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Phononic and photonic band gap structures: modelling and applications

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Abstract

Photonic crystals (PhCs) are artificial materials with a permittivity which is a periodic function of the position, with a period comparable to the wavelength of light. The most interesting characteristic of such materials is the presence of photonic band gaps (PBGs). PhCs have very interesting properties of light confinement and localization together with the strong reduction of the device size, orders of magnitude less than the conventional photonic devices, allowing a potential very high scale of integration. These structures possess unique characteristics enabling to operate as optical waveguides, high Q resonators, selective filters, lens or superprism. The ability to mould and guide light leads naturally to novel applications in several fields.
Band gap formation in periodic structures also pertains to elastic wave propagation. Composite materials with elastic coefficients which are periodic functions of the position are named phononic crystals. They have properties similar to those of photonic crystals and corresponding applications too. By properly choosing the parameters one may obtain phononic crystals (PhnCs) with specific frequency gaps. An elastic wave, whose frequency lies within an absolute gap of a phononic crystal, will be completely reflected by it. This property allows realizing non-absorbing mirrors of elastic waves and vibration-free cavities which might be useful in high-precision mechanical systems operating in a given frequency range. Moreover, one can use elastic waves to study phenomena such as those associated with disorder, in more or less the same manner as with electromagnetic waves.
The authors present in this paper an introductory survey of the basic concepts of these new technologies with particular emphasis on their main applications, together with a description of some modelling approaches.

Keywords: Phononic crystals; Photonic crystals

1. Photonic band gap structures

In 1987 E. Yablonovitch [1] and S. John [2], proposed a three dimensional structure able to completely inhibit spontaneous emission and to strongly localize the light, respectively. The focus point of the above mentioned works is the idea that a periodic arrangement of dielectric or metallic elements can exhibit polarization and/or direction

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depending on the band gap regions for certain frequency ranges, where the propagation of the electromagnetic waves is forbidden. This property depends on the material, frequency of operation and crystal lattice property.

One-dimensional (1D) periodic structure is the simplest photonic crystal usually used as reference model to understand the formation of the band diagram [3], showing stop band regions. Two-dimensional (2D) photonic crystals are more difficult to fabricate than 1D photonic crystal, but their increased complexity, even if still quite less than three dimensional (3D) photonic crystal, is largely compensated by the wide field of applications in integrated photonic circuits. However, index contrast and existence of PBGs, can be properly combined to obtain a confinement in three directions, as in slab waveguides 2D PhCs. These properties can be exploited for realizing low loss waveguides with very large curvature angles, and resonant cavities with high quality factors.

A sort of doping, similar to that one used in semiconductors is required for implementing specific functions in the PhCs. In this case doping is achieved adding or removing a certain amount of dielectric material, thus breaking the crystal periodicity. The translational symmetry of the periodic lattice is disturbed when defects are introduced and the consequence of this is that Bloch mode can not still be considered a solution of the Maxwell's equations. When a defect is introduced in a perfect crystal, one ore more localized evanescent mode can be created within the PBG. The parts of the crystal on both sides of the defect behave like mirrors where modes exponentially decay and light is trapped in the space between the mirrors. Since the distance between the mirrors is of the order of the light wavelength, the modes are quantized. Therefore, due to the presence of defects corresponding to frequencies inside the photonic band gaps, localized mode can exist.

Type and size of the defect define the shape and the properties of the localized states, such as frequency, polarization, symmetry, field distribution. The defects can be classified as point defects or extended defects. Point defects determine the presence of e.m. modes at discrete frequencies, while extended defects result in the presence of transmission bands inside the photonic band gap of the unperturbed photonic crystal.

2. Phononic band gap structures

Analogously to the photonic crystals, PhnCs make use of the fundamental properties of waves, such as scattering and interference, to create band gaps where waves cannot propagate through the structure. A periodic array of inclusions forms a crystal lattice. The periodic variation of density and/or elastic constants of the structure changes, in turn, the speed of sound in the crystal and this causes the formation of a phononic band gap. The band gap centre frequency, width and depth are detemined by the size, periodicity and geometry of the lattice and by the properties of both background material and inclusions.

The periodic variation in the density and/or speed of sound forming a phononic crystal can be achieved by making air holes in a solid background material. Also the phenomenon of negative refraction has been observed in phononic crystals. Controlling the dispersion properties for phonons both inside and outside the band gap, new effects and related applications could be found.

Acoustic waves (waves passing through a gas or a liquid) or elastic waves (those passing through a solid) differ from light waves in several ways. Acoustic and elastic waves cannot travel through a vacuum as light waves. Moreover, a light wave can have two independent polarizations, while an elastic wave in a homogeneous solid has three independent polarizations: two of these are transverse (shear waves) and one is longitudinal (a compression wave). Shear waves are not supported in liquids and gases, so an acoustic wave has just one longitudinal polarization.

The propagation of mechanical waves in a medium is usually described by a dispersion relation between frequency ω and wave vector, $\boldsymbol{k}$, that can be even quite complicated in inhomogeneous materials.

The mechanism governing the formation of the band gap is based on Bragg reflections due to the crystal periodicity. As in case of photonic crystals, the 1D crystal composed by alternating layers of two differente materials can be used for intuitively understanding how band gaps form. In general, the regularity of the arrangement of scattering elements of the phononic crystal gives rise to the Bragg reflections of the sound waves inside the crystal. The constructive or destructive interference of the waves creates ranges of frequencies at which waves can both propagate through or are blocked by the crystal. The condition for constructive interference is obtained when the lattice constant a is comparable to the wavelength λ. Since the frequency at the centre of the band gap, ω_c, is inversely proportional to the lattice parameter: $\omega_c \sim 1/\lambda \sim 1/a$, by simply changing the size of the unit cell, a band gap can be formed at any frequency or wavelength. The width of the band gap depends on the crystal structure and increases when the contrast of the densities and sound velocities between the material of the scattering elements and that of backgound material also increases. Therefore, to increase band gap means to use materials with a large acoustic impedance mismatch. Moreover, the position and width of the band gap depend on the propagation direction because the path difference depends on the angle of incidence. Some phononic crystals structures form band gaps for any propagation direction, that are known as complete band gaps. Other materials possess partial band gaps that only stop waves travelling in certain directions. A 1D crystal does not have a complete band gap because its mechanical properties are periodic in one direction. When the wave vector forms right angles to the propagation direction, it will not be reflected, then there will not be any band gap in this direction.

To design a PhnC having a complete band gap the density and sound velocities need to vary in all three directions of space. However, not all 3D periodic structures will form a complete phononic band gap.

Moving from a liquid, which supports only the longitudinal polarization, to a solid background material, which can support both longitudinal and transverse polarizations, larger band gaps can be achieved. If one want to create a complete phononic band gap, structures having band gaps for both longitudinal and transverse waves in the same frequency region must be designed. This could be more difficult than designing structures for photonic crystals where electromagnetic waves have only transverse modes.

The existence of full bandgap was demonstrated both theoretically and experimentally for 2D and 3D phononic crystals [4]. The formation and width of complete band gaps depend on the contrast in density and/or sound velocities and elastic constants of the involved materials. Another parameter influencing the formation of a complete band gap is the crystal geometry. In any case the ”ideal” phononic structure has not yet been found and even a comparison among different material systems is difficult. Examples of large complete band gap in 3D were reported for arrays of spherical inclusions of a low density fluid in a high density host fluid [5] while in 2D structures large band gaps were found for rectangular and hexagonal arrays of air cylinders in water [6].

Moreover, the introduction of defects within the structure allows sound waves with frequencies in the band gap to be trapped near a point-like defect or guided along linear defects.

3. Modelling approaches

From the point of view of the fundamental physics involved, phononic crystals are even more challenging than photonic crystals to be modelled theoretically because of a number of additional parameters have to be considered such as density and Lamè coefficients and an extra polarization of the wave inside the crystal. The strong coupling between longitudinal and transverse waves is another complicating factor to take into account. Main parameters in designing both photonic and phononic crystals are the fill factor the index contrast between the inclusions material and the host material. These parameters control the location and size of the bandgap.

Most of the modelling approaches here described are used for both PhCs and PhnCs.

The Plane Wave Method (PWM) [7] is largely used for the computation of band diagrams. For investigating photonic crystal slabs, because of the lack of periodicity along the etching direction, one can use the Supercell Method (SCM) [8]. However, the accuracy is a growing function of the decoupling between adjacent supercells, therefore, this method results to be computationally very expensive for the theoretical analysis of complex photonic crystal-based devices.

Although the PW method is very powerful even for the calculation of the dispersion relations of acoustic and elastic waves, it fails in some cases, such as for PhnCs in mixed (fluid/solid) composites and for structures where the material contrast between inclusions and host is very high. In this last case very large-step functions need an extremely large number of Fourier components to ensure enough accuracy.

Bloch-Floquet Method (BFM) [9] is based on the Bloch waves and Floquet's theorem. It is used for studying layered structures formed by homogeneous regions along the direction normal to the propagation plane. It is most useful for analyzing PhCs slab with 2D periodicity where the finite size of the PhC lattice, together with the presence of both cladding and substrate, has to be taken into account. Bloch-Floquet method allows calculating the modes even for complex propagation constant, e.g. the leaky modes and the modes at frequencies within the band gaps. Transmission and reflection spectra can be evaluated together with the out-of-plane losses in a very short computer time.

The Finite Difference Time Domain (FDTD) [10] is a very general method useful to calculate the transmission and reflection spectra of 2D guided–wave PBG devices, but computation of band diagrams is rather difficult. A good level of accuracy requires a very small discretization step, thus involving large CPU time, in particular for the analysis of structures with a refractive index variation in three dimensions. Moreover, the high contrast discontinuities, cause large reflections and so a huge number of time steps has to be considered before the field reaches a significant steady state.

FDTD method is well known in the acoustics and seismology communities but has been only recently to the study of phononic crystals. The most important advantage, together with the general properties of giving the field at any point inside and outside a sample, at every time, and in both frequency and time domains, is that it can be applied in systems with arbitrary material combination and in systems with arbitrary configuration of the scattering elements, giving the possibility to study also defect states.

The Finite Element Method (FEM) [11] requires a very dense grid of finite elements where high refractive index discontinuities are present and this produces an increase of computation time, particularly in the analysis and design of complicated photonic crystal slab devices and complex phononic crystal structures, although good accuracy can be achieved.

The Scattering Matrix Method (SMM) [12] allows the evaluation of both field distributions and transmission spectra. When scattering centres with circular cross section are considered, the CPU time can be minimized by exploiting the Bessel-Hanken functions for the em field expansion. However, the computational complexity scales with the third power of the number of holes or rods in the BG device, and so even this method can hardly be used for the design of large photonic/phononic crystal structures.

Green's functions [13] are a mathematical artifice which facilitates the solution of differential equations when the boundary conditions are known and the excitation of the structure is made by means of point source. The Green's function of a complicated system can be found by a matrix multiplication involving several Green's functions of a much simpler system. Such approach has been applied to the study of multilayer systems and photonic crystal slabs.

The Multiple Scattering Theory Method (MST), derived from the traditional Korringa-Kohn-Rostoker (KKR) method [14] developed for the calculation of the electronic structure of solids, appears to be numerically efficient for simulating several both photonic and phononic crystal structures. MST is able to both calculate dispersion relations for mixed composites and for high contrast composites and transmission of finite slabs of those composites, both periodic and random, also showing a good agreement in comparison to experimental results.

4. Applications

4.1. Photonic crystals applications

The importance of the PhC structures in the development of the integrated photonics strongly depends on the large variety of devices that can be realized on a single chip, with a better performance with respect to the conventional photonic devices.

The existence of photonic band gap can suitably be exploited for realizing high efficiency optical reflectors. The high index contrast of the elementary cell makes this mechanism very efficient, and reflectivity values higher than 90% can be obtained [15].

Breaking the perfect periodicity of a PhC lattice creates available photonic states within the photonic band gaps. These new energy states are associated to wave functions and the structure behaves as optical resonant microcavity. The resonant frequencies depend on the cavity and defect geometry. Very high quality factors can be achieved due to the efficient confinement mechanism based on photonic band gap effects. The structures reported in literature are particularly suitable in telecommunication and sensing devices as multiplexer/ demultiplexer devices and add/drop filters. Where the quality factor (Q) is a critical parameter, Fabry-Perot cavities using high efficiency reflectors have been proposed [16-17].

Another interesting property is the very small mode volume, that can assume values also very close to the minimum value theoretically allowed [18]. This effect can be exploited for fabricating very efficiency LED and lasers without threshold in principle.

PhC resonant cavities can be used for realizing lasers with very small size. A higher selectivity and single mode operation in a waveguide laser can be achieved by including in the cavity a PhC mirror placed [19]. A tunable single mode laser can be also realized by using cavities delimited by PhCs, exploiting the refractive index variation due to a temperature change

PhCs allow to realize optical waveguides based on physical effects different from the conventional total internal reflection [20], by exploiting the effect of linear defects. An optical beam with a wavelength within the photonic band gap can not penetrate in the PhC and will be forced to propagate along the axis of the linear defect. The advantage of the PhC waveguides with respect to the conventional waveguides consists of the capability of guiding optical signals along paths with very large curvature angles. Curvature angles as large as 60° in hexagonal lattices and 90° in square lattices have been reported.

PhC resonant cavities can be easily coupled to optical waveguides and this advantage open interesting possibilities of realizing components that are building blocks of the photonic circuits [21]. Same basic principle enables the operation of channel-drop filters [22].

PhC fibres (PCF) are a new class of optical fibres based on the use of periodic dielectric structures. They are able to overcome some typical issues of the conventional silica fibres in telecommunication systems, such as losses, non linearities, and limited tuning, due to low index contrast between guiding core and cladding.

Two types of PCF there exist: bandgap guiding fibre (PBF) and index guiding fibres (PCF). In PBFs, the photonic crystal lattice has the property of confining the light by means of the mirroring function realized by the crystal, while in PCFs the lattice is made by air holes within a guiding dielectric material, with a resulting effect of reducing the cladding refractive index.

PCFs able to maintain the polarization state (PMF) have been demonstrated. To get PMFs, a strong birefringence is introduced in the fibre. The input signal must have a polarization state along one of the main axis of the fibre. Under these conditions, the light polarization will be preserved even in presence of curvatures, because the wave numbers, that are different for the two polarization states, do not create any mode coupling when in presence of irregularities of the structure. PCFs allow obtaining birefringence values up to one order of magnitude higher than the conventional PMF fibres, because some asymmetries can be more easily introduced and designed.

Dispersion effects occurring in PhCs can found several applications in the field of passive devices. Supercollimators and superprisms are well known examples. In the PhCs regions with a constant curve gradient of $\omega(\mathbf{k})$, and regions with a propagation direction for the e.m. energy changing very rapidly can both exist. Then, those regions with gradient constant can be exploited for realizing the supercollimators [23], where the refracted waves, associated to different wave components, can propagate in parallel directions, giving an optical beam that appear to be perfectly collimated.

Different is the operating principle at the basis of the superprisms. Conventional prisms have a spectral selectivity that is too low to be employed as mux/demux in WDM systems. Photonic crystals allow, however, to change the dispersion properties of the material, achieving a condition satisfying the required performance. The crystal can be designed so that in the spectral region of interest the isofrequency curves show a strong sensitivity to small variations in frequency, changing in shape from concave to convex forms. Devices of this type have a high spectral resolution and can be used in the modern DWDM systems. The big advantage consists in the possibility of demultiplexing/multiplexing a large number of signals by using a single component at micrometric scale.

4.2. Phononic crystals applications

The field of PhnCs is only about 10 years old and the search for the best phononic structure is still ongoing. Phononic crystals will provide new components in acoustics and ultrasonics fields, offering functionalities and level of control comparable to the light field.

It is useful to classify phononic crystals into sonic, ultrasonic and hypersonic crystals, depending on the operating frequency. Each class leads to different applications and involves different technological approaches. Sonic crystals (1 Hz – 20 kHz) are important in sound manipulation, communication and information transfer. Still, these structures need to be several meters wide to create a phononic band gap in the sonic range and this could make them impractical for many devices. In the ultrasonic regime (20 kHz – 1 GHz) the wavelengths are much shorter than in the sonic regime and then the phononic crystals are also much smaller (from centimeters to fractions of millimeters). This aspect, together with the negative refraction property, could lead to several applications for phononic crystals.

Examples are imaging and non-destructive testing. Wavelengths in the hypersonic range (>1 GHz) are shorter than those in the ultrasonic regime. The behavior of hypersonic phonons is crucial for many physical phenomena in materials, as an example, the interaction between electrons and high-frequency phonons, that determines the efficiency of spontaneous light emission in silicon and other semiconductor materials that having an "indirect" electronic band gap. Controlling the phonons in silicon could lead to highly efficient silicon-based light-emitting devices. Further applications are acousto-optics, signal processing and thermal management.

As in photonic crystals, the PhnCs having a wide bandwidth act as acoustic mirrors that can reflect a large fraction of the acoustic energy incident on the crystal. In case of micro-phononic crystals this property results to be useful for isolating resonating structures such as Coriolis gyroscopes, microresonators, filters and oscillators. 1D Bragg acoustic mirrors have been proposed [24] to isolate thin film AlN resonators in cellular phone duplexers. The use of a mirror rigidly attached to the substrate improves the power handling and immunity to vibration. This isolation capability is limited in 1D Bragg mirror, in particular when the waves do not propagate exactly in the direction perpendicular to the stack. Vibrating thin film resonators not only produce acoustic energy that is not normal to the substrate but also a small percentage of acoustic energy is converted into shear modes. For these reasons, phononic crystals to be used for isolating resonators and filters have typically 2D and 3D periodicity [25].

Removing scattering elements in a phononic crystal can create defects in that structures, such as waveguides that route and bend acoustic signals [26]. Phononic crystal waveguides can be used for miniaturizing acoustic delay elements in signal processing and delay line oscillators. The miniaturization of the delay line is based on 'slow sound'. This effect is due to the fact that wave propagating through the guide resonates at the same time and this slows the group velocity by orders of magnitude, allowing a reduction in the size of the device to be used for getting a given time delay. The principle is similar to 'slow light' in photonic crystals. Tapered waveguides can be used for miniaturized impedance matching, collimation and focusing in acoustic imaging applications such as medical ultrasound.

Waveguide can be also used to decouple the design of the transmitting/receiving element in an acoustic imaging system from the size of the aperture. Reduction of the aperture size of each element in an acoustic imaging array reduces to get high density. An example of routing and focussing of signals from an array of large, high dynamic range capacitive micromachined ultrasonic transducers to a group of apertures by means of a set of phononic crystal waveguides is given in [27].

The reduction of the aperture size and the possibility of more dense imaging array reduce the need of creating synthetic apertures, used to solve the problems of image resolution in low-density arrays.

By introducing defects in a phononic crystals allowed states within the band gap can be created and they are strongly localized in the defect region. Then, an interesting field of application of phononic crystal technology is the area of high Q cavities and filters.

At macro-scale cavities and filters have been demonstrated [28] in defected solid/water phononic crystals. Micro cavities have been proposed in 2D phononic crystal with the advantages of increasing the frequency selectivity and reducing the insertion loss. Point defect cavities with quality factors approaching 10^4 have been proposed. Further advantage of phononic crystal based cavities and filters are the ability to decouple the high Q resonator and electro-acoustic transducer design. Phononic crystals allow realizing micro-scale cavities in high Q materials, such as Si, SiO_2 and W, while the electro-acoustic transduction is performed peripheral to the cavity using high-efficiency piezoelectric couplers, so overcoming the problem of searching a trade-off between Q and motional impedance, typical in microresonator technology. Drop and series/drop phononic crystal waveguide cavities for distributed stripline resonators commonly used in microwave filters are proposed in [29]. The properties that makes these waveguide based filters interesting devices are, first, that phononic crystal waveguides are broadband compared to phononic crystal cavities, and then frequency division multiplexers and demultiplexers can be implemented by using a waveguide and a series of cavities. Furthermore, phononic crystal waveguide cavities can be realized by changing the lattice constant in proximity to the waveguide. Very high Q have been achieved in photonic crystals by means of this approach.

One of the interesting aspects of the photonic crystals is their capability of making superlenses, i.e. lenses not diffraction limited, with materials having a negative refractive index. On the basis of the first demonstrations in this sense the research has been also focused on the possibility of making superlenses for acoustic waves.

Negative refraction in phononic crystals is possible due to multiple scattering of sound waves at the solid-air interfaces. A sound wave impinging at a specific angle on a phononic crystal can be seen as having two components:

one travelling parallel to the surface, and one that moves at right angles to it. Negative refraction will occur if the direction of the parallel component is reversed while that of the normal wave does not change.

Requirements for negative refraction in phononic crystals have been discussed in [30].

An application of hypersonic phononic crystals could be the thermal management. Thermal energy in solids is transported mainly by electrons and phonons. The electronic contribution is important for materials with a large number of free carriers, such as metals, while the thermal conductivity of dielectric materials and many semiconductors is determined mainly by the phonons.

The flow of phonons and, then, the thermal conductivity of a solid could be reduced by the existence of a phononic band gap, resulting to be very useful for thermoelectric devices that directly convert thermal energy into electricity because able to improve the performance of devices such as Peltier thermoelectric coolers, thermocouples and thermoelectric energy generators.

Due to the operating frequencies the hypersonic crystals require 3D periodic patterns at submicron and nanometre scale and this implies the use of specific fabrication techniques, such as two-photon lithography, holographic interference lithography and self-assembly, more challenging with respect to the standard manufacturing techniques used for sonic and ultrasonic crystals.

Materials having both photonic and phononic properties are now under investigation. The basic ideas under both phononic and photonic band-gap materials are the same, thus the research effort has been also focused on the possibility of finding materials that exhibit both types of band gap. Hypersonic crystals, that have lattice constants in the range of visible or infrared wavelengths, seem to satisfy this requirement. A theoretical demonstration was given [31] for crystals consisting of a square or triangular 2D array of air holes in silicon. The simultaneous presence of photonic and phononic band gaps allows to localize both sound and light in the same region and this strongly increases the acousto-optical interactions. As an example, in [32] it was suggested to use these structures to generate intense sources of coherent monochromatic phonons, which could be known as "phonon lasers".

5. Conclusions

The basic concepts of the photonic and phononic crystal technologies have been reviewed in this paper with particular emphasis on their main applications, together with a description of some modelling approaches.

Research efforts must be spent on the improvement of the proposed devices, on the development of new materials and new devices, mainly with reference to those having simultaneously both the phononic and photonic band gap.

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