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Photonic Crystals, Photonic Wires and Photonic Bandgaps: Some Basics: A

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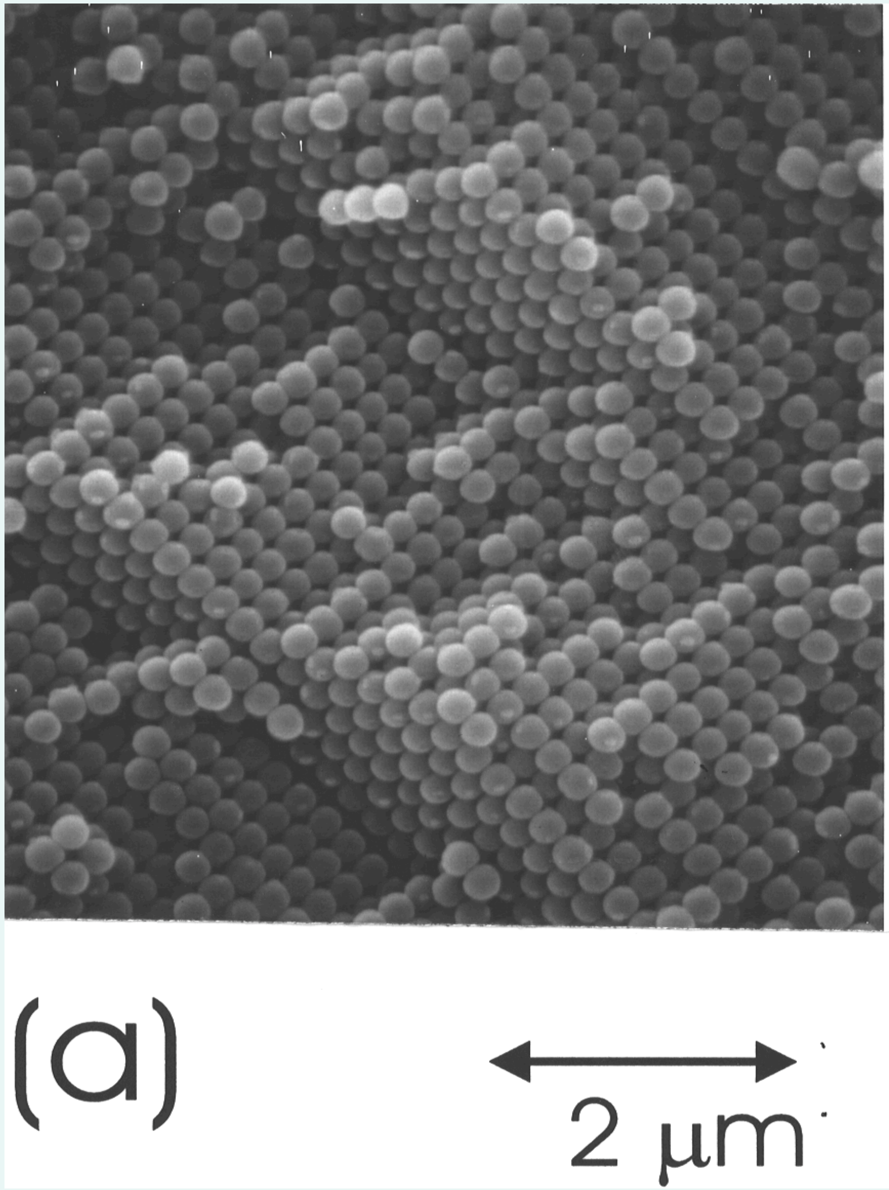
Bare opal: Electron Micrograph

Sub-micrometre (typically ~300 nm dia.) colloidal silica spheres. Cleaved material surface shows both *square* packing associated with (100) planes and *hexagonal* packing associated with (111) planes. Made in Russia.



S.G. Romanov, N.P. Johnson and C. Sotomayor-Torres

Summary

- What are photonic crystals (PhCs)/bandgaps/ microstructures?
- Why are photonic bandgap (PBG) properties interesting?
- Why use III-V semiconductors for photonic bandgap devices?
- Extracting light more efficiently from LEDs
- Spontaneous emission inhibition
- Stimulated emission possibilities
- Brillouin zones, Bloch modes, equi-frequency surfaces (EFS) and band-gaps.

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What are photonic crystals/ bandgaps/microstructures?

- ***Photonic crystals*** have a regularly **periodic refractive index** variation in one, two or three-dimensional space.
- Photonic crystals may be called ***Photonic microstructures*** (nanostructures) when they are formed by using lithography and etching processes.
- Photonic crystals exhibit ***full*** **photonic bandgap *(PBG)*** behaviour if there is a range of frequencies (photon energies) - i.e. a stop-band - over which *electromagnetic wave propagation is strongly inhibited*, no matter what direction of propagation or polarization condition is considered. This typically requires a refractive index ***contrast*** of ~2:1 or more.

What are photonic crystals/bandgaps/ microstructures? (cont)

- ***Incomplete*** PBG behaviour may also be useful. **Directional** or **polarisation-dependent** behaviour provides **selectivity** within or at the edges of the stop-band. One-dimensional PBG = > strong directionality.
- **Variation of periodicity** (e.g. ***Chirp***) may be useful?
- **Fibre Bragg-gratings, DFB lasers**, etc. all use 'photonic bandgap' **(stop-band)** behaviour. Chirped **(quasi)-periodicity**, amplitude-weighting and **step phase-jumps** are often used to provide the required **time- or frequency-domain** (*filter*) properties.
- **Transmission features** within the stop-band can be very useful: i.e. formation of ***photonic crystal microcavity***.

What might photonic bandgap components be good for?

- Photonic bandgap devices may possibly be used in optical telecommunications, displays, sensors and detectors - and elsewhere.
- Lasers, LEDs, photodetectors, WDM multiplexing and demultiplexing, OEICs and PICs, pulse compression and variable delay, etc.
- Performance enhancements: reduced threshold current (density), reduced device size (i.e. compactness), enhanced non-linearity,…….

Why was the photonic bandgap concept introduced?

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- ***Photonic Bandgap*** **behaviour** was recognised by ***E. Yablonovitch*** in 1987, ['Inhibited Spontaneous Emission in Solid-State Physics and Electronics', *Phys. Rev.Letts*, **58**, pp. 2059 - 2062, (18 May 1987)] to be a potentially useful effect.
- Yablonovitch pointed out that preventing the escape of photons from a source by surrounding it uniformly with a stop-band medium would shift the balance from predominantly spontaneous emission towards the situation where stimulated emission would predominate. This statement is essentially the same as saying that a **reduced threshold for lasing** is created by **omni-directional stop-band behaviour**.
- He also pointed out that in all systems, following the Einstein equations, there is always ***spontaneous emission*** occurring alongside ***absorption*** and ***stimulated emission.***

Spontaneous emission & stimulated emission

- **Spontaneous emission and stimulated emission always occur together. (Einstein A and B coefficients). But typically LEDs *predominantly* produce *spontaneous emission* and *lasers* predominantly produce *stimulated emission*.**
- **The *threshold* of lasing is the *transition* between mainly spontaneous emission and mainly stimulated emission.**
- **Strong(er) periodic feedback makes lasing easier to achieve, because it restricts spontaneous emission - and particularly so, if there is a frequency selective 'defect-state' incorporated into the periodic feedback structure.**

Why was the photonic bandgap concept introduced (cont.)?

- **For LEDs (light emitting diodes),** it is desirable that light (photon) generation be primarily by spontaneous emission, provided that the high ***internal*** quantum efficiency that really is available from diode heterostructures can be converted into high ***external*** quantum efficiency.
- But the characteristic problem of LEDs has been that their external QE is very much lower than their internal QE, because of the ***high refractive index (>3)*** of the semiconductor. The high RI means that much of the light that is generated does not escape from a cuboidal 'box'.

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Why is spontaneous emission preferable to stimulated for many purposes?

- **LEDs (light emitting diodes)** do not need to be spectrally very narrow - e.g. for people to see images on multi-colour displays, traffic lights, etc.
- The coherence of predominantly stimulated emission used in semiconductor lasers makes them problematic for safety reasons (not eye-safe). Coherent light leads to **coherent scattering** effects, e.g. from rough surfaces - speckle - i.e. heterodyne noise, which is a much larger fluctuation than for incoherent light.
- Reliability is greater for cheap volume manufacture of LEDs than semiconductor lasers. Material quality can be inferior, so epitaxial growth perfection can be less. The stimulated emission process tends to concentrate at defects, e.g. dark-line defects?

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Why III-V Semiconductors?

- III-V semiconductors are used in the vast majority of the world's lasers. 100 million (?) lasers, 100 billion (?) LEDs are produced per year. (A thousand times more LEDs than lasers!)
- Both as LEDs and lasers, III-V semiconductors provide, still, the most efficient and direct means of converting electrical power into optical power.
- III-V semiconductors are the preferred materials for light generation in a spectral range from the blue/uv to the mid/far infra-red.
- III-Nitrides => Phosphides/Arsenides => Antimonides

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Why III-V Semiconductors? (cont.)

- Most LEDs for visible wavelength light emission are based on single crystal wafers of the semiconductor ***gallium phosphide (GaP).***
- i.e. the **substrate** on which the epitaxial heterostructure is grown, with various alloy compositions of the form $Ga_xAs1^{-}{}_{x}P/Ga_yAs_{1-y}P$, **may well be GaP** - although:
- At the longer wavelength end of the visible spectrum, the substrate used may be gallium arsenide GaAs.
- GaP is an indirect (electronic) bandgap semiconductor.

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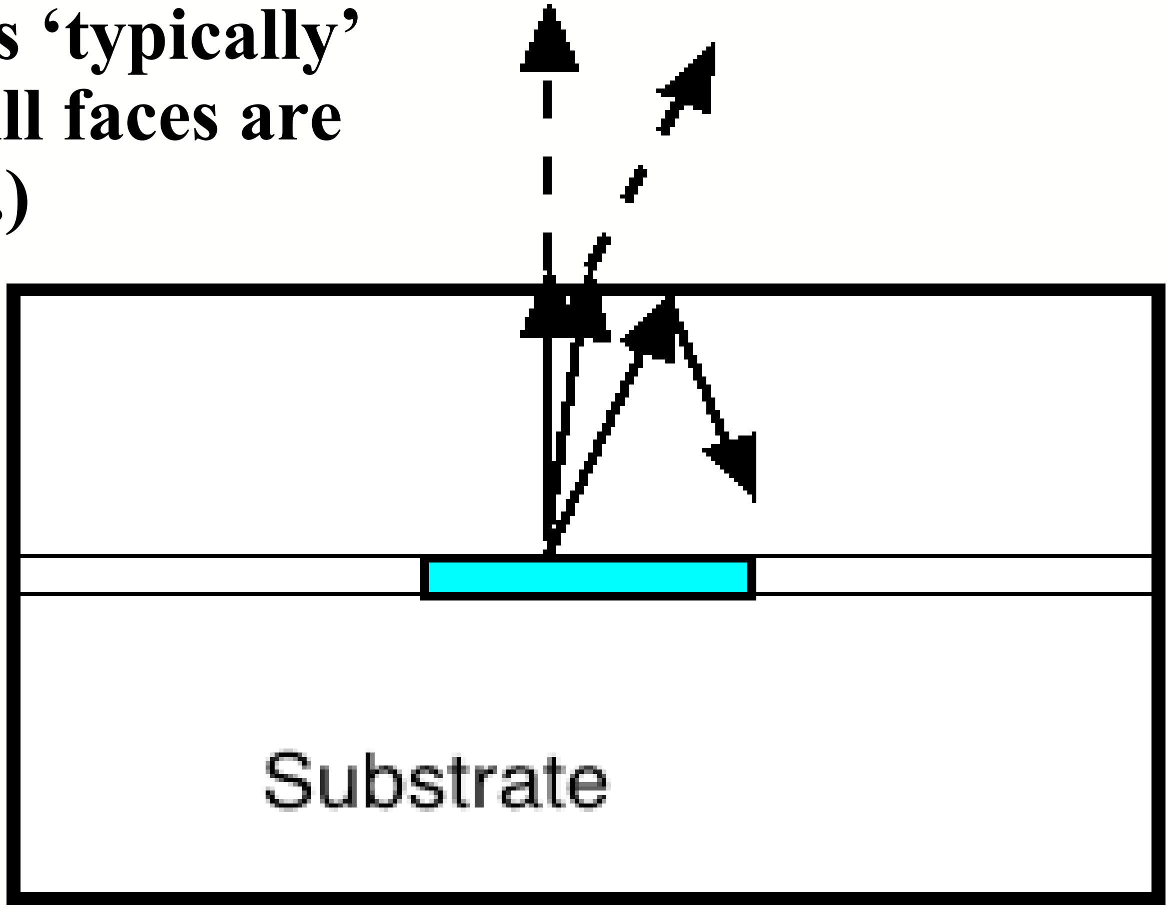
Why III-V Semiconductors? (cont.)

- Indirect band-gap semiconductors are typically NOT good light emitters - e.g. silicon. (But people are still trying to make good light emitters based on silicon. This is hard work!)
- So, why use gallium phosphide (GaP)?
- Gallium phosphide is transparent through a large part of the visible spectrum, but not the blue part.
- GaP can become a good (enough) current-injection electroluminescent semiconductor by special doping processes (oxygen, nitrogen atoms) that create ***states in the (electronic) bandgap.***

LEDs: where does the light go - or not go?

- LED 'box' is 'typically' a cuboid. (All faces are rectangular.)



- Active region is in a thin layer grown epitaxially, usually on a high refractive index semiconductor substrate.
- Substrate may be ***transparent*** - or may ***not*** be?
- There are six nominally equivalent faces on a cuboid.

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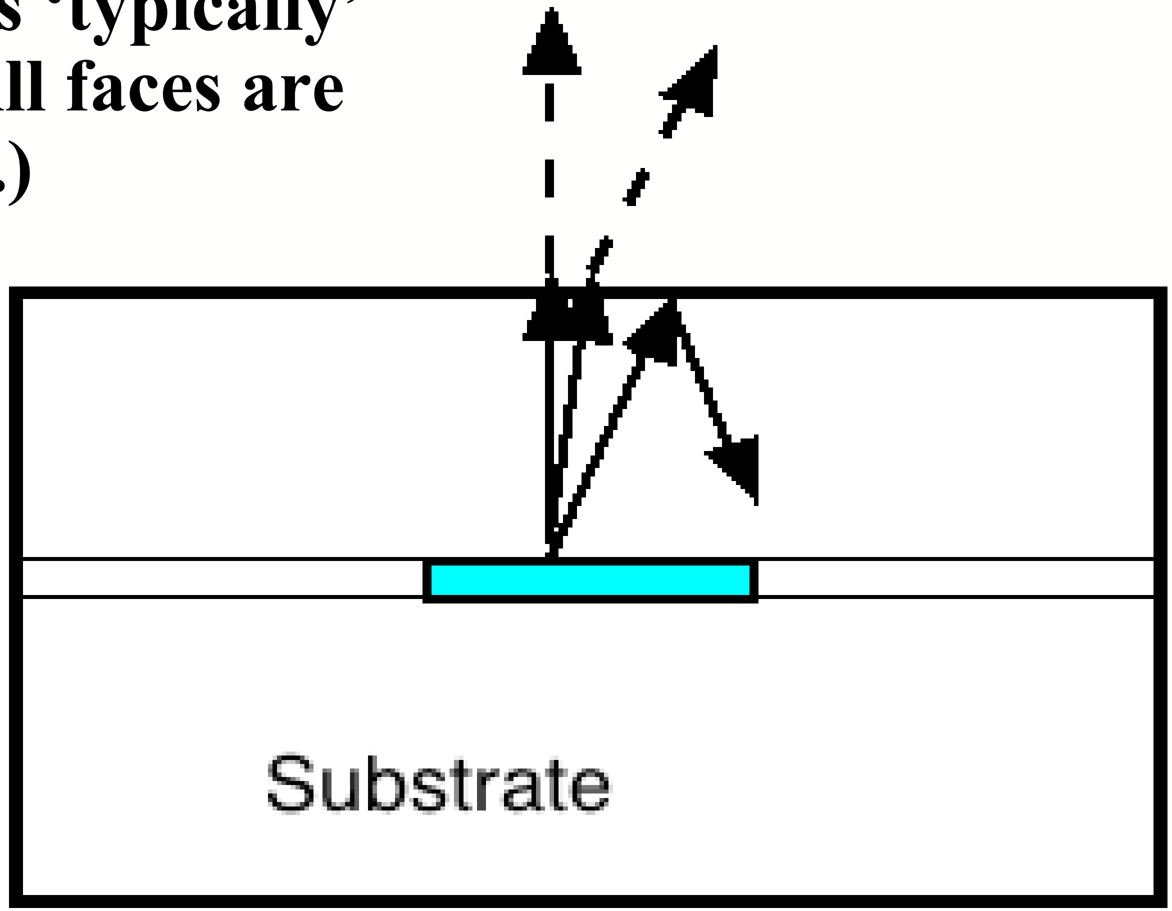
Why doesn't the light come out easily from the high-index cuboidal box?

- ***Light generated in the core*** (active region) of the optoelectronic component (LED) strikes boundaries at a wide range of angles. (360 degrees nominally).
- ***Rays bend away from normal*** on exit into air according to ***Snell's law*** (Descarte's law in France).
- But, for a high refractive index box in air, rays already bend to satisfy ***total internal reflection*** (TIR) condition at small angles away from normal incidence.
- Solid geometry calculation for the ***exit cone*** reduces possible ***external efficiency*** to ***maximum of ~3%.*** (Assuming that only top emitted light is useful.) (Refractive index of emitter ~3.)
- ***Reflected light*** may well undergo ***absorption*** without photon re-generation ('re-cycling') occurring, particularly if substrate electronic band-gap is smaller than emitted photon energy.

Where does the light go - or not go?

- LED 'box' is 'typically' a cuboid. (All faces are rectangular.)

- Active region is in a thin layer grown epitaxially, usually on a high refractive index semiconductor substrate.
  - Substrate may be transparent - or may not be?



- There are six nominally equivalent faces on a cuboid.

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What are the possible ‘cures’ for the TIR problem?

- *a) Transparent box* with six faces - increases possible external efficiency by up to six times. ***h ~= 24 %***
- But external *mirror system* is required to re-direct light in desired direction. (Bigger effective source area - *reduced brightness*.)
- *b) ‘Upside-down’ Truncated* square-base *pyramid geometry* together with transparency - rays always bounce out after multiple reflection. *(Lots of sawing and polishing ?!)* ***h ~= 50 %***
- *c) Microcavity LED* (1D PhC) with large area. ***h > ~20 %***
- May use both top and bottom emission, plus edge (guided) light.
- *d) Embed 3D PhC into the LED*. (Must overcome damage and other problems due to fabrication processes such as RIE.)

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Spontaneous emission control

Light generated within a solid body must escape effectively if it is going to be useful.

'Typically' the solid body has many available modes of oscillation which are excited *incoherently* over a 'fairly wide' spectral range by the emission process.

'Typical' LEDs operate *predominantly* via spontaneous emission - and can fairly readily exhibit nearly 100% *internal* quantum efficiency. (Defined e.g. as photons per electron.)

But *total internal reflection* (t.i.r) occurs where the radiated light strikes the large index-contrast boundary at a moderately oblique ANGLE, so the *external* quantum efficiency may be much less than the internal quantum efficiency.

Spontaneous emission control (cont)

A full PBG 3-D photonic crystal can (in principle) eliminate all of the available modes of oscillation in the spectral range of the emission process, thus giving complete inhibition of radiation out of the 'LED box'.

Photons are bosons, so many photons can occur in the same mode. So the emission process may be channeled spectrally

Limiting or eliminating the possibility of spontaneous emission significantly increases the probability of obtaining *stimulated* emission.

- LED-type semiconductor structures (typically using *direct-bandgap* III-V semiconductors) may have **very high INTERNAL quantum efficiency** for the ***spontaneous emission*** process, e.g. more than 90%. Photon generation by electron-hole pair recombination.

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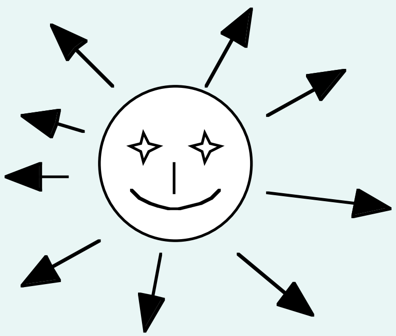
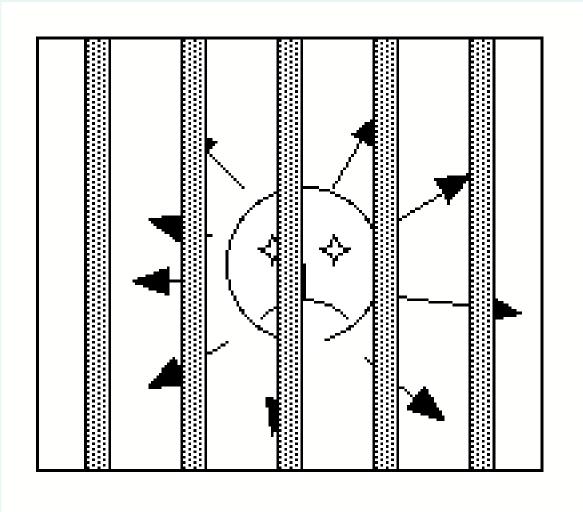
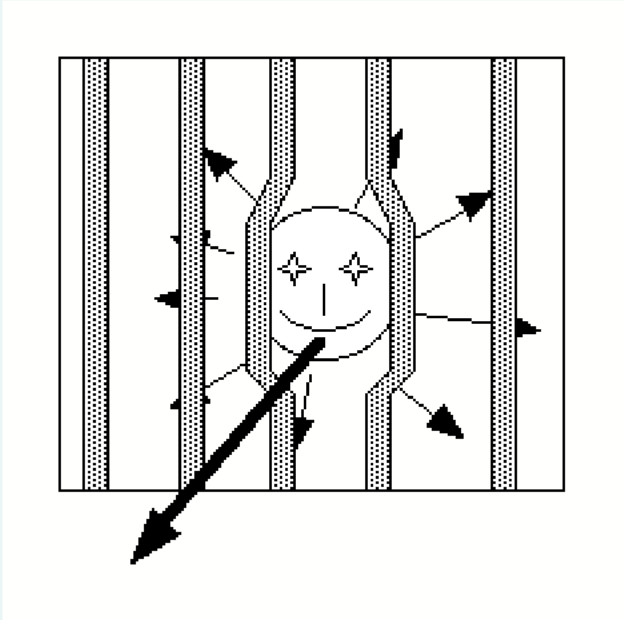
Spontaneous emission control



Unrestricted emitter



Emission completely prohibited.



Emission via selected modes allowed by defect.

Stimulated emission

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- The sequence of diagrams just shown is also a close analogy for the way a DFB laser works, although the typical semiconductor DFB laser has only *one dimensional periodicity*.
- So the standard DFB laser arrives at its lasing threshold with a lot of spontaneous emission already happening.
- Above threshold, the stimulated emission process grows very rapidly because the newly stimulated photons are directionally very selective.
- The demonstration by Salt Lake City group of *photo-pumped lasing* in 3D-PhC (dye-solution infilled into synthetic opal) DID NOT REQUIRE FULL PBG behaviour.
- In the index-matched limit it showed lasing action with ZERO REFRACTIVE INDEX CONTRAST, relying purely on *gain-modulation alone*.

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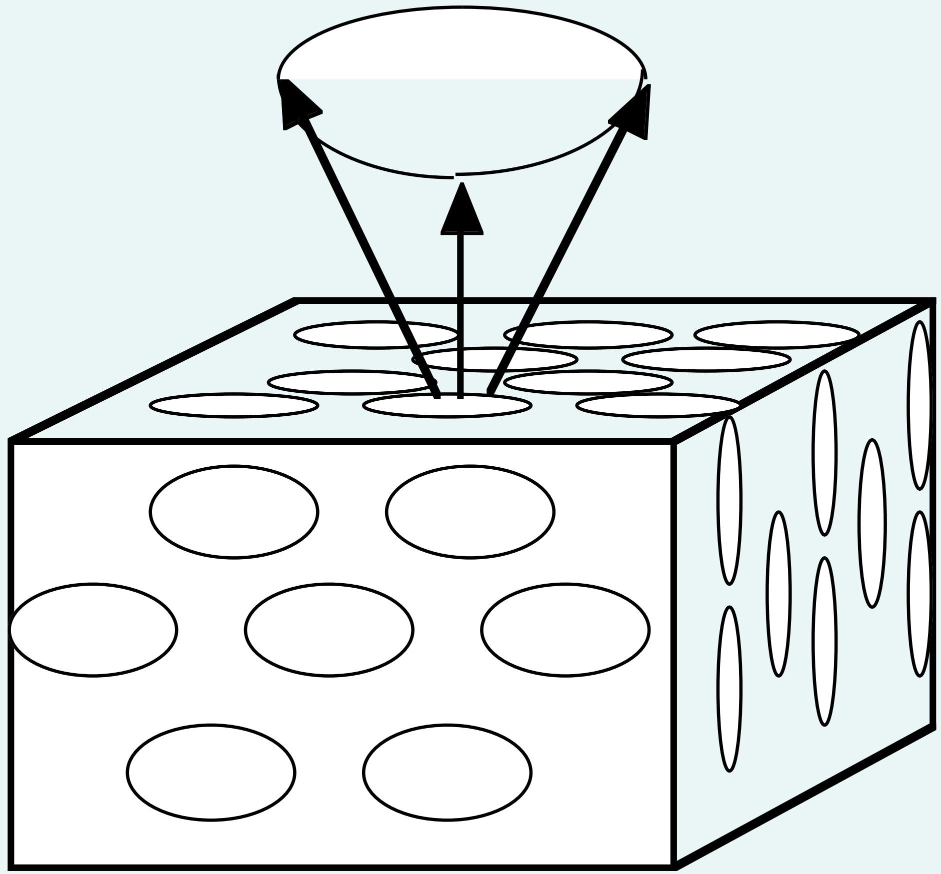
3D (PBG) PhC light emitter

- Large index-contrast 3D PhC structure throughout the high index ‘light-box’ ‘forbids’ emission in most directions/frequencies.
- Limited size *defect channel* directs frequency selected light out of the box (within escape cone).
- Substantially divergent output beam if the defect channel ‘exit spot’ is small.



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Quantum energy-frequency relations

- **In simple quantum language, the photon energy and optical frequency are related by:**
- $E = hf = hn = (h/2p)\ w =$ ***'h-bar'.*** w
- **where (given that we all want to pass ourselves off as engineers some of the time), the energy E is in Joules, f or n are both the cyclic frequency in Hertz, the angular frequency w is in radian/second and**
- h **is Planck's constant, which has the value of ~6.6×10^{-34} Joule.second.**

Quantum momentum relations

- We also need to consider the (quasi-)momentum associated with a photon of propagation constant k:
- De Broglie tells us that *momentum*:
  - $p = h/l\ =(h/2p).k =$ ‘h-bar’$.k$
- This applies even for ‘particles with zero rest-mass’, such as photons. But for photons, the free-space (vacuum) value of k is simply the same as:
  - $k_0 = w/c$, where c is the velocity of light in free-space.
- In a medium with refractive index n:
  - The wave-vector, $k = n.\ k_0$

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Some definitions

- Photonic Bandgap behaviour is a feature of electromagnetic wave propagation in periodic structures.
  - More generally we are talking about BAND-STRUCTURE.
- Wave propagation in periodic structures is inherently dispersive, i.e. the *phase* velocity *depends on frequency*. The phase velocity is a vector quantity - and it is, by definition parallel to the wave propagation vector. We therefore have the phase velocity definitions that follow, with he second form giving a proper vectorial version:

$$v_p = \omega/k = (\omega/\underline{k}.\underline{k})\underline{k}$$

- Using the word 'photonic' has the same connotation as using the word 'electronic' when talking about the properties of semiconductors. i.e. we routinely mix *particle* language into descriptions of *wave phenomena*.

Definitions (continued)

- **i.e. it's the ratio of the y-axis value to the x-axis value in a plot of ω versus k that gives the *phase velocity*, where ω is the angular frequency (radians per second) and k is the wave vector magnitude.**
- ***Group* velocity is defined as the *slope* of the dispersion curve, i.e.**
  - $v_g = d\omega/dk$
- ***But Group velocity* and *phase velocity* are both VECTORIAL properties of a medium (in three-space). So the group velocity definition should be understood as meaning the use of the *gradient operator* in vector calculus.**

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Definitions (continued further)

- In the characteristically ANISOTROPIC situation of a periodic medium, **group velocity and phase velocity are only collinear along 'high-symmetry' directions**; i.e., in general, the wave-front normal is not parallel to the energy transport direction.
- **In general: phase-velocity and group-velocity are non-collinear.**
- Even a one-dimensionally periodic medium (e.g. a simple grating) in two-space or three-space may be strongly anisotropic.
- The classic electronic engineering contexts for periodic structures are *artificial* (lumped element) *delay lines* and the *'slow-wave'* structures used in *microwave electron tubes*, such as travelling-wave amplifiers (TWAs) and backward wave oscillators (BWOs).

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Light lines and heavy photons, etc.

- It is often useful to use the free-space *light-line* as a reference marker - or the *substrate light-line* (thinking about planar waveguide situations).
- The light line is a straight line through the origin of an ω-k diagram.
- The slope of the *light-line for free-space* is simply the velocity of light c, i.e. $3\mathrm{x}10^{8}$ $\mathrm{m.s^{-1}}$
- In general, the *light-line for a specific medium* has its slope given by c/n, where n is the medium refractive index.
- **Strictly guided Bloch modes** of a layered open waveguide photonic crystal structure must have an effective refractive index which is larger than the external media indices, so they **must lie *below all* the relevant light-lines**.
- Heavy photon behaviour occurs when the group velocity is significantly smaller than the modal phase velocity.

Light lines and planar (slab) waveguides

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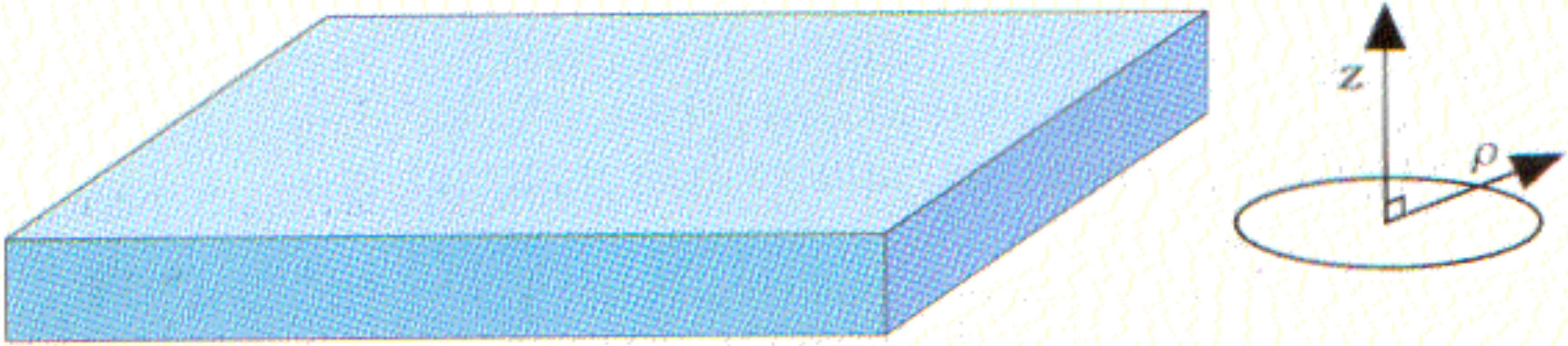
The waveguide 'layer' has finite thickness *a* in the *z*-direction - and it extends to infinity in all in-plane directions.

As shown, it is a thin membrane with 'air' (refractive index n = 1) above and below it. To be 'single-moded' at optical frequencies, it would need to be approximately 0.3 μm thick - or less!

Refractive index of slab might be as high as n = 3.5 in a semiconductor.



Light lines and modes for a planar (slab) waveguide with 'air' above and below.

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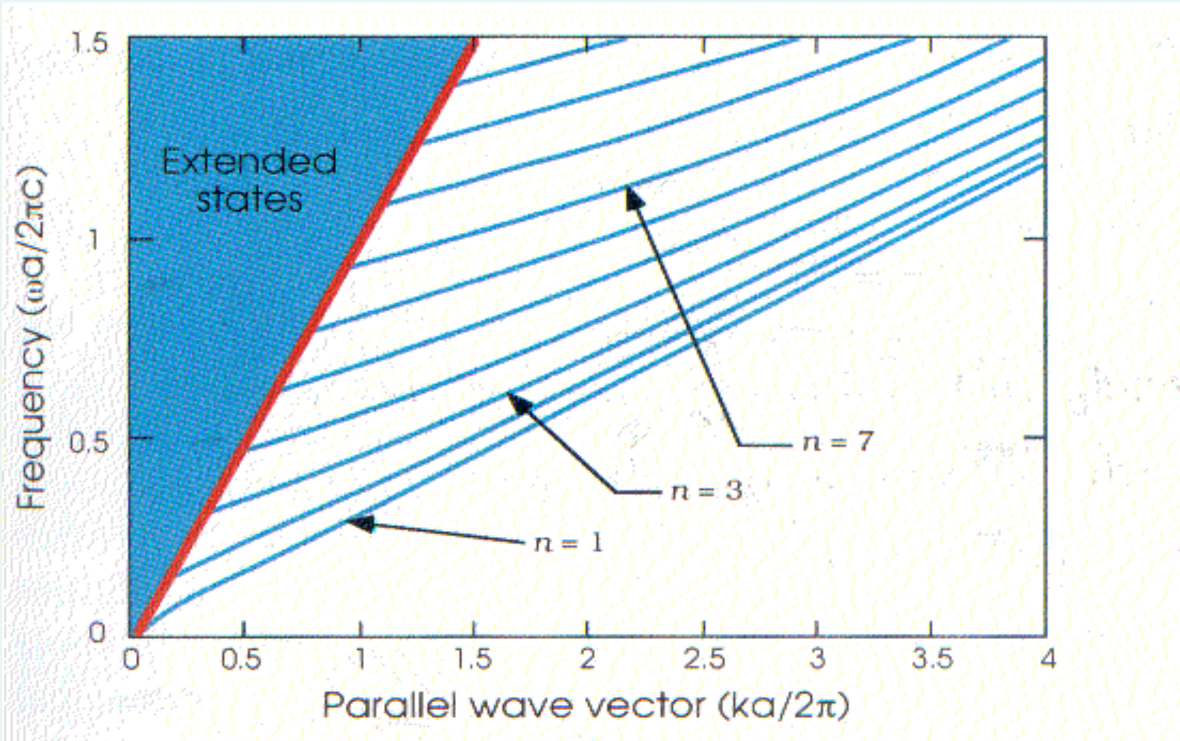
The labels ***n*** are used to identify the truly-guided (confined) modes of the slab. The modes decay evanescently above and below the slab. The spectrum of guided modes is ***discrete***.

All modes exhibit cut-off behaviour below specified frequencies that depend on the thickness and index, except for the lowest mode of the perfectly symmetric slab.

(Typical guided-mode literature uses labelling from n = 0.)



'Heavy' photons

- Heavy photon behaviour is typically observed as the Brillouin zone-boundary is approached, i.e. where the dispersion curve starts to look (locally) parabolic.
- In waveguide photonic crystals, *'anti-crossing' phenomena* may be observed due to the *coupling*, e.g., of modes with different nominal polarisation states. This anti-crossing phenomenon is a form of *mini-stopband behaviour*.
- Heavy photon behaviour is identified with *reduced group velocity*, i.e with *particle-like behaviour*.
- *Control* of the group-velocity (or *group-delay)*, with *large changes in velocity* resulting from *small changes in frequency* looks interesting for device purposes. But the situation may be too critically dependent on the *precision of fabrication*, on *temperature*, etc.
- *'Make a virtue out of necessity'* and think *'sensors'?*

The effects of periodicity: Bloch modes

- ***Solutions*** **of Maxwell's Equations for propagation in loss-less periodic media** ***are themselves periodic*****.**
- **This is effectively the same as saying that the** ***solutions take the form of Bloch waves*****. (Bloch-modes or Floquet-Bloch modes). See Joannopoulos et al.**
- **The Bloch modes at a single frequency for a photonic crystal structure are described by the product of a complex exponential propagation term (for each axis) multiplied by** ***a term which has exactly the periodicity of the photonic crystal structure*****, i.e. (in 2-space):**
    - $\exp(jk_x x).\exp(jk_y y) \times u(x,y)$

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The effects of periodicity: Bloch modes (cont)

- where *u(x,y)* has the **periodicities of the photonic crystal**. It has a 2D discrete Fourier-spectrum in k-space for a 2D-PhC.
- In our 3D-Universe, the function *u(x,y)* will also have z-dependence that is determined by the detailed **'vertical'** distribution of the 2D PhC structure, e.g. a waveguide layer with holes in it, typically supported by a substrate that has a refractive index greater than that of air, but less than that of the waveguide layer.
- *Bloch waves* are typically **partial standing waves**, so they can transport optical power. They become **pure standing waves** at the **Brillouin zone boundaries**, i.e. at the band-edges - where the **slope of the W-k diagram goes to zero** - and the group velocity is therefore also zero.

Bloch modes and Brillouin zones

- **For a lattice constant a, the relevant wave number is $2\pi/a$**
- **In particular, a purely standing wave situation occurs when the Bragg condition is satisfied. (= stop-band edge situation.)**
  - **Bragg condition: $k = k_B = +/- \pi/a$ x *(non-zero integer)***
- **This condition occurs at different photon energies (frequencies) for different possible Bloch modes of the PhC lattice.**

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Bloch modes and Brillouin zones

- In general the *periodic function* could be complex, but it *might be real*, and it can be expressed as a *complex Fourier series expansion* of complex exponential components with both positive and negative k-vector terms that are integer, non-zero multiples of the wave-number determined by the lattice constant.
- We now present some analysis based on a recent paper: B.Lombardet et al: 'Fourier analysis of Bloch wave propagation in two-dimensional photonic crystals', Proc. SPIE, vol 5450, pp.150-.., (2004). They choose to analyse a square lattice of high dielectric-constant rods in a low-index background, but the results apply more generally.
- The Fourier series representation of a Bloch wave may be written as:

$$H_k(r) = \sum_{n,m} h_{n,m(k)}.H_0.\exp\left[i\left(k + G_{n,m}\right)r\right]$$

Bloch modes and Brillouin zones

- The form given is relevant, in particular, to TM modes - which have an H-field that lies purely in the lattice plane. Alternatively they are known as E-modes (because their E-field component, in a 2D-periodic lattice of infinite cylinders, is purely 'vertical' - i.e. along the axes of the cylinders). Joannopoulos et al. point out that the computational problem is easier to solve for the TM situation.
- The summation is made over the plane waves with propagation directions specified by the reciprocal lattice vectors at the Brillouin zone boundaries, $G_{n,m}$. H_o gives the magnetic field strength in A/m. The partial waves have the normalisation condition:

$$\sum_{n,m} \left| h_{n,m(k)} \right|^2 = 1$$

Bloch modes and Brillouin zones

- ‘Solution’ means finding the values of the coefficients $h_{n,m}$.
- The corresponding electric field-strength, *E*, and the electric flux density, *D*, are then obtained from Maxwell’s curl equations.
- Expressing the Bloch modes in terms of their Fourier plane-wave decomposition also makes it readily possible to evaluate the power flow via the Poynting vector, summed over all of the individual plane waves that make up the Bloch wave:

$$\langle S_k \rangle_{t,s} = \left\langle \mathrm{Re}\left(\frac{E \times H^*}{2}\right)\right\rangle_s = \sum_{n,m} \frac{1}{2}\mu_0 h^2_{n,m(k)} . H_0^2 . \left(\frac{\omega}{k^2_{n,m}}\right) k_{n,m}$$

- The time-averaged Poynting vector gives the **(local) power-flow per unit area** (units: Watt/m²) and its direction. Note that the phase velocity and group velocity are collinear for each constituent plane wave.

Bloch modes and Brillouin zones

- **If we are happy to identify group velocity with energy velocity, we can use the energy density (in Joule/m³) expression to calculate the group velocity:**

$$\langle \mathrm{E}_{\boldsymbol{k}} \rangle_{t,s} = \left\langle \frac{1}{2} \cdot \frac{\boldsymbol{BH}^*}{2} + \frac{1}{2} \cdot \frac{\boldsymbol{ED}^*}{2} \right\rangle_{s} = \sum_{n,m} \frac{1}{2} \mu_0 \boldsymbol{h}^2_{n,m(k)} . \boldsymbol{H}_0^2$$

- **At optical frequencies, the relative magnetic permeability is always assumed to be 1. But the *E-D* relationship varies between regions of high and low refractive index.**

- **The energy density expression above, together with the Poynting vector expression already quoted (noting the typo in our source paper), gives the group velocity via:**

$$v_g = \frac{\langle \boldsymbol{S_k} \rangle_{t,s}}{\langle \mathrm{E}_{\boldsymbol{k}} \rangle_{t,s}} = \sum_{n,m} \boldsymbol{h}^2_{n,m(k)} \cdot \left(\frac{\omega}{\boldsymbol{k}^2_{n,m}} \right) \boldsymbol{k}_{n,m}$$

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Bloch modes and Brillouin zones

- The expression just given says that the **Bloch wave group velocity** is the **vectorial sum of the velocities** of the constituent plane waves, as *weighted* by the relative power coefficients.
- *Benoit et al* then examine various situations and, in particular, ones where the biggest contribution to the power flow may come from a plane wave with a propagation constant located in a Brillouin zone other than the first Brilloun zone.
- They conclude that their structures, over a range of parameters, **never show left-handed medium behaviour**, as defined by the condition that $\underline{k}.\underline{v}_g$ is negative.

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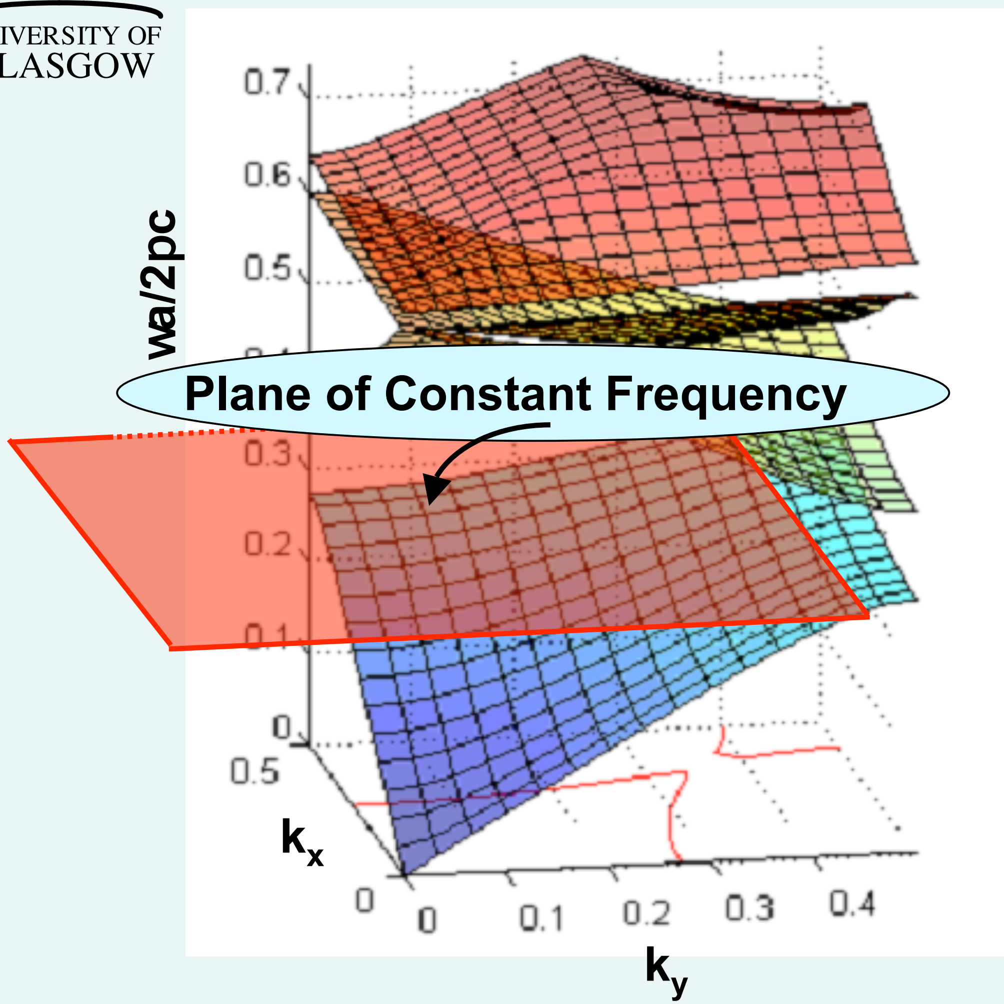
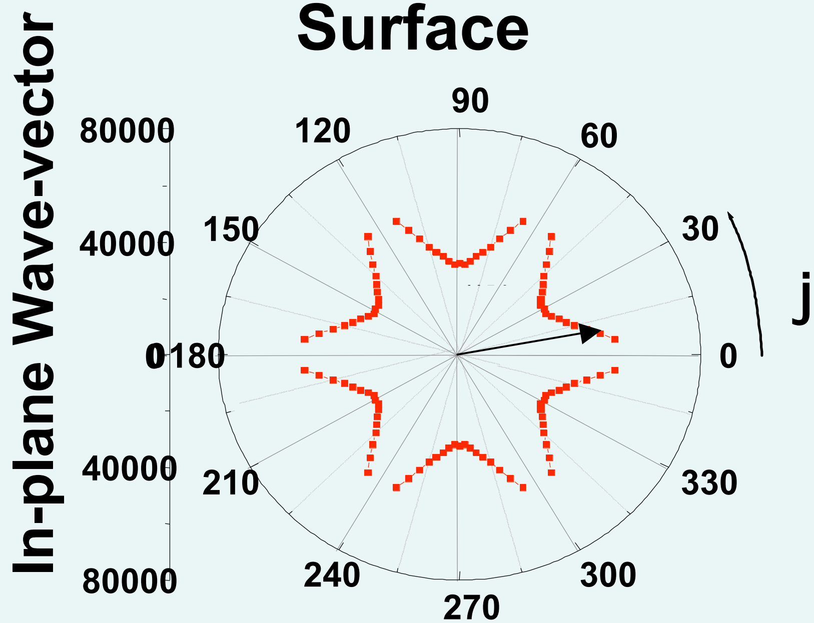
Equi-Frequency Surfaces



Dispersion Surfaces

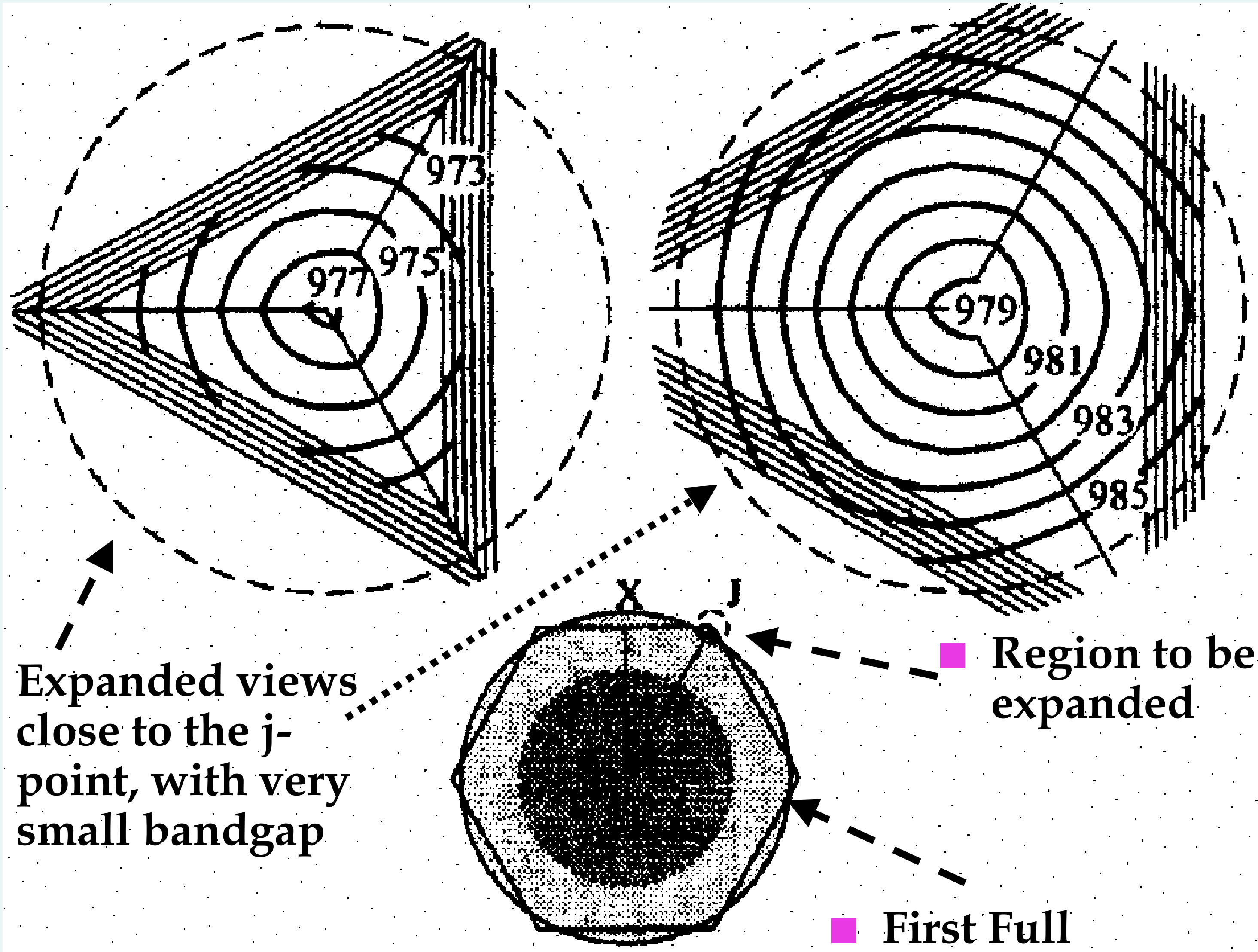
Measured Equi-frequency Surface



Triangular ('hex') PhC lattice of holes in high dielectric constant medium. Leaky Bloch modes.

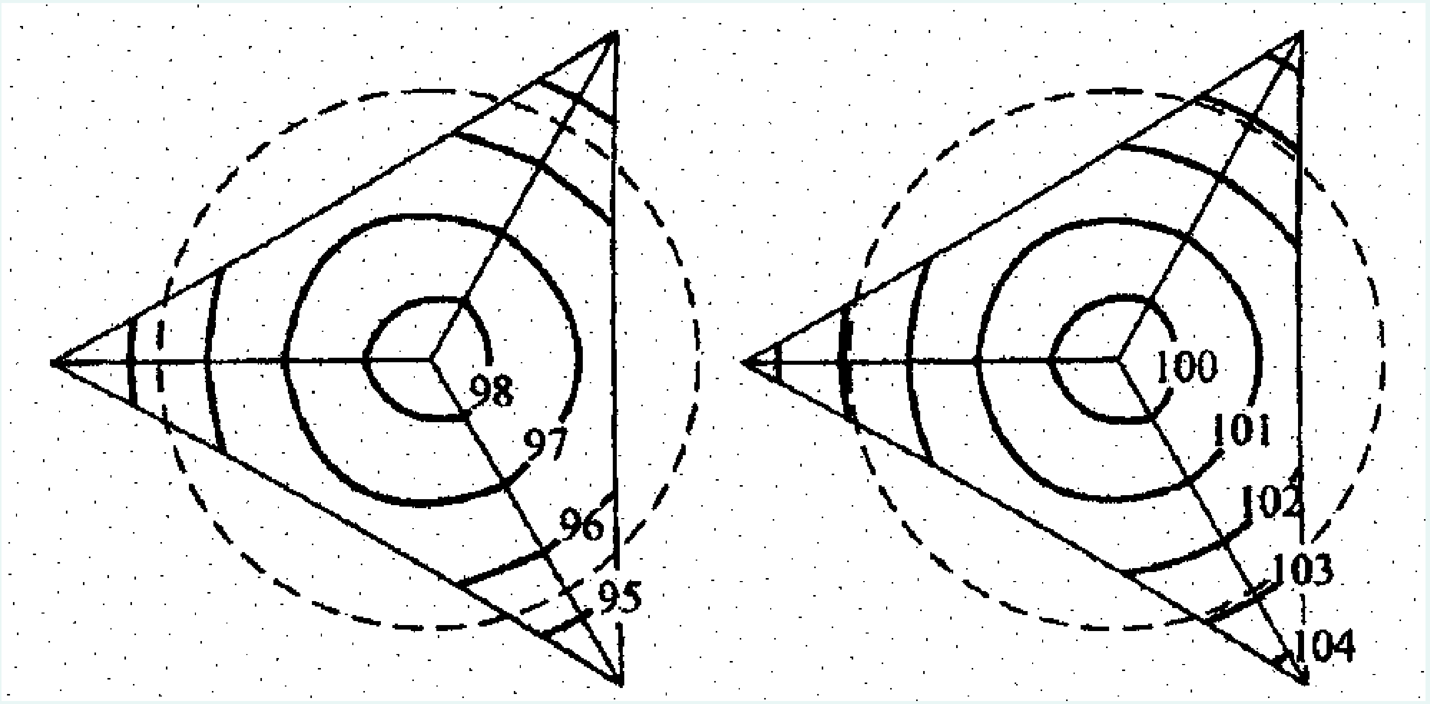
Equifrequency surfaces (EFS) in 2D k-space

- Strongly periodic, high vertical index-contrast waveguide
  - see: E.Silvestre et al, APL, 77, 14th Aug. 2000, pp. 942-944.



- Expanded views close to the j-point, with very small bandgap
- Region to be expanded
- First Full Brillouin zone

Dispersion surfaces in 2D k-space



- Blow-ups around J-point at fixed frequency with *hole-radius* (/nm) as parameter. Remember J-point is same as K-point elsewhere.

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Negative refraction and super-prisms

- Particularly near Brillouin-zone edges, the group velocity, which is normal to the equi-frequency surface, may change its direction rapidly as the propagation direction (phase velocity) is changed by small amounts - or the magnitude of the k-vector is changed.
- Super-prism behaviour (very strong chromatic dispersion) may occur at the interface between two different PhC regions (or between a plain medium and PhC region): giving rapid changes in the propagation direction in the second medium, as frequency is changed. Possibly useful for wavelength de-multiplexing in WDM communication systems.
- Negative refraction is a possible result of the diffractive behaviour that occurs at interfaces. Dielectric PhCs can behave as negative index media, without being ‘Left-Handed’.