# Propagation of light near the band edge in one-dimensional multilayers

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Optical systems offer rich modulation in light propagation, but sufficient quantitative descriptions lack when highly complex structures are considered since practical structures contain defects or imperfections. Here, we utilize a method combining a data-fitting method and a time-resolved system to describe light propagation near the band edges in one-dimensional structures. Calculations after optimization of the method show little deviation to the measurements.

**Keywords:** light propagation, band edge, light localization

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## 1. Introduction

The propagation of light in the optical systems has attracted interests in research. Due to different constructions of structure, the optical systems show distinct properties of light propagation. Periodic and quasi-periodic structures, with their feature sizes comparable to the wavelength of light, have bandgaps and pseudo-gaps.[1–3] In addition, the latter exhibits properties which periodic crystals do not have, such as self-similar properties[4,5] and critical states.[6] Although band gaps do not appear in a totally random structure, numerous work has reported on intriguing effects. In terms of multiple scattering, light localization can exist in structures with disorder introduced,[7–12] as its electronic counterpart in solids firstly predicted by Anderson.[13] This stimulates exploration in research of studying and modulating light propagation, and inspires many studies on weak localization,[14,15] random lasing,[17–20] light diffusion,[21–25] etc.

Modulation of light propagation[26–28] motivates different constructions of photonic structures. Strong stretching pulses are observed through the band-edge states in Fibonacci multilayers,[6,29] and the optical modes are also reported as ones with fast decay in a positional-disordered multilayer.[30] In higher-dimensional structures, strong scattering changes light propagation[31] in random medium and group-velocity dispersion near the band edge in periodic structures.[32] However, disorders or imperfections are inevitably contained in practical structures. This may result in different or even undesirable light transport. It is efficient to characterize a structure with simple design, but it is nearly impossible for highly complex structures with disorders or imperfections. Some methods of characterization even need theoretical assumptions ahead. Nevertheless, work on the characterization of structures is still limited in quantitative methods.

In this work, we illustrate quantitatively that numerical simulations of light propagation become closer to the measurements in one-dimensional (1D) multilayers of periodic and Fibonacci types, without any assumption made ahead. Combined with a data-fitting method based on the Levenberg–Marquardt (LM) algorithms[33] and a time-resolved system, simulations show slight deviations of spectra and time constants to the measurements, although the simulation before optimization shows huge deviation. Such a method can be extended for characterization for more different and complex optical systems and stimulate further applications of light propagation.

## 2. Results and discussion

The studied 1D structures are periodic and Fibonacci, consisting of layers of two materials, $SiO_2$ and $TiO_2$. The Fibonacci multilayer belongs to the quasi-periodic structures and forms in a specific fashion[1,6,29]

$$F_i = F_{i-2} + F_{i-1}, \tag{1}$$

where in our work $F_0$ is chosen to be the layer of $TiO_2$ and $F_1$, $SiO_2$, and $i$ is 12 so that the 12-order Fibonacci structure contains 233 layers. As a comparison, the periodic structure is constructed with 232 layers. Due to little absorption in the near-infrared regime, these two materials create an advantageous condition for measurements of localization near the band edge. Therefore, the band gaps of the periodic and the Fibonacci multilayers are designed to be centered at 1.62 μm and 1.74 μm, respectively. The samples, between 25 μm and 30 μm thick, are fabricated on the substrate K9 glass with the thickness of 1.5 mm. Transmittance spectra are measured at

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normal incidence by Fourier infrared spectrometer. Figure 1 (black dashed lines) shows the transmittance spectra near the band edges of the periodic (left panel) and the Fibonacci structures (right panel).

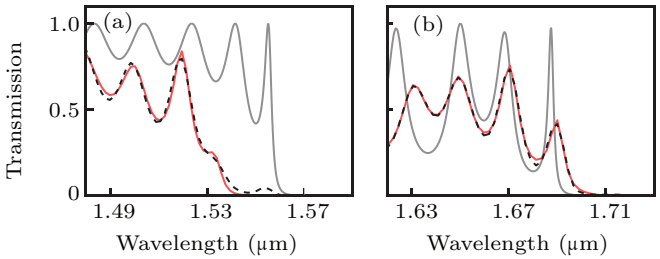



**Fig. 1.** Transmittance spectra of the samples with (a) the periodic and (b) the Fibonacci structures, respectively. In each panel, transmittance spectra obtained in calculations before optimization (grey solid lines), after optimization (red solid lines) and measured by Fourier infrared spectrometer (black dashed lines) are all normalized.

To carry out the comparison between calculations and measurements of the spectra, we employ the finite-difference time-domain method (FDTD) to obtain the spectra. As can be seen in Fig. 1, the measured (grey solid lines) and the calculated (red solid line) spectra are totally different in both structures. The spectral shift in wavelength and the sharp edges of the band gap are observed in the calculated spectra in comparison with the measured spectra. This deviation may indicate that the samples are not exactly the same as designed, and may lead to different numerical descriptions of the behaviors of light propagation in time domain.

To find out where this deviation originates from, we apply a data-fitting method based on the LM algorithms to optimize the parameters of multilayers. In this method, the gradients can be obtained through the back-propagation algorithms, and the process of optimization is achieved in a reasonable time. It uses initial values of thickness and refractive index of each layer in 1D structures, and alters them layer by layer, according to the measured spectra. When finishing this process, it generates a set of optimized parameters for structures of which the spectra can fit better to the measurements. In our optimization, the refractive index is given by the Cauchy's equation, and only the thickness is set for optimization. As a result of the optimization, the method produces random parameters for both types of the samples, and the optimized thickness fluctuates randomly from its designed values. This verifies that the two samples are not perfectly periodic or quasi-periodic in thickness. The imperfections could be introduced during the complicated fabrication. Moreover, as presented in Fig. 1 (red solid line), the calculated spectra after optimization are slightly deviated from the measurements.

To compare the properties of light propagation near the band edges in time domain, we build a time-resolved system. It works as follows. First, a femtosecond pulse of laser goes through a beam splitter, divided into two directions. One goes through the sample and the other through the delay-line which scans in the propagating direction. These two separated beams meet again at a nonlinear crystal at a small angle, focused and overlapping mostly to produce a sum-frequency generation (SFG) signal. The two original light beams and their second-harmonic generation signals are blocked. The SFG signal is detected by a photodetector placed behind as the delay-line moves, and a pulse envelope is recorded in time domain after the process finishes. The duration and repetition rate of the pulse are 150 fs and 1 kHz. As shown in Fig. 2, the pulse is more stretching and delayed in the long-time tail (black solid lines) when the wavelength is near the band edge, while the pulse decays much faster (red solid lines) as the wavelength moves away from the band gap. Additionally, the Fibonacci structure possesses an oscillatory profile in the pulse envelope (Fig. 2(b), black solid line), which could be explained by mode beating.[6] All the pulses shift later after 2 ps mainly because of the delay which the substrate introduces. We can see that the light propagation near the band edge is strongly and differently modulated in these two structures.

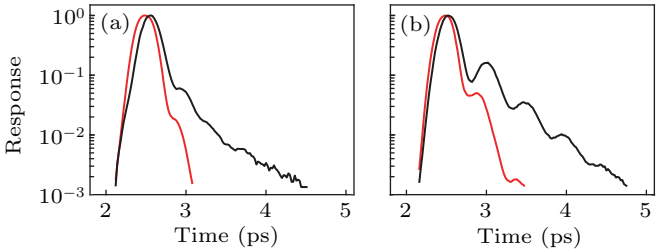



**Fig. 2.** Measured transmitted signals of (a) the periodic structure and (b) the Fibonacci structure in time domain. Red and black solid lines represent responses passing at wavelengths within the pass band and near the band edge, respectively.

For further details of light propagation near the band edges, we vary the wavelength of light pulses near the band edges in these two structures. Two time constants are used here: delay time and decay time.[6,34] Delay time is calculated as the difference of the center of mass of envelopes between one pulse propagating through the sample and one through only the substrate. Decay time is the time constant obtained by fitting an exponential-decay function to the long-time tail of the pulse envelope. As shown in Fig. 3 (black dots), the time constants both show an increase near the band edge as wavelength increases for the periodic and the Fibonacci structures. In addition, in the periodic structures (Figs. 3(a) and 3(b)), both of the time constants remain unchanged at first, and decrease slightly in the bandgap, while in Fibonacci structures (Figs. 3(c) and 3(d)), they exhibit a constant increase as wavelength increases. These different changes of light propagation in the Fibonacci structure could result from the effect of the pseudo-gap. All the error bars in measurements are standard deviations in experiments.

What we are more concerned about in terms of the results is how well numerical simulations and measurements can fit.

Therefore, we firstly use the same initial values before optimization to simulate pulses transporting through multilayers by the FDTD method. In the simulation, the pulse duration is set to be 150 fs and the wavelength varies as used in the measurements. The calculations (Fig. 3, grey dots) show a large deviation from measurements: the time constants are three to four times larger near the band edges in both structures, although they match well at first. The deviation of the time constants indicates again that the samples are not in perfect order or quasi-order. Then, we use the optimized parameters obtained before, to reconstruct multilayers, and simulate pulses propagating in the structures under the same conditions, as shown in Fig. 3 (red dots). Surprisingly, the calculated delay and the decay time increase more slightly near the band edges, and fit better with the experimental results. The comparison again illustrates that the samples contain disorder in thickness, and this disorder could be introduced in the fabrication of samples. Notice that in the periodic structure, both of the time constants in simulations after optimization reach the highest values at a shorter wavelength, compared to the measured one. This could be explained by the fact that the transmittance spectrum after optimization is slightly deviated near the band edge.

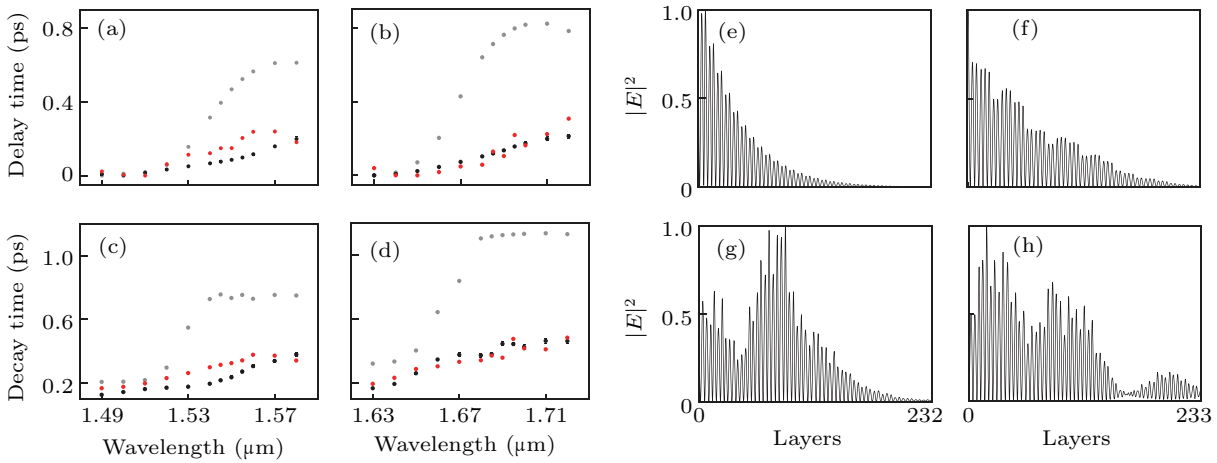



**Fig. 3.** Delay time (a) and decay time (b) of the periodic structure, and delay time (c) and decay time (d) of the Fibonacci structure near the band edges. The grey and the red dots represent simulation results before and after optimization, and the black dots, the experimental measurements. A constant is subtracted from the results of the delay time. The calculated intensity distributions (e)–(h) near the band edges of two structures. (e) and (f) The periodic and the Fibonacci structures before optimization. (g) and (h) The periodic and the Fibonacci structures after optimization.

To find out why there is a huge difference in light propagation between calculations before and after optimization, we could turn to the existence of extended necklace states,[30] which exhibit more symmetric pulses with fast decay compared to localized states. As can be seen in Fig. 3, the intensity distributions are calculated near the band edges of the structures. Figures 3(e) and 3(f) illustrate that before optimization, the intensity decays exponentially, which shows light localization. Figures 3(g) and 3(h) show different profiles, which are the onset of the necklace states. Also, these extended necklace states can coexist with the localized states in the samples. Thereby, the emergence of the necklace states could be responsible for the measurements to have such a huge drop from the calculation before optimization.

## 3. Conclusion

We compare the time-resolved results between the periodic and the Fibonacci structures, and between simulations and measurements. Light propagation is strongly modulated near the band edge in the periodic and the Fibonacci multilayers. Without any assumption made ahead, the deviations between simulations and experiments reduce or even disappear after optimization. The deviations could be the result of the disorder which can be introduced in the process of the fabrication. Using the data-fitting method, combined with the time-resolved system can help to study light propagation in more disordered and complex structures, and to offer desirable designs of the structures to obtain the modulation in light propagation.

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## References

[1] Steurer W and Sutter-Widmer D 2007 *J. Phys. D* **40** R229
[2] Vardeny, Z V, Nahata A and Agrawal A 2013 *Nat. Photon.* **7** 177
[3] Xu X S, Chen H D and Zhang D Z 2005 *Chin. Opt. Lett.* **3** S194

[4] Gellermann W, Kohmoto M, Sutherland B and Taylor P C 1994 *Phys. Rev. Lett.* **72** 633
[5] Dal Negro L, Stolfi M, Yi Y, Michel J, Duan X and Kimerling L C 2004 *App. Phy. Lett.* **84** 5186
[6] Dal Negro L, Oton C J, Gaburro Z, Pavesi L, Johnson P, Lagendijk A, Righini R, Colocci M and Wiersma D S 2003 *Phys. Rev. Lett.* **90** 055501
[7] John S 1984 *Phys. Rev. Lett.* **53** 2169
[8] Arya K, Su Z B and Birman J L 1986 *Phys. Rev. Lett.* **57** 2725
[9] John S 1987 *Phys. Rev. Lett.* **58** 2486
[10] Wiersma D S, Bartolini P, Lagendijk A and Righini R 1997 *Nature* **390** 671
[11] Stöerzer M, Gross P, Aegerter C M and Maret G 2006 *Phys. Rev. Lett.* **96** 063904
[12] Schwartz T, Bartal G, Fishman S and Segev M 2007 *Nature* **446** 52
[13] Anderson P W 1958 *Phys. Rev.* **109** 1492
[14] Van Albada M P and Lagendijk A 1985 *Phys. Rev. Lett.* **55** 2692
[15] Sapienza R, Mujumdar S, Cheung C, Yodh A G and Wiersma D 2004 *Phys. Rev. Lett.* **92** 033903
[16] Lawandy N and Balachandran R 1995 *Nature* **373** 204
[17] Wiersma D S and Lagendijk A 1996 *Phys. Rev. E* **54** 4256
[18] Cao H, Zhao Y G, Ho S T, Seelig E W, Wang Q H and Chang R P H 1999 *Phys. Rev. Lett.* **82** 2278
[19] Fallert J, Dietz R J B, Sartor J, Schneider D, Klingshirn C and Kalt H 2009 *Nat. Photon.* **3** 279
[20] Yao K, Feng G Y, Yang L L, Yi J Y, Song Y S and Zhou S H 2012 *Chin. Opt. Lett.* **10** 082901
[21] Rossum M C W van and Nieuwenhuizen T M 1999 *Rev. Mod. Phys.* **71** 313
[22] Conti C and Fratalocchi A 2008 *Nat. Phys.* **4** 794
[23] Levi L, Krivolapov Y, Fishman S and Segev M 2012 *Nat. Phys.* **4** 794
[24] Sarma R, Golubev T, Yamilov A and Cao H 2014 *Appl. Phys. Lett.* **105** 41104
[25] Schittny R, Kadic M, Bückmann T and Wegener M 2014 *Science* **345** 427
[26] Notomi M 2000 *Phys. Rev. B* **62** 10696
[27] Wang D, Wu J Z and Zhang J X 2016 *Chin. Phys. B* **25** 064202
[28] Lv Z G and Teng H 2021 *Chin. Phys. B* **30** 044209
[29] Ghulinyan M, Oton C J, Dal Negro L, Pavesi L, Sapienza R, Colocci M and Wiersma D S 2005 *Phys. Rev. B* **71** 094204
[30] Bertolotti J, Gottardo S, Wiersma D S, Ghulinyan M and Pavesi L 2005 *Phys. Rev. Lett.* **94** 113903
[31] Watson G H and Fleury P A and McCall S L 1987 *Phys. Rev. Lett.* **58** 945
[32] Imhof A,Vos W L, Sprik R and Lagendijk A 1999 *Phys. Rev. Lett.* **83** 2942
[33] Fan L J, Chen A, Li T Y, Chu J, Tang Y, Wang J J, Zhao M X, Shen T Y, Zheng M J, Guan F, Yin H W, Shi L and Zi J 2021 *Light: Advanced Manufacturing* **2** 395
[34] Peatross J, Glasgow S A and Ware M 2000 *Phys. Rev. Lett.* **84** 2370