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ReflectSim: an open-source software for teaching optical light reflection of nanostructured materials

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Abstract

Leveraging computational resources for modern physics education has become increasingly prevalent, especially catalyzed by the COVID-19 pandemic when distance learning is widely implemented. Herein, we report an open-source software for students and instructors to on-demand simulate optical reflection behaviors of one-dimensional photonic crystals (1D-PCs), a model system for understanding light–matter interactions relevant to materials science and optical physics. Specifically, our MATLAB application, ReflectSim, employs an adapted transfer matrix method simulation and can account for the effects of several critical material design parameters, including interfacial roughness and layer geometry, to determine the reflectance spectrum of user-defined 1D-PCs. By packing our codes into a graphical user interface, this software is simple to use and bypass the requirement of any coding experiences from users, which can be widely used as an education tool in high school/undergraduate classrooms and K-12 outreach activities. We believe that ReflectSim provides great potential for assisting students in understanding optical phenomenon in nanostructured layered materials and relevant scientific concepts through enabling more engaging learning experiences.

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S Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)

1. Introduction

Integrating simulation tools into STEM education can enhance students' learning experience for understanding complex concepts [1–3]. To address this need, a variety of open-source simulation software has now been developed to cover a wide range of scientific subjects for K-12 teaching, outreach, and undergraduate research. For example, wildfire propagation and its underlying dynamics can be demonstrated using simple MATLAB-based models, which have been incorporated into high school and college curricula [4]. Connecting visual representations with numerical simulations can enable students to efficiently grasp how the proximity of reactive elements affects the spreading of associated combustion reactions. This lesson can be broadly applied as a model for teaching chemical, ecological, and societal processes. The advantages of using interactive simulation software for STEM education are also exemplified in many other activities such as undergraduate research. Particularly, during COVID-19, students can use computational resources to remotely engage in lab activities. As a result, simulation software can provide an important platform for enhancing the teaching and mentoring infrastructures in STEM education [5, 6].

Understanding and controlling light–matter interactions is of central interest for various technological applications such as communication [7, 8], renewable energy [9, 10], and sensing technologies [11, 12]. Photonic crystals are a class of materials that can display structural color by manipulating propagation of electromagnetic waves using at least two materials with distinct refractive indices [13]. Briefly, PCs can effectively reflect desired wavelengths of light through organizing different components into periodic nanostructures, including one-, two-, and three-dimensional geometries. Among them, one-dimensional photonic crystals (1D-PCs) represent the simplest configuration, which have been utilized in many commercial products such as large-scale architectural artwork. These materials typically use alternating layers with different refractive index to control light reflection through varying the layer thickness and/or composition. A comprehensive understanding of 1D-PC light reflection behaviors can be obtained using transfer matrix method (TMM) through solving Maxwell's equations, which models how electromagnetic waves propagating within the entire dielectric media [14, 15]. While several TMM simulations have been established in the literature for predicting reflecting behaviors of PCs [15–18], these calculations sometimes do not take account of several important factors such as the non-uniformity between different layers, and can only provide a rough estimation [16]. Moreover, most conventional simulations are not packaged with a graphical user interface (GUI) which may limit their scope as a broad educational resource. As such, development of simple-to-use TMM simulation software is beneficial on multiple fronts, including for (1) high school and undergraduate courses to teach lessons on basic optical phenomena such as constructive and destructive interference; (2) undergraduate and graduate research for developing advanced 1D-PC systems with informed structure–property relationship; and (3) outreach for providing engaging materials science/physics examples to K-12 students. We also recognize that 1D-PCs can provide an excellent opportunity for understanding the

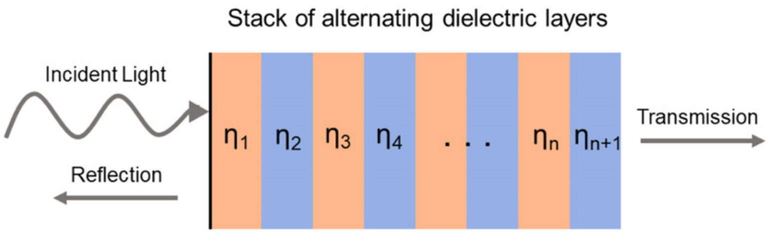

Figure 1. Schematic representation of a stack of dielectric layers with varying optical lengths, η. The distinct optical length of each layer determines the phase variation of propagating electromagnetic waves, illustrating the optical behavior of the dielectric structures through TMM.

correlation between material characteristics, light reflecting spectrum, and the corresponding structural color through leveraging visually enhanced learning experiences (e.g. color display from input material structural parameters). These examples provide important insights about light–matter interference in several relevant STEM courses such as introductory physics and optics at the high school and undergraduate level.

In this work, we develop an open-source TMM simulation software, ReflectSim, for modeling the reflectance behavior of 1D-PCs, which can be tailored to account for several variables such as interfacial roughness and complex layer geometry. Additionally, our MATLAB code has been outfitted with a GUI, bypassing the requirement of any coding experience to enable its efficient use by a broad education community. ReflectSim can be used in the classroom to teach students about the fundamental nature of optical phenomena associated with 1D photonic structures, while providing additional insights such as how interfacial roughness affects the corresponding optical reflecting properties, which are challenging for students to directly calculate using Maxwell equations. It can also be employed in undergraduate/graduate research projects for demonstrating how optical behaviors can be manipulated through materials and system design.

2. Transfer matrix method simulation

TMM can be used to determine the optical properties of a given photonic structure by simulating how light propagates upon interacting with domain interfaces throughout the entire sample [17]. This is accomplished by dissecting the structure into individual domains and collectively solving their corresponding Maxwell's equations, as demonstrated in figure 1.

To provide a brief background, the propagation of incident electromagnetic radiation through the system can be controlled by several key factors, including domain thickness, the refractive index contrast of different media, and interfacial roughness. Specifically, the product of domain refractive index and thickness determines the wavelengths that will be in-phase and constructively interfere upon reflection at the interfaces. The combination of contrast in refractive index between distinct domains and the total number of interfaces present in a given structure controls the amount of reflected light at a particular wavelength. These variables can directly impact the propagating electromagnetic wave at the interfaces of the layer in terms of Fresnel coefficients, as well as the phase difference the wave experiences upon interaction with the bulk of the dielectric layer. When the matrices are combined to comprehensively describe the behavior of the electromagnetic wave through the layer, the layer transfer matrix is given, which is demonstrated below:

$$m_n = \begin{bmatrix} \cos(\Phi_n) & -\dfrac{\mathrm{i}}{n_{ij}} \sin(\Phi_n) \\ -\mathrm{i}n_{ij} \sin(\Phi_n) & \cos(\Phi_n) \end{bmatrix}, \tag{1}$$

where n_n is the wavelength dependent refractive index for a given layer and Φ_n is the phase variation induced by propagation through the corresponding layer. In equation (1), phase variation can be described as

$$\Phi_n = \frac{2\pi}{\lambda}(\eta_n), \tag{2}$$

$$\eta_n = n_n d_n, \tag{3}$$

where in equation (2), λ is the wavelength of incident light and η_n is the optical length for a given layer within the 1D-PC stack. The optical length is determined by the product of the refractive index (n_n) and thickness (d_n) of the layer (equation (3)). The interaction between adjacent dielectric domains can be described by assigning the layer transfer matrix (equation (1)) to the individual domains (m_n and m_{n+1}), and relating the corresponding matrices to equations (4) and (5). Collectively, this would result in the system transfer matrix which described the effects of interactions with all of the interfaces in the structure in terms of individual Fresnel coefficients, as well as the culmination of phase changes which occur as a result of propagating through the bulk of the layers:

$$M_n = m_n \bullet m_{n+1}, \tag{4}$$

$$M = \prod_i^n M_i = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}, \tag{5}$$

where M_n represents interactions between adjacent layers, and M is the characteristic matrix of the entire structure which accounts for contributions from each domain. The identities of this representative matrix are used to determine the reflectance of the modeled structure at a given wavelength while including interactions at top (e.g. air/1D-PC) and bottom (e.g. substrate/1D-PC) interfaces, using the following equations:

$$r = \frac{(M_{11} + M_{12}n_\mathrm{m})\,n_\mathrm{s} - (M_{21} + M_{22}n_\mathrm{m})}{(M_{11} + M_{12}n_\mathrm{m})\,n_\mathrm{s} + (M_{21} + M_{22}n_\mathrm{m})} \tag{6}$$

$$R = |r|^2, \tag{7}$$

where n_m and n_s are the refractive index of the medium and substrate, respectively, r is the reflection coefficient, and R is the total reflectance of the structure at the specific wavelength. These calculations will then be carried out over a range of wavelengths to simulate the full reflectance spectrum from 300–1200 nm of a user-defined 1D-PC structure. It is worth noting that the TMM in its current state does not account for losses that occur as a result of diffraction, but only describes the theoretical reflectance behavior of the structure.

3. Matlab simulation using adapted transfer matrix method

Compared with established codes/scripts for conventional TMM simulations, several modifications have been incorporated in our software to further impart functionality and applicability

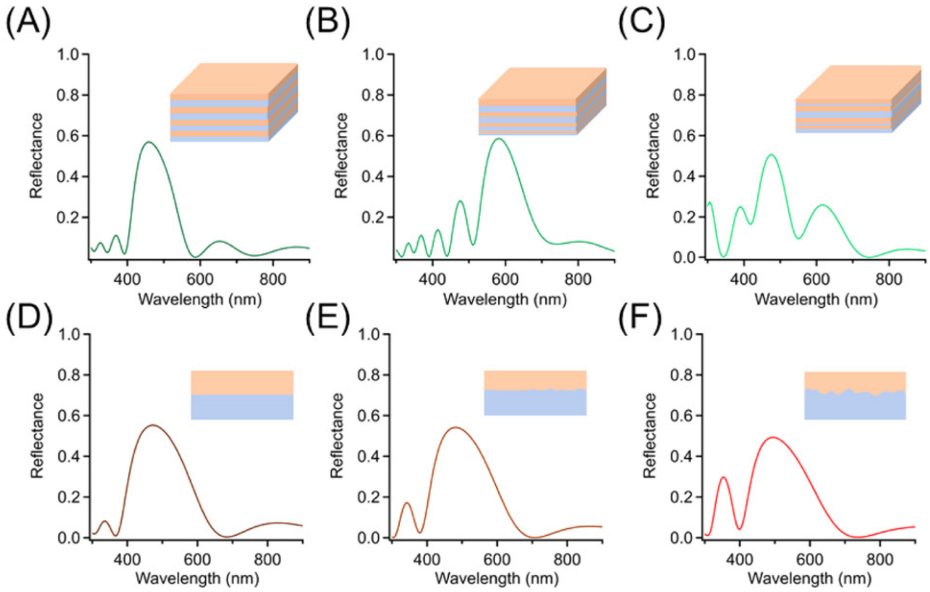

Figure 2. The effects of layer geometry on a 1D-PC constructed from high and low refractive index layers with refractive indexes of 1.6 and 1.31, respectively, are shown in (A)–(C). (A) describes uniform layers of 60 nm and 105 nm result in the presented spectrum. By increasing these thicknesses by 10 nm with each subsequent bilayer from bottom to the top (B), the reflectance spectrum is shifted to higher wavelengths accompanied by a change in shape. (C) When the layers of the 1D-PC are irregular (table S1), the reflectance decreases as a result of incoherence and the reflectance peak shape is altered. (D)–(F) demonstrate the effect of interfacial roughness on the reflectance performance of 1D-PCs. When no roughness is included into the reflectance calculation (D), the reflectance peak is well defined, and uniform. With increasing interfacial roughness between each film (E)–(F), the primary peak becomes less uniform with the emphasized presence of secondary peaks and the reflectance performance decreases by roughly 10% from (D) to (F).

to a broad range of user groups. First, the use of a GUI in our software removes the requirement of coding experience for its implementation as an educational tool. Additionally, we have incorporated several key features to allow users to on-demand design 1D-PCs, such as the ability to input thicknesses of each individual layer, include interfacial roughness into the reflectance spectra calculations, and embed wavelength-dependent refractive index data. Aiming at maximizing the impact of our software in education and outreach, below provides a detailed description about the improvements and operating procedures of ReflectSim.

3.1. Adaptations to the transfer matrix method

(1) Most TMM software available from the literature considers periodic alternating layers throughout a model 1D-PC. While such geometry is commonly used to describe 1D-PCs, changes in the thickness of different layers can give rise to altered optical behaviors such as shifting of the reflectance peak or variations in the spectrum shape. Therefore, it is necessary to establish the ability of simulation software to predict the effect of irregular layered structures on 1D-PCs. RelectSim is capable of modeling 1D-PCs of various geometries by assigning a distinct matrix to each individual layer with user-defined parameters, including refractive

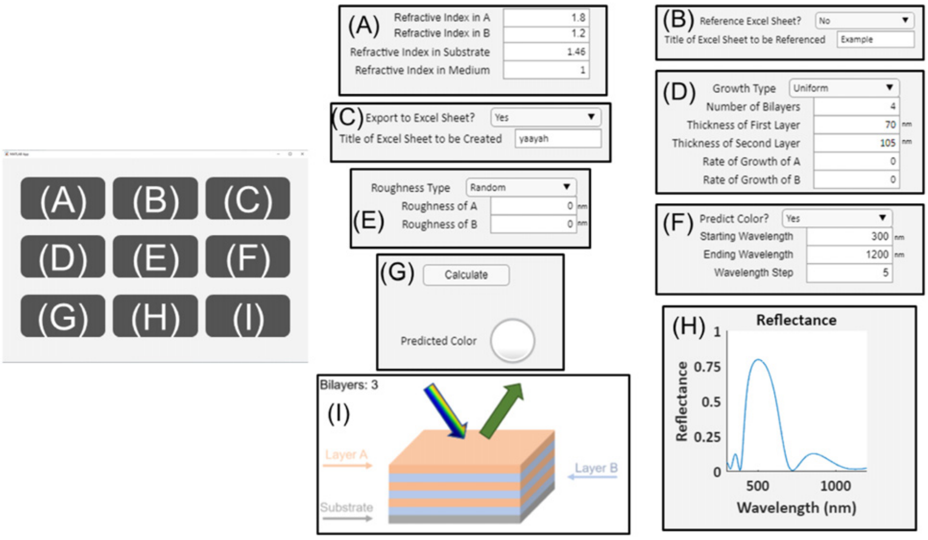

Figure 3. GUI utilized by the TMM MATLAB code. The GUI is separated into multiple sections relevant to the data entered by the user including (A) and (B) refractive index values, (C) data export option, (D) thicknesses and geometry of the layers within the structure, and (E) interfacial roughness variations. (F) allows user to select whether color will be displayed and the range of wavelength for simulation. Upon calculation (G), the results of the TMM calculations are displayed in the reflectance plot (H), which can also be exported to a Microsoft Excel file for further use. (I) shows a schematic illustration of a 1D-PC.

index and thickness. Specifically, layer thickness can grow by an integer or by a factor with each iteration from bottom to top. Alternatively, each layer thickness within the 1D-PC can be introduced through entering them as a list in the GUI. Figures 2(A)–(C) demonstrates the effect of different layer geometries on the reflectance performance of the 1D-PC. Disrupting the uniformity of the layered structure by increasing the thickness of selective layers (figure 2(B)) or fabricating layers with irregular thicknesses (figure 2(C) and table S1 (https://stacks.iop.org/EJP/43/035303/mmedia)) can result in shifts in the primary reflectance peak and decreases in the overall reflectance.

(2) Interfacial roughness can play a significant role on controlling the overall reflectance behavior of 1D-PCs, as demonstrated by many experimental examples in the literatures [19–22]. To take this factor into consideration, a simple method was employed in ReflectSim to introduce interfacial roughness in the 1D-PCs. This is accomplished by incorporating varying degrees of incoherent scattering of incident light into the phase variation at each domain interface [23]. By adding random variations in thickness to the pre-determined optical length, roughness-induced incoherence is included for understanding the optical behavior of 1D-PCs. In our calculations, a term dedicated to interface roughness is added into the phase variation as follows:

$$\Phi_n = \frac{2\pi}{\lambda}\left(\eta_n + \rho_n\right) \tag{8}$$

$$\rho_n = \beta * \varepsilon, \tag{9}$$

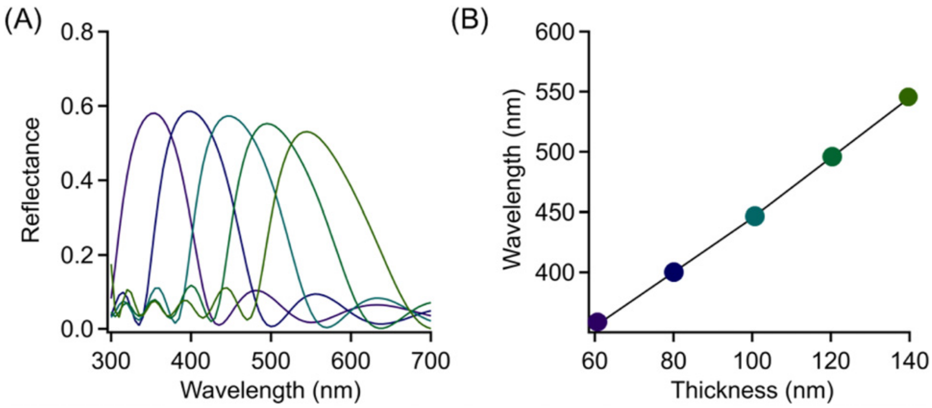

Figure 4. (A) Sample data of modelled 1D-PCs which shift to longer wavelengths upon increasing thickness of the layers within the theoretical structure. (B) Primary reflectance peak position as a function of increasing layer thickness of the low refractive index layer, while maintaining the thickness of the high refractive index layer.

where ρ_n is the interfacial roughness factor consisting of two random terms (β and ε) generated by MATLAB, within the ranges of 0 to π and -1 to 1, respectively. β represents the magnitude of the phase shift, where $\beta = \pi$ represents complete incoherence and values of $0 < \beta < \pi$ are in the case of partial incoherence which is representative of the case of surface roughness. The value ε determines if the shift is positive or negative, and both terms are generated from a Gaussian population of values between their respective boundary conditions. The calculations are performed over multiple iterations with distinct random phase variations, resulting in a closer approximation of 1D-PCs reflecting behaviors as roughness is inevitable in practical systems from processing. Additionally, options are provided to the user for defining the roughness of each interface in the unit of nanometers within the GUI. As shown in figure 2(D), a 1D-PC sample with no roughness and four bilayers has a peak reflectance of 56% at 470 nm. Upon the addition of distinct roughness to each layer described in table S2, incoherence is introduced into the reflected light and the reflectance decreases approximately 10% depending on the severity of the input interfacial roughness in our model study (figures 2(E) and (F)).

(3) Refractive index is a wavelength-dependent material property. However, most TMM models only use a constant value for describing the refractive indices to conduct simulation (typically at the wavelength of 532 nm). To precisely predict reflectance spectra of 1D-PCs, wavelength-dependent refractive index of the dielectric layers must be included in the calculation. Herein, we build up a function to allow users to input a two-column list of wavelengths and the corresponding refractive index. This matrix will be employed in equation (3) to accurately determine the light reflecting behavior of the 1D-PC. This is an optional function, as users can still simply input a constant refractive index value when wavelength dependent refractive index data is not available, or a quick estimate is preferred.

3.2. Graphical user interface and operating procedures

The adapted TMM simulation is packaged into an ergonomic GUI to enable its ease of use for broad groups in K-12 education/outreach and undergraduate/graduate research. Figure 3 displays the GUI of our software, separated into multiple subsections where users can input relevant information/data to define the simulation, including the refractive index and thickness of different layers in 1D-PCs, the number of bilayers, geometry of the layers throughout the structure, and interfacial roughness variations. Once a particular model with detailed parameters is determined, the reflectance spectrum is subsequently calculated and shown within the GUI, which can be exported to an Excel file for further use. In the refractive indices section (figure 3(A)), the optical properties of each layer, as well as the medium and substrate can be introduced. If the user prefers to include wavelength-dependent refractive index, the dropdown menu in the references section (figure 3(B)) should indicate 'yes' for data input. Similarly, if the data needs to be exported to a spreadsheet, 'yes' should be chosen in the dropdown menu under the export section (figure 3(C)), and a desired name for the Excel sheet should be added. Layer thicknesses and general geometries of the modeled 1D-PC are entered into the growth section shown in figure 3(D). Specifically, the dropdown menu contains four options for defining 1D-PC geometries: step-wise, geometric, uniform, and customized. In 'uniform' models, the 1D-PC contains alternating layer thicknesses that are homogenous throughout the entire sample. Selecting 'step-wise' or 'geometric' increases the initial indicated layer thicknesses by a desired integer thickness (in nanometers) or a relative percentage, respectively. In 'customized' geometry, users can enter the value of the specific thicknesses for each layer. The roughness section (figure 3(E)) contains a dropdown menu, providing users options of 'no roughness', 'random' roughness, and 'defined' roughness. The section in figure 3(F) allows the user to define a wavelength range of interest for simulating the reflectance spectrum, accompanied by an additional option to display the corresponding color of the 1D-PC. This is accomplished by assigning an RGB value to each wavelength and determines the collective RGB result from the simulated spectrum; weighing the contribution of each wavelength by its corresponding reflectance value. After pressing the 'Calculate' button in figure 3(G), the simulation will be performed, and the results will be shown in figures 3(G) and (H) including both spectrum and color. Figure 3(I) provides a representative 1D-PC geometry to assist the user for visualizing the structure and understanding necessary structure parameters. Overall, the GUI in our software is designed to allow its easy use for enabling the ReflectSim to be an engaging and widely applicable educational resource.

4. Sample lessons using ReflectSim

Two example lessons are provided to demonstrate the potential use of ReflectSim as an educational resource for understanding structure–property relationship of 1D-PCs, as well as the basic light–matter interaction concepts. By performing multiple simulations with only varying the thickness of the alternating dielectric layers, multiple reflectance spectra can be calculated to demonstrate the effect of thickness on the wavelength of light reflected by the structure, as depicted in figure 4.

Specifically, increasing the thickness of the low refractive index ($n = 1.31$) layer from 60 nm to 140 nm while maintaining the thickness of the high refractive index layer ($n = 1.6$; thickness = 60 nm) results in red-shifting of the primary reflectance peak from 355 nm to 545 nm. Accordingly, our software can directly display the color so that the effect of the increased layer thickness can be visualized to the students, allowing them to easily understand the interference of the reflected light upon manipulating the nanostructures of 1D-PCs. Furthermore, ReflectSim can be used to demonstrate the effect of varying the geometry of the modeled 1D-PC systems. Students can simulate multiple 1D-PCs based on uniform layered structures of different thicknesses and record their reflectance spectra. Following this step, the students can simulate 1D-PCs constructed of combinations of the uniform layered structures they previously simulated and compare the differences in the reflectance spectra.

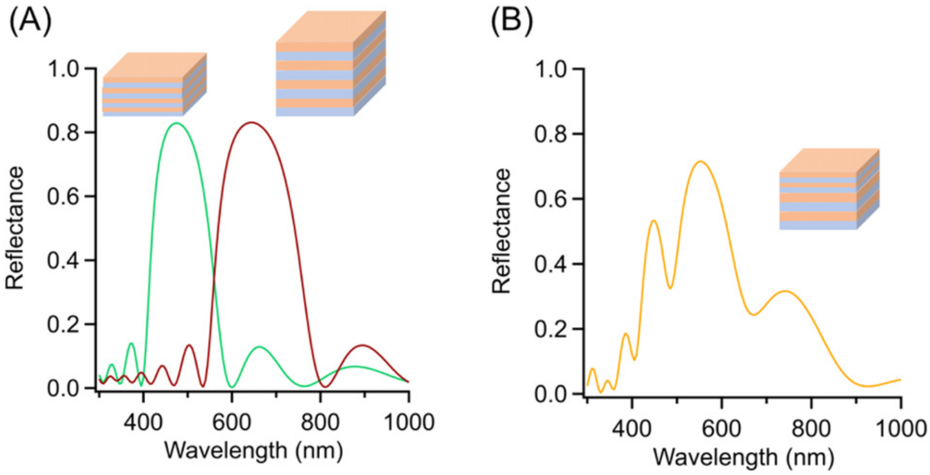

Figure 5. (A) Reflectance spectra of two six bilayer 1D-PCs with uniform layered structures. (B) Reflectance spectrum of a modeled six bilayer 1D-PC which consists of three bilayers of each of the 1D-PCs displayed in (A).

Figure 5(A) depicts sample data of two uniform structures each containing a total of six bilayers with reflecting peaks at 475 nm and 640 nm which are constructed from alternating layers of 70 nm/105 nm and 100 nm/130 nm, respectively. Figure 5(B) depicts the optical light reflectance behavior of a 1D-PC fabricated from three characteristic bilayers of both 1D-PCs in figure 5(A). The result is an intermediate of the reflectance behaviors of the two uniform systems caused by destructive and constructive interference between the two spectra. By comparing the reflectance spectra of the uniform systems compared to systems with combinations of layer thicknesses, the students will be able to directly observe the contributions of the different layers into the reflectance behavior of the 1D-PCs and how these parameters change the resulting color, as shown in figure 5. Such observation is valuable in understanding constructive and destructive interference when electromagnetic waves interact with nanostructured materials. Through these example lessons, it is evident that ReflectSim can be used as a supplementary tool to inform students upon their first introduction to optics, electromagnetic waves, or other relevant fundamental physical phenomena, while providing following advantages: (1) significantly improved throughput for generating results to obtain fundamental structure–property relationship for 1D-PCs, as conventional calculations would be relatively time consuming especially for systems containing complex layer geometry, (2) upon obtaining sufficiently large database from students, it may provide an opportunity for inverse materials design (i.e. from color to structures), which could be difficult through directly using Maxwell models, (3) engaging students with visual evidence and examples, which is a proven method for enhancing physics learning outcome [24], (4) extend the physics education to students may have limited education background/resources, and thus promote the inclusivity of STEM education. Overall, we believe that ReflectSim can help students deconvolute the initially complex concepts behind constructive and destructive interference in waves for use in introductory physics courses, as well as remove the need to code simulations for students.

5. Conclusions

ReflectSim, a versatile and easy-to-use TMM based simulation software, has been developed as an educational tool for high school/undergraduate level physics and materials science courses, research activities, as well as for outreach. The adapted TMM simulation of ReflectSim is able to account for many different user-defined parameters, such as interfacial roughness and layer geometries, which allows students and instructors to explore a wide material design space for 1D-PCs. Additionally, the application has been packaged into a simple GUI, allowing it to be easily used regardless of coding experience. Manipulating the user-defined variables in the GUI can provide unique opportunities to inspire and assist students in understanding important light–matter interaction concepts such as interference in electromagnetic waves.

Author contribution

CK and MR contributed equally to this manuscript.

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