

# Photonic crystal heterostructures—resonant tunnelling, waveguides and filters

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## Abstract

Photonic crystal heterostructures are concatenations of photonic crystals differing in refractive index or lattice geometry. They can be fabricated using self-assembly of colloidal spheres. In this paper we present a review of the devices enabled by such colloidal heterostructures, along with an envelope approximation used to efficiently study their properties. We show that the approximation is well suited for studying polymer photonic crystals. We also provide a comparison between the envelope approximation and a tight-binding method used to study defects in photonic crystals.

**Keywords:** Photonic bandgap materials, photonic crystals, heterostructures, K dot P theory, envelope approximation

## 1. Introduction

Photonic crystals, structures with a periodic modulation of their refractive index in two or three dimensions [1, 2], have received significant attention in the past two decades. Understanding of their behaviour has grown through extensive experimental and theoretical investigation.

On the experimental front, both two-dimensional and three-dimensional structures have been fabricated. Two-dimensional structures [3] consist of an array of holes etched lithographically in a slab; index guiding is used to confine light to the slab. Two-dimensional photonic crystals use an established fabrication technique and simplified simulation programs. Three-dimensional structures have been fabricated by advanced semiconductor processing [4], by self-assembly of colloidal spheres from a dispersion [5] or by holography in a polymer photoresist [6]. Fabrication of self-assembled or holographic structures is much simpler, and after semiconductor infiltration they may exhibit a complete band gap.

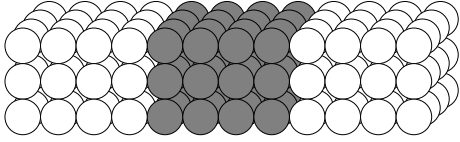
Wavelength filters, waveguides with sharp bends and microcavities with high quality factors [7] have been proposed and fabricated. Demonstrated devices using photonic crystals typically rely on defects introduced in the perfectly periodic crystal. Most such devices have been based on two-dimensional crystals in which defects are controlled in the lithographic process. The size of a hole may be modified, or the hole removed completely, in order to produce a point defect. Line defects are produced by removing a row of holes.

Three-dimensional crystals fabricated by self-assembly or holographic techniques do not typically lend themselves as directly to controlled local modification. Point defects have been introduced in such crystals [8] in a less pre-programmable fashion.

Photonic crystal heterostructures have recently been introduced as an alternative to defects to create devices in three-dimensional colloidal photonic crystals [9–11]. They consist of concatenations of different photonic crystals which differ in band structure—through differentiation in refractive index, lattice period or even lattice type. An example structure is shown in figure 1. Fabrication of such structures by sequential self-assembly has been demonstrated [12], as has controlled self-assembly of polymer photonic crystals on patterned substrates [13].

The flow of light in photonic crystal heterostructures extends further the analogy with electronic wavefunctions inside semiconductors—an analogy which substantially motivated research in photonic band-gap materials. Semiconductor quantum electronics employs heterostructures to create resonant barriers and superlattices to select electrons of a given energy, and also to provide high-mobility channels in high-electron-mobility transistors (HEMT). Photonic heterostructures would seek to exploit the fact that light of a certain frequency will find different allowed or forbidden bands in the different photonic crystals.

Just as in the electronic counterpart, a method is needed to allow forward design of photonic crystal heterostructures.



**Figure 1.** A photonic crystal heterostructure: dark spheres are of a different refractive index to white ones.

Structures must be engineered to meet a given set of requirements rather than being simulated purely numerically and optimized iteratively. Existing photonic crystal simulators fall mostly into two categories. The first type assumes an infinitely periodic structure and computes bands and modes. The second type makes almost no assumption on the structure, and solves Maxwell's equations in a general medium.

In the case of heterostructures, the first type cannot be used, since the junctions break the periodicity. The second type of simulator will be inefficient in heterostructures for it ignores the presence of large regions of perfect local periodicity. The size and complexity of the numerical computations becomes truly onerous in three-dimensional crystals.

What is needed is an algorithm that will combine the two types of simulation: it will exploit the fact that large sections of the crystal are periodic, but allow this periodicity to extend over finite regions. Such a method—an envelope approximation—has been introduced recently in the photonic domain [9–11]. Inspired by the envelope approximation used to model semiconductor heterostructures [14], it reduces each region of photonic crystal to its dispersion relation. These parameters are then used to calculate the behaviour of the envelope of the electromagnetic wave in the heterostructure. The method is useful both for simulation of devices, as well as for forward design of structures to meet given specifications. In this paper we review the envelope approximation method for photonic crystal heterostructures and provide examples of its application in colloidal photonic crystals.

We conclude our introduction by noting related problems previously studied. Superstructure gratings exhibit periodicities on two scales and are analysed using a tight-binding approximation employing coupled mode equations [15]. Light propagation in a non-linear photonic crystal has been studied using a multiple-scale approach [16] which finds the envelope modulating the Bloch modes of the crystal, in a similar fashion to the envelope approximation. Simulation algorithms have been proposed to deal with junctions and defects: *Multem* [17] computes the transmittance of a periodic layer of spheres, and allows almost arbitrary layers of this type to be stacked. However, it is quite intensive numerically. A method has also been proposed [18] similar to the electronic tight-binding approximation for semiconductors: using localized waves, it is ideally suited for the analysis of point or line defects. We discuss in section 4 the relationship of the envelope function method with complementary simulation approaches.

## 2. The envelope approximation framework

The object of our model is to simplify the solution of the wave equation

$$[\nabla^2 + \omega^2 \mu \epsilon - \nabla \cdot (\nabla \cdot)] \mathbf{E} = 0 \quad (1)$$

in a photonic heterostructure defined by its dielectric constant:

$$\epsilon(\mathbf{r}) = \epsilon_b + \epsilon_f(\mathbf{r})[1 + \Delta_s(\mathbf{r})]. \quad (2)$$

We have separated the dielectric permittivity into three parts: a constant background permittivity,  $\epsilon_b$ ; a fast oscillation,  $\epsilon_f$ , defining the photonic crystals; and a slow variation,  $\Delta_s$ , describing the heterostructure.  $\Delta_s$  is allowed to have jumps, but these should be separated by several lattice constants of the underlying crystal.

Within a region of homogeneous photonic crystal, solutions of the wave equation take the form of Bloch modes:

$$\mathbf{E}_{n,\mathbf{k}} = \mathbf{u}_{n,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (3)$$

We express the electric field inside a heterostructure as a superposition of the bulk Bloch modes:

$$\mathbf{E}(\mathbf{r}) = \sum_n \mathbf{W}_n(\mathbf{r}) \mathbf{u}_n(\mathbf{r}) \quad (4)$$

$\mathbf{W}_n$  represents an envelope modulating the Bloch modes of the bulk crystals. As described in [10] and [11], we can find an equation for this envelope which does not include the fast-varying refractive index of the photonic crystals. In this way we treat the crystals as if they were homogeneous materials, except that appropriate parameters are used to take account of the effects of the photonic crystal. These parameters are obtained from the properties of the bulk crystals used in the heterostructure. We may employ either the Bloch modes [10] or the dispersion relations [11] for this purpose. Ignoring the background dielectric constant,  $\epsilon_b$ , we write the envelope equation as

$$\mathbf{H}\mathbf{W}(\mathbf{r}) = \omega^2 \mu [1 + \Delta_s(\mathbf{r})] \mathbf{W}(\mathbf{r}). \quad (5)$$

$\mathbf{W}$  is a column vector containing the envelopes for all the bands.  $\mathbf{H}$  is a matrix operator with the following elements:

$$\begin{aligned} H_{n,m} \equiv & - \left\{ (\nabla^2 + k_0^2 - \omega_m^2 \mu \epsilon_b) u_{n,m} \right. \\ & + \sum_p \kappa_{p,n,m} \left( \frac{1}{j} \frac{\partial}{\partial p} - k_{0p} \right) \\ & \left. - \sum_p \sum_q \left[ \left( \frac{\partial^2}{\partial p \partial q} + k_{0,p} k_{0,q} \right) u_{n,p,m,q} \right] - \omega_n^2 \mu \delta_{n,m} \right\}. \end{aligned} \quad (6)$$

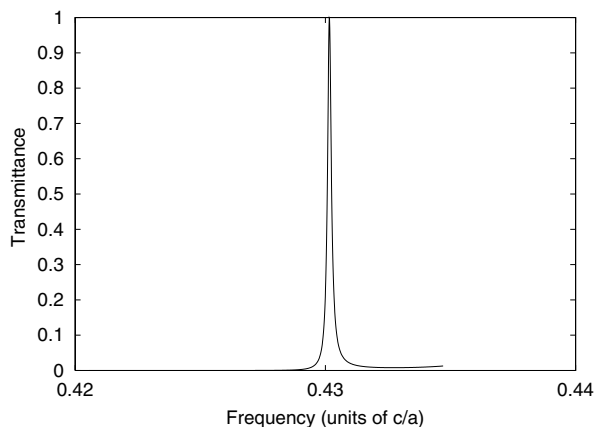
$u_{n,m}$ ,  $u_{n,p,m,q}$  and  $\kappa_{n,m}$  are constants computed from the Bloch modes of the crystal.  $\omega_m$  and  $\omega_n$  are the frequencies of the Bloch modes,  $k_0$  is the wavevector of the Bloch modes,  $p$  and  $q$  represent the three directions  $x$ ,  $y$  and  $z$ .

Alternatively, the equation for a single band  $n$  can be written as a function of the band frequencies instead of the Bloch modes:

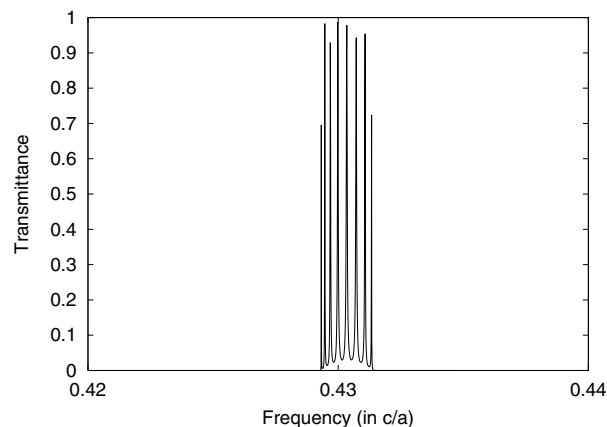
$$\omega_n^2(-i\nabla) \mathbf{W}_n(\mathbf{r}) = \omega^2 [1 + \Delta_s(\mathbf{r})] \mathbf{W}_n(\mathbf{r}) \quad (7)$$

$\omega_n^2(-i\nabla)$  describes the exact dispersion relation of the given band.

$\Delta_s$  represents a perturbation to a bulk photonic crystal. Depending on its strength, it may be taken into account in one of two ways. For small perturbations we may assume small



**Figure 2.** The transmittance of the resonance double barrier.



**Figure 3.** The transmittance of a superlattice with eight layers.

changes in the Bloch modes, and need only account for the bulk properties of one type of crystal, with the heterostructure described with the term  $\Delta_s$ . For stronger perturbations, or for interfaces between crystals of different lattice geometries, this is no longer appropriate. We need to obtain a general solution in each crystal separately. The heterostructure solution is then found from these general solutions and the application of boundary conditions at the interface. This is similar to what is done with semiconductors, in which a Schrödinger-like equation, with suitably chosen effective mass, is solved for each material, and the solutions are connected at the interface.

Considering the individual photonic crystals as regions of known, homogeneous band structure puts the focus onto the effects of the heterojunctions. The dimensions and characteristics of a structure may be determined directly without the need for complex optimization algorithms.

### 3. Photonic heterostructure devices

We classify the applications of photonic crystal heterostructures into two categories depending on the direction of propagation of the light. In analogy to semiconductor electronics, we call the case where light must cross heterointerfaces ‘perpendicular transport’ and the case where light forms a mode with the propagation vector parallel to the interfaces ‘parallel transport’.

#### 3.1. Perpendicular transport

When light crosses a number of heterojunctions and propagates through a number of photonic crystals, it encounters different dispersion bands in the different crystals, potentially falling inside the stop band of certain materials. In such cases the electric field will decay exponentially. If the region is wide enough, the decay will be complete, and all the energy will be reflected. If they are narrow, some energy will be allowed to traverse them, as in quantum mechanical tunnelling. Combining allowed and forbidden regions allows us to set up cavities for light, and to control the tunnelling through the forbidden regions. Through judicious choice of heterostructure geometry and dimensions, the transmittance and reflectance spectra of these structures may be precisely engineered.

The simplest example of a perpendicular transport device is the resonant double barrier. This is the example of figure 1 in which a layer of one photonic crystal is enclosed between two layers of a different crystal. Near the frequency of interest, light is allowed in the centre layer and encounters a forbidden region in the side layers. The centre region functions as the *well* and the sides form the *barriers*.

Light at a resonant well frequency will tunnel through the first barrier, be reflected a number of times between the barriers and then tunnel through the second barrier. Light at any other frequencies is not allowed in the well. The transmittance of the structure will be high only for the frequency of the resonant state. The operation of this device is similar to that of a Fabry–Perot interferometer. The barriers act as mirrors, while the well forms the centre cavity. The width of the transmittance peak depends on the strength of the barriers. Stronger barriers will confine light longer in the centre cavity, with a better frequency selectivity. A stronger or longer barrier will give a narrower resonance peak. The transmittance of such a structure is shown in figure 2. For illustrative purposes, a photonic crystal with simple cubic geometry is employed with the spheres touching one another. The centre region includes four layers of spheres of index 1.5 in air, while the side crystals have 32 layers of spheres of index 1.4. These indices are typical of colloidal polymer or silica photonic crystals. The position of the peak obtained from the envelope approximation agrees with full numerical simulations within 0.2%.

To obtain a transmittance peak of a certain width, with a flat top, the structure in figure 1 needs to be repeated a number of times to create a periodic alternation of the two crystals. This periodicity imposed on a second scale creates a superlattice which will give rise to a new set of allowed and forbidden *minibands*. As we bring two identical wells close together, their modes will interact and their energy levels will split. As more and more wells are brought together, we will obtain many states, very closely spaced, which will ultimately merge into a miniband. Allowed minibands will have a transmittance close to unity. They are abruptly separated from the forbidden bands which have a very low transmittance. In figure 3 we show the transmittance spectrum of a structure with eight periods in which we can observe the closely spaced states. The non-uniformity in the heights of the peaks is due to the finite number of frequencies included in the simulation.

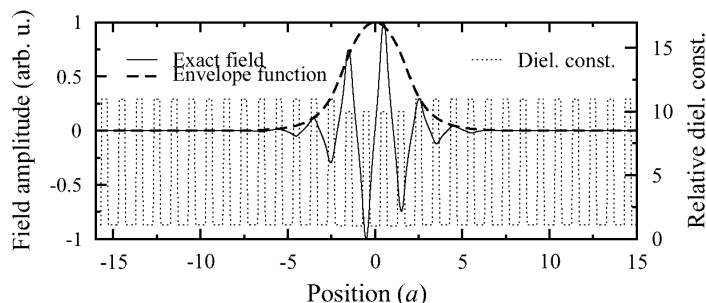


Figure 4. The profile of a guided mode.

Perpendicular transport has been observed experimentally in colloidal photonic crystal heterostructures [12]. These structures consist of thin crystal layers composed of colloids of different sizes deposited on top of each other.

### 3.2. Parallel transport

Photonic heterostructures can also be used to confine light propagating parallel to the interfaces. They act as a waveguide, where both the core and the cladding are made of photonic crystals. The requirement is that light falls in an allowed band in the core, but encounters a stop band in the cladding.

In conventional dielectric waveguides, the core must have a higher refractive index than the cladding in order to confine light through the mechanism of total internal reflection. Photonic heterostructure waveguides do not have this restriction, potentially confining light even if the average index in the core is lower than in the cladding. In figure 4 we show the profile of a mode guided in a slab waveguide with lower average index in the core than in the cladding. The solid curve represents the electric field obtained from full numerical simulations. The dashed curve represents the envelope of the mode computed using the envelope approximation. In most cases the envelope provides enough information when designing such waveguides, indicating whether a mode is guided or not. As described in [11], the envelope approximation can also be used to compute the single-mode condition for these waveguides in a manner similar to the single-mode condition of dielectric waveguides.

## 4. Comparison of modelling techniques

In this section we compare the envelope approximation with the tight-binding technique presented in [18]. Both methods use the Bloch modes of the bulk crystals in order to calculate properties of non-periodic structures more efficiently. In the tight-binding method waves are expressed as a superposition of localized Wannier functions. Interactions between the localized waves are limited to nearest neighbours. The parameters of the Wannier functions are obtained by fitting their frequency eigenvalues to the true eigenvalues obtained by full simulations. As required by the initial assumptions, the Wannier functions decay rapidly to almost zero within one lattice constant.

Having determined the functions for bulk crystals, deviations from periodicity are expressed in the Wannier function basis with coefficients obtained by numerical

integration. Due to the localized nature of the basis set used in the tight-binding method, the method is ideal for defects of the order of one lattice constant. Larger defects are less well described using the same basis set. On the other hand, a transfer matrix method using the tight-binding framework has been introduced [19] to address heterostructures which have deviations from periodicity on a larger scale. The tight-binding approximation, being based on localized states, is better suited to crystals with a high index contrast and with high-index regions that are well separated, such as is the case with thin rods in air. The method has so far been deployed only in two-dimensional photonic crystals.

The envelope approximation, in contrast, is designed to work with heterostructures in which the heterojunctions are well separated. This creates the conditions necessary for separation of the length scales of the crystals and the heterostructures. The method is suited to photonic crystals with both high and low index contrast. Two versions exist—one which is useful only with structures that present a weak perturbation from a bulk crystal and one which is more generally applicable. It was found that the envelope approximation provides good results for heterostructure layers at least four lattice constants thick.

## 5. Conclusions

In this paper we have reviewed the envelope approximation, and its use with heterostructure devices for both perpendicular and parallel propagation. We have also presented a comparison between the envelope approximation and a tight-binding method for the analysis of defects in photonic crystals.

Since the envelope approximation allows us to treat photonic crystals almost as one treats homogeneous materials, many of the well established techniques developed for these materials can be adapted to photonic crystals. As an example, the transfer matrix method and the beam propagation method, developed for junctions between homogeneous materials, can be applied to photonic crystal devices.

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