from 27 to around 100, the consistency error is found to decrease by a factor of 4. Thereafter, the consistency error saturates, no longer decreasing appreciably for larger N_G . The implication is that beyond this point, the error in the FLAME-slab result is dominated by discretization error, rather than the error in the RCWA basis functions.

Next, we investigate how the consistency error varies with the spatial discretization. In Fig. 4.10, we plot ξ versus N_x for fixed $N_G = 97$, and three different choices of $N_G^{(\text{target})}$. All other parameters in the calculation are kept fixed, and the same as in the previous Fig. 4.9. For all three values of $N_G^{(\text{target})}$, the consistency error scales as $\sim 1/N$ within the tested range of N_x . It also decreases with increasing values of $N_G^{(\text{target})}$, indicating convergence toward the “true” solution.

4.6 Conclusion

We have devised a numerical method based on FLAME [41], “FLAME-slab”, which is suitable for solving the wave scattering problem in amorphous photonic slabs. The FLAME procedure generates finite-difference stencil coefficients from a set of basis functions, which are computed using by calling external solver (the RCWA-based program S^4 [44]) as a subroutine. The subroutine solves the wave scattering problem for a set of periodic “local lattices” which are much smaller in size than the actual structure being handled by the FLAME-slab calculation. Moreover, for slab structures containing locally similar elements (e.g., rods that are placed randomly but have identical geometry and dielectric constants), the local lattice solutions only need to be evaluated once, and re-used with the help of interpolation. The

boundary conditions are handled using Fourier transforms, which can benefit from the Fast Fourier Transform (FFT) speedup.

One advantage of the FLAME-slab method over traditional finite-difference and finite-element methods is that a relatively coarse grid can be used without sacrificing accuracy. In the present implementation, for instance, the grid consists of only three horizontal layers (z_+ , z_0 , and z_-).

In future work, we seek to implement the scheme for fully three-dimensional slab structures. More investigation is also needed with respect to the best way to treat the outgoing boundary conditions; instead of the FFT-based scattering conditions described in Section 4.2.3, it may be possible to use boundary element techniques or partially-matched layers [7]. It will also be interesting to explore other methods of generating the basis functions, apart from RCWA, including the Vertical Mode Expansion Method (VMEM) [82].

Chapter 5

Conclusions and Future Directions

In this thesis, I have studied amorphous photonic structures in context of random lasing and photonic topological insulators, and developed a computational method to solve the wave scattering problem efficiently for this class of disordered structures.

In the first part of the thesis, I have shown numerically that high Q -factors, on the order of 10^5 , can be achieved in 2D amorphous photonic structures consisting of dielectric rods connected with veins, for the transverse magnetic (TM) polarization relevant to quantum cascade lasers (QCLs). This Q -factor enhancement is not possible using structures consisting of air holes embedded in dielectric, because such designs do not open TM photonic band gaps (PBGs) efficiently. Our study indicates that rod-and-vein designs are highly promising for lowering the lasing threshold, and including the multi-modal performance, for electrically pumped random QCLs.

The samples studied in this chapter were of fixed size, and the localization length was not systematically studied. In future, it would be interesting to rigorously study the mode localization, and investigate the interplay of Anderson localization and localization due to PBG effects. The next step would be to model the lasing

behavior, possibly using a method such as Self-consistent Ab-initio Laser Theory [87–89], to study the conditions under which strongly multi-modal lasing can occur.

In the second part of the thesis, I presented a numerical study of amorphous lattices of gyromagnetic rods, showing the existence of robust, strongly non-reciprocal edge states. It was observed that even when the disorder was very strong (weak short-range order), there was still a substantial enhancement in the isolation ratio (I_R), implying the presence of the edge states. The study was done using a microwave-regime design, using ferrite materials biased by a magnetic field to break time-reversal symmetry. In order to make the results in this work more experimentally relevant, it would be interesting to extend the concept of amorphous photonic topological insulators to optical-regime structures that do not require time-reversal symmetry breaking, such as arrays of helical optical waveguides.

In the last part of the thesis, I devised a numerical method to efficiently solve the wave-scattering problem in amorphous photonic slab structures having short-range order. This novel method, called “FLAME-slab”, is based on the Flexible Local Approximation Method (FLAME) scheme, using Rigorous Coupled Wave Analysis (RCWA) as a subroutine to calculate the basis states. The boundary conditions in the outermost layers are handled through Fast Fourier Transforms (FFTs). A key advantage of this method, compared to standard finite element or finite difference methods, is that it does not require very large meshes; for instance, the computation of solutions can be done using as few as three grid layers across the thickness of the slab. Thus far, I have only implemented this method for solving two-dimensional problems (where the slab lies in the x direction and the out-of-plane direction is z). In the future, I plan to extend the implementation to handle fully 3D structures (where the slab lies in the x - y plane). If successful, this would provide a more efficient way to study a variety of disordered slab structures, as well as other slab designs such as aperiodic lattices and topological defect structures

[26, 27, 30, 33, 54, 62, 90, 91].

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