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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

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Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
**MINIWORKSHOP ON**
**QUANTUM WELLS, DOTS, WIRES**
**AND SELF-ORGANIZING NANOSTRUCTURES**
**11 - 22 AUGUST 1997**

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# "Electromagnetic Forces in Nanostructures"

**M.I. ANTONOYIANNAKIS**
**Imperial College**
**Condensed Matter Theory Group**
**Department of Physics**
**Prince Consort Road**
**London SW7 2BZ**
**U.K.**

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**These are preliminary lecture notes, intended only for distribution to participants.**

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# ELECTROMAGNETIC FORCES
# IN
# NANOSTRUCTURES

M. I. Antonoyiannakis & J. B. Pendry

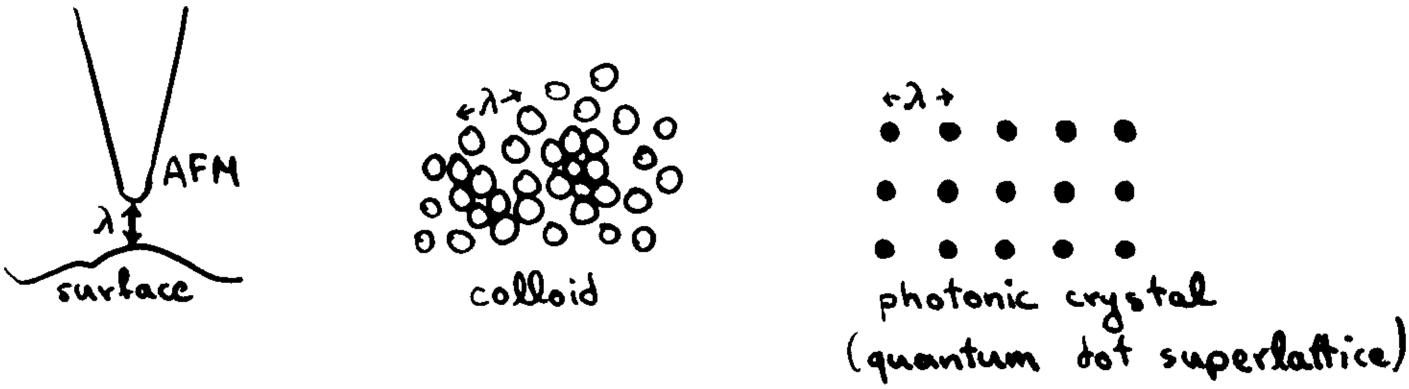
Condensed Matter Theory Group
Physics Dept
Imperial College - London

Also in this group:

- F. J. Garcia - Vidal [Univ. Autonoma, Madrid]
- A. Ward
- J. A. Porto
- I. Watson
- T. Pitarke [Univ. Euskal Herriko, Bilbo]
- L. Martín - Moreno [Univ. Zaragoza]
- P. Bell [Shell UK]
- F. Wijnands [Philips, Ipswich]

INTRODUCTION

Photonic materials: possess structure at scale of wavelength of light




By adjusting the geometric and dielectric properties of a photonic material, we can control the optical properties at will, e.g:

- no allowed optical modes at certain ranges of frequencies (photonic band gaps)
- introduce defects in crystalline order
  ⇒ localisation of light
  ⇒ inhibition of spontaneous emission
- resonant scattering & enhanced non-linear effects

leading to device applications, e.g:

- perfect mirrors
- thresholdless lasers
- single-mode LED's
- materials with $\epsilon_{eff} = 0$

etc.

Of all nanostructures, photonic crystals have received most attention since they support most of the above <u>and</u> are theoretically tractable

Where do we find photonic crystals ?

Nature ⟶ gemstone opals
⟶ butterfly wings

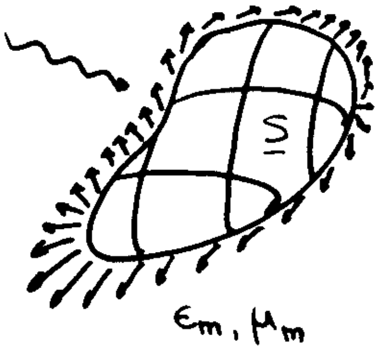
Laboratory ⟶ intense methods the past 10 years
⇓
artificial opals at scales from mm → μm

| ELECTRONIC BAND STRUCTURE (EBS) | | PHOTONIC BAND STRUCTURE (PBS) |
|---|---|---|
| Schrödinger | Equation | Maxwell |
| $E \sim k^2$ (approximate) | Dispersion relation | $E \sim k$ (exact) |
| Scalar, $\Psi(\underline{r}, t)$ | Wave nature | Vector, $\underline{E}(\underline{r}, t, \sigma)$ polarisation |
| Fermionic | Particle nature | Bosonic |
| Strong | Particle-particle interactions | Absent |
| $\ell \sim \mathring{A}$ | Typical scales T/ℓ | $\ell \gtrsim 100$ nm |

Due to similarities/differences above, PBS will display distinct features not present in EBS.

OUR INTEREST - General formulation of EM effects in nanostructures, based on reflection coefficients.

OUR METHOD - MAXWELL STRESS TENSOR FORMALISM




$$F_\alpha = \oint T_{\alpha\beta}\, dS_\beta \quad , \alpha,\beta = \{x,y,z\}$$

$$T_{\alpha\beta} = \epsilon_0 \epsilon_m E_\alpha E_\beta - \frac{1}{2}\delta_{\alpha\beta}\, \epsilon_0 \epsilon_m \cdot E_\gamma^2 + \mu_0 \mu_m \cdot H_\alpha H_\beta - \frac{1}{2}\delta_{\alpha\beta} \cdot \mu_0 \mu_m \cdot H_\gamma^2$$

Comments:

(a) Integration over closed $\underline{S}$ surrounding the body is a consequence of momentum conservation, i.e.

| | | |
|---|---|---|
| force on system | = | change in net momentum entering the system |
| $\underline{F}$ | $= \frac{dp}{dt}$ | |

MOMENTUM - BALANCE PICTURE

(b) $F_\alpha = \oint T_{\alpha\beta}\, dS_\beta \Rightarrow F_\alpha = \int \frac{\partial T_{\alpha\beta}}{\partial x_\beta} dV$

$T_{\alpha\beta}$ has dimensions of energy-density

i.e.

| | | |
|---|---|---|
| force on system | is | due to spatial variations in the system's energy |

$$\underline{F} = -\nabla U$$

ENERGY - GRADIENT PICTURE

c) We are interested in EM effects on macroscopic bodies in nm scales

$\Rightarrow$ treat matter as continuum
$\Rightarrow$ classical Maxwell's equations apply

} CONTINUUM PICTURE OF MATTER

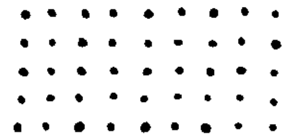
$\Rightarrow$ must time-average harmonic fields of $\omega \sim eV$
[since no macroscopic object can respond synchronously to THz oscillations]

Under these conditions, our methodology applies to :

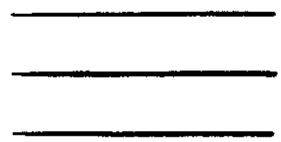
- purely electric; purely magnetic effects
- full electromagnetic effects
- real and virtual photons [e.g. vacuum fluctuations]
- travelling (real wavevector $\underline{k}$) and evanescent fields (complex $\underline{k}$)
- dielectric and metallic objects
- objects of any shape and size
- any frequency ranges for light incident on object

# OUR NUMERICAL APPROACH -

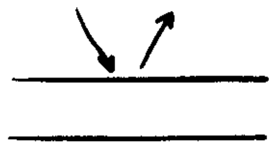
Discretise Maxwell's equations on a mesh [Real Space Quantisation]



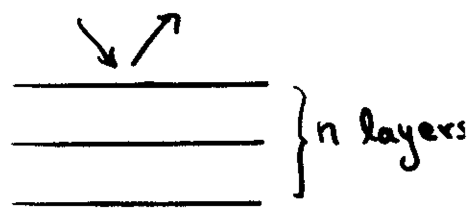
Divide our system into layers



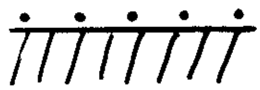
Reflection coefficients for single layer derived - R(1)



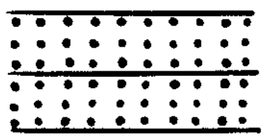
Multiple scattering formalism → R(n)




E, H fields outside

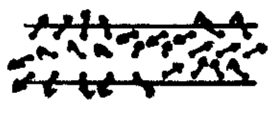


Propagate fields inside the system using the Transfer Matrix Formalism



Fields everywhere

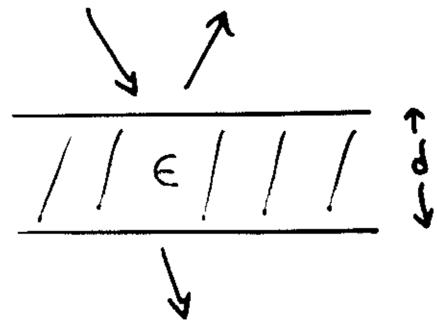
$T_{\alpha\beta}$ (forces) calculation




· J.B. Pendry J. Mod. Opt. 41, 209 (1994)

· P.M. Bell et al Comp. Phys. Com. 85, 306 (1995)

RESULTS




- Homogenous medium

  - Infinite thickness d

L1: Full reflection ⇒ $F = 2 \cdot P_{inc}$ at normal incidence
[e.g. metal, $\omega < \omega_{plasma}$]

$P_{inc}$ … incident radiation pressure

$P_{inc} = \frac{I_0}{c_0}$ ($I_0$ … power, $c_0$ … speed of light in vacuum)

L2: Full absorption ⇒ $F = P_{inc}$
[e.g. dielectric at Brewster angle, metal at $\omega > \omega_p$]

  - Finite thickness d

L3: Full transmission ⇒ $F = 0$
[e.g. thin sheet of metal at $\omega > \omega_p$]

L1, L2, L3 are the natural limits for total radiation forces on a macroscopic body, and cannot be exceeded unless resonance conditions are met.

⇒ Momentum-balance picture justified

Force calculated also from $\underline{F} = -\nabla U$

⇒ Energy-gradient picture justified

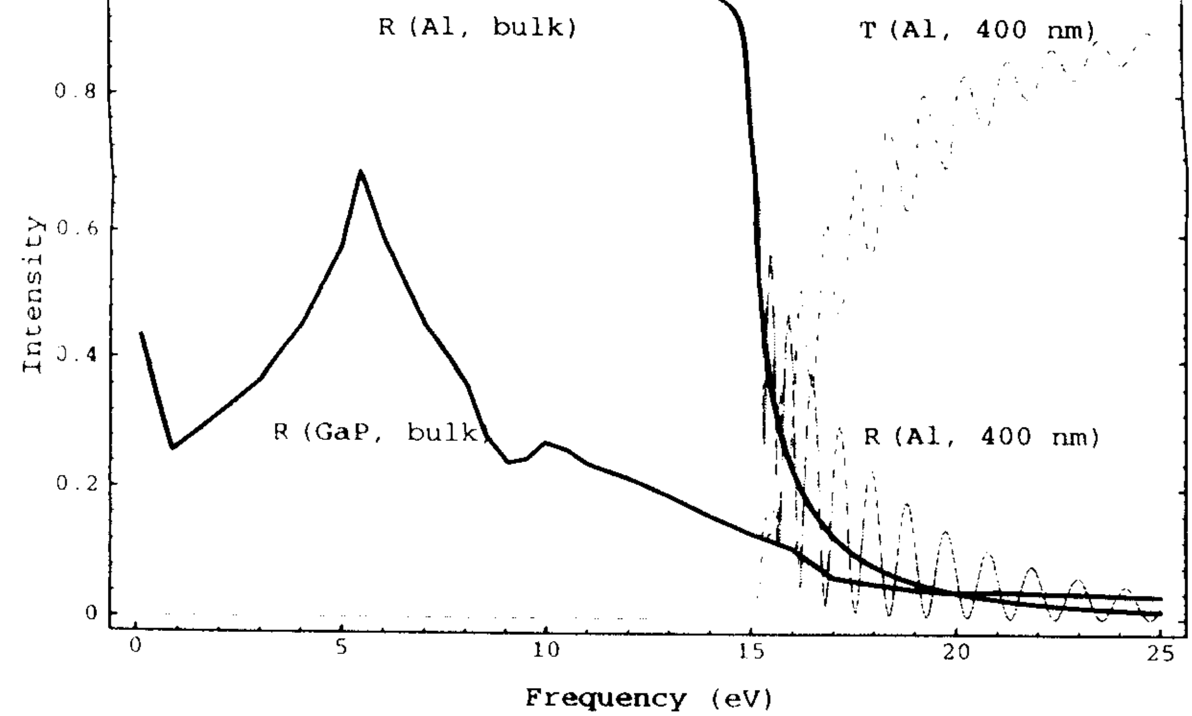



Fig.1: Intensity of reflected light for semi-infinite (black lines) and finite (400 nm, grey lines) homogeneous media for normal incidence. For the semi-infinite systems the transmittance is zero (not shown) , whereas for 400 nm it is finite (shown in broken grey lines). The ripple structure is due to multiple reflections of the waves from the sides of the finite sample (Fabry-Perot oscillations).

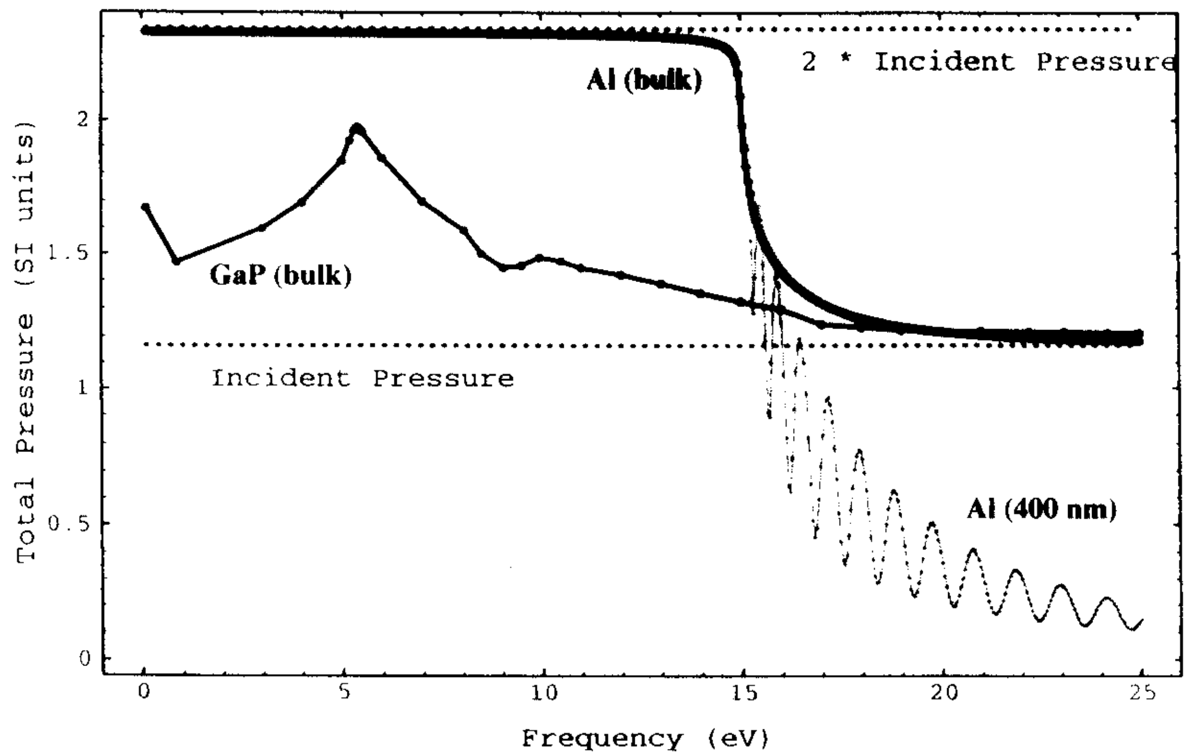



Fig.2: Pressure on a homogeneous medium of infinite (GaP and Al, black curves) and finite (Al, grey curves) thickness. Light is normally incident along the $+z$ direction and has power $I_0 \sim 3.5 \times 10^8$ W/m$^2$. Positive values for the pressure imply that the light is pushing the system. (i) For the infinite medium, the pressure is calculated with the stress-tensor method analytically (solid black lines) and numerically (dotted black lines) in perfect agreement. It ranges from $P_{inc}$ (full absorption) to $2P_{inc}$ (full reflection). (ii) In contrast, a layer of finite thickness experiences a pressure with a zero lower bound, corresponding to full transmission through the layer. For this system the pressure is calculated numerically with the stress-tensor method (solid grey line) and with the energy-gradient method (dotted grey line).

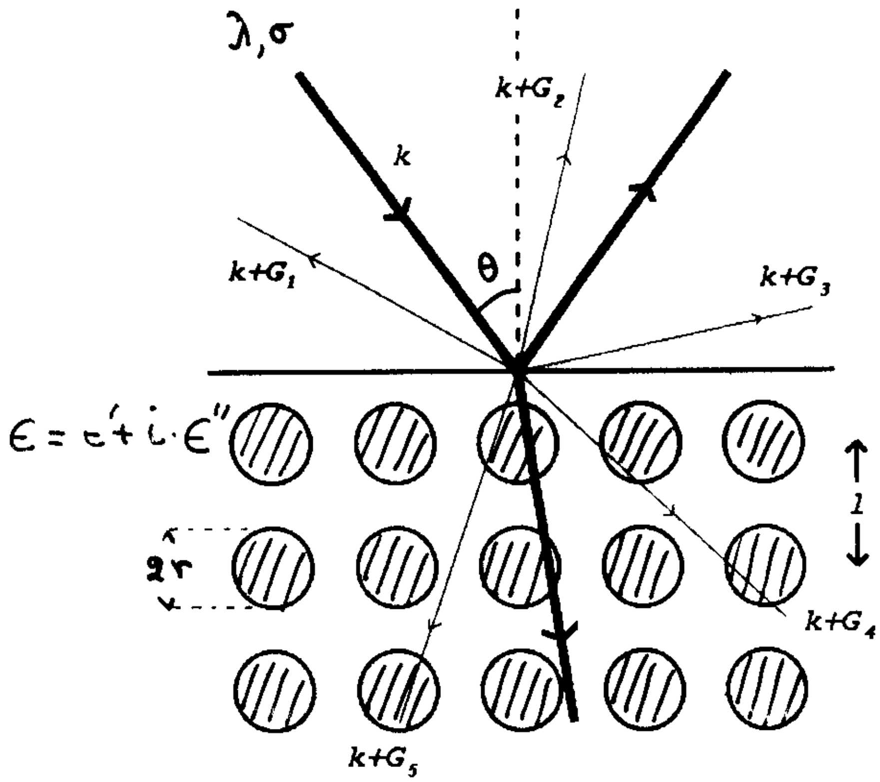
• Photonic crystal (dielectric)

Simple cubic arrangement of spheres

$\epsilon = 8.9$ (GaP)

$l = 900$ nm

$r = 365$ nm




filling fraction

$f = \frac{4\pi}{3} r^3 / l^3$

3 cases (limits) :

- $\lambda \gg r, l$ : Continuum approximation
  $\epsilon(\underline{r}) \to \epsilon_{eff} = f \cdot \epsilon + (1-f)$
- $\lambda \sim l$ : Multiple scattering effects
  → PHOTONIC BAND GAPS
- $\lambda \sim \lambda_{MIE}$ : Resonant features at frequencies of EM eigenmodes of single spheres (MIE modes)

All three cases are present in photonic band structure and transmission spectra :

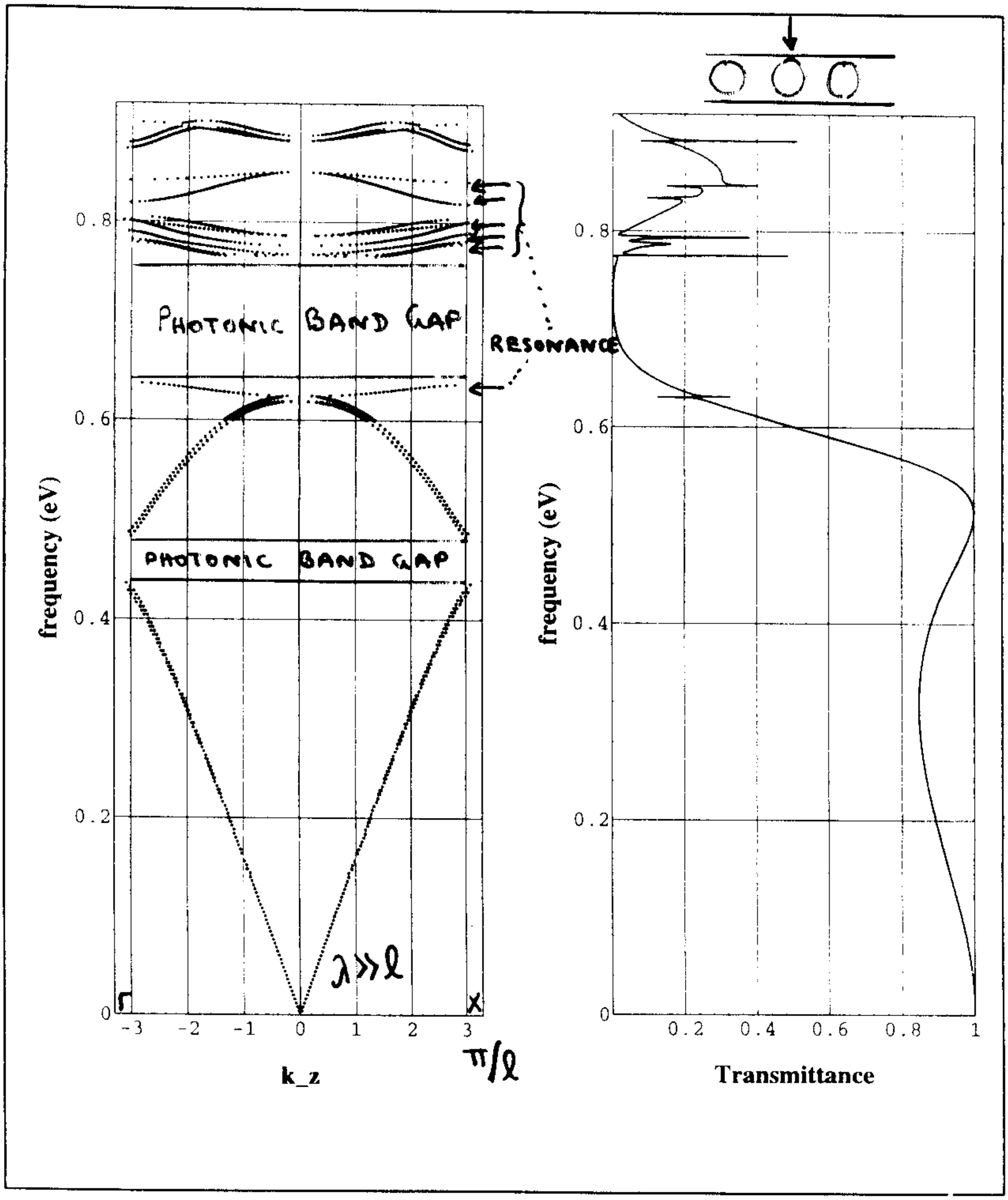



Fig.3: Photonic band structure along the $\Gamma X$ direction for a simple cubic lattice and transmittance for a crystal one layer thick.

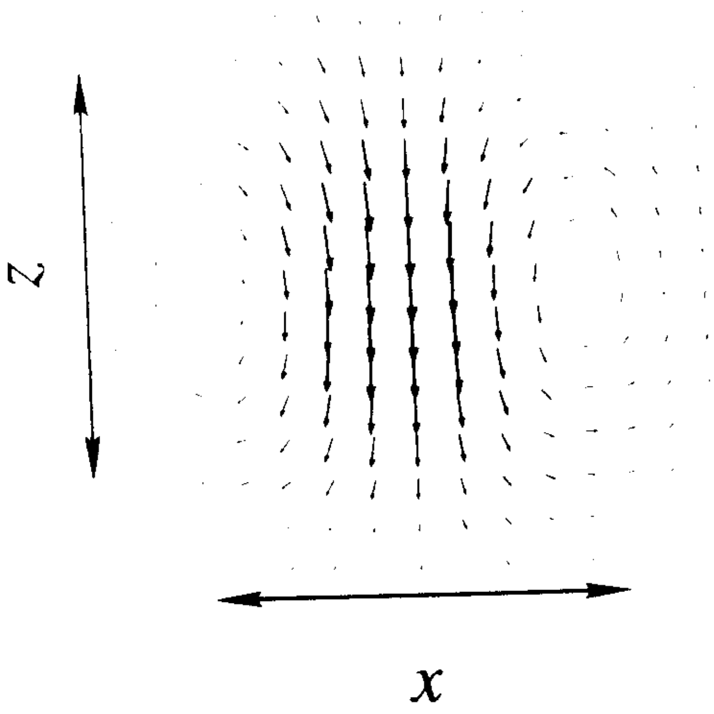
to confirm

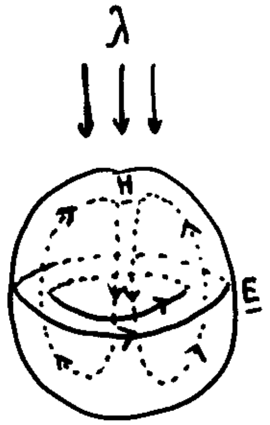
$\omega_0 = 0.629$ eV

magnetic dipole mode

$b_1^1$

# H-field




# E-field

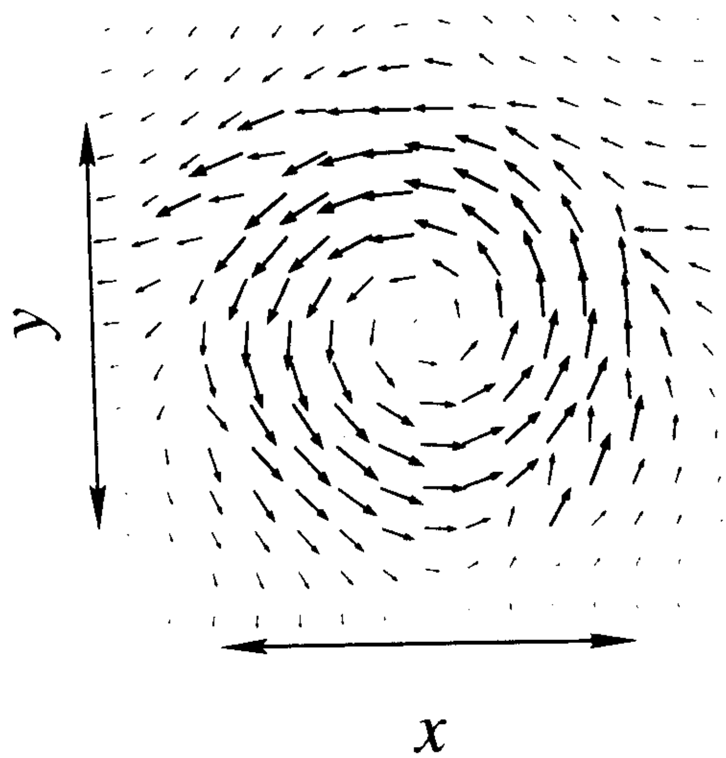
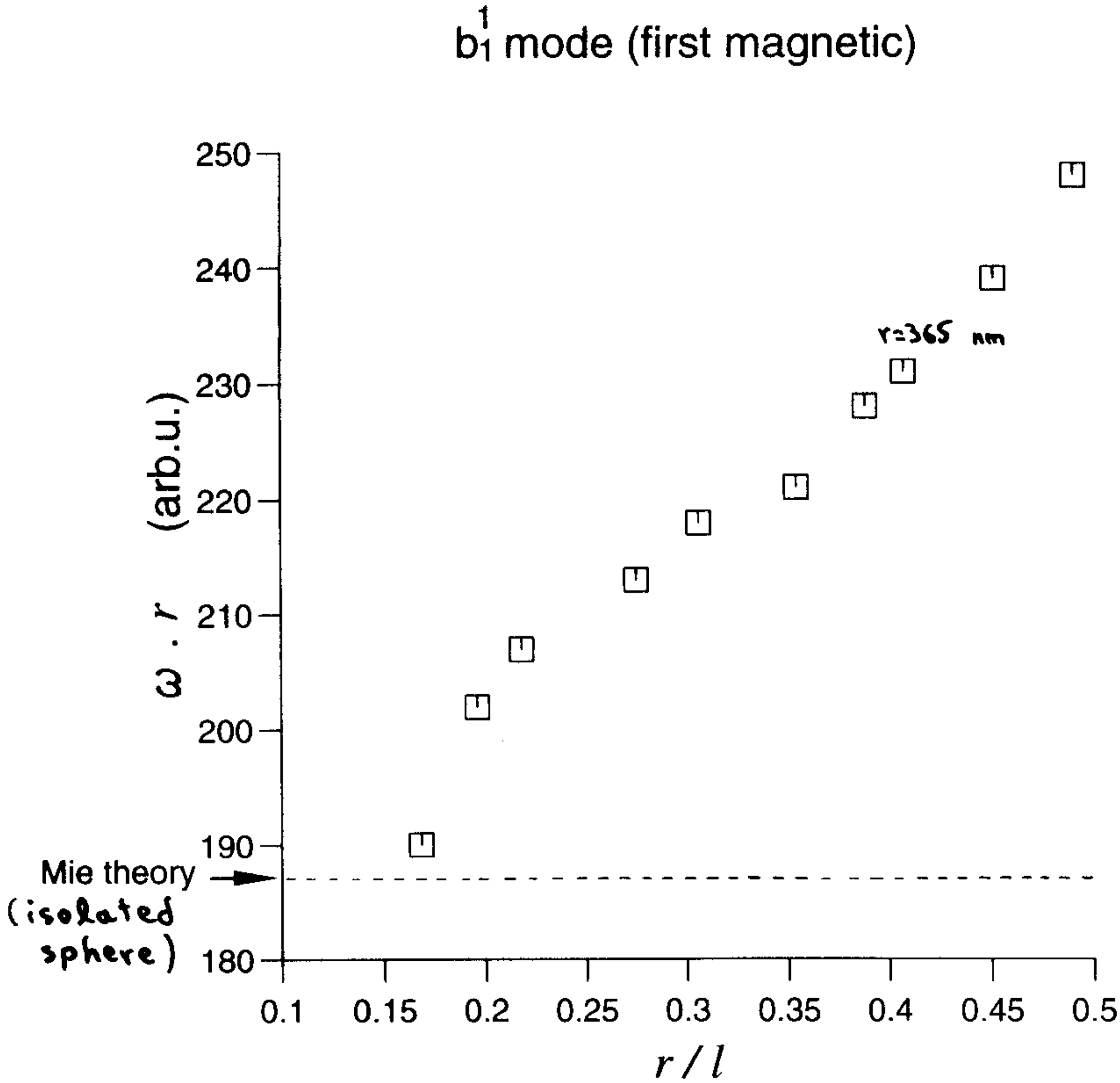



Fig.4: Field distributions within a unit cell of the photonic crystal in the lowest heavy-photon band mode. The light is $s$ polarised, normally incident from the $z$ direction. **H** fields are shown on a cross section $xz$ through the centre of the sphere. **E** fields are shown on a cross section $xy$ through the centre of the sphere. The arrows indicate the sphere edges. The field distributions are identical to those predicted by Mie theory for the $b_1^1$ mode.

Position of sharp features on $\omega$ axis compared to expected result of Mie theory for isolated sphere:

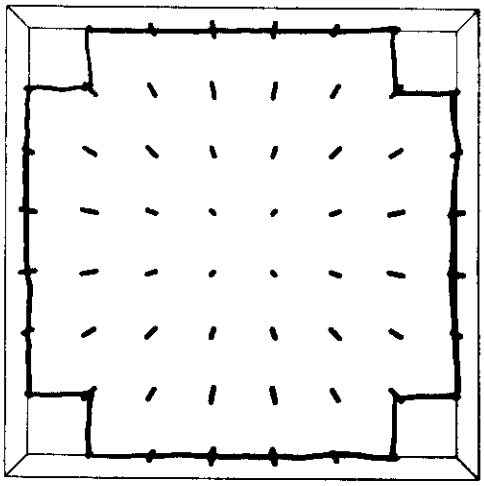
$$\text{Mie theory}: \quad \omega_{MIE} \cdot r = \text{const}$$



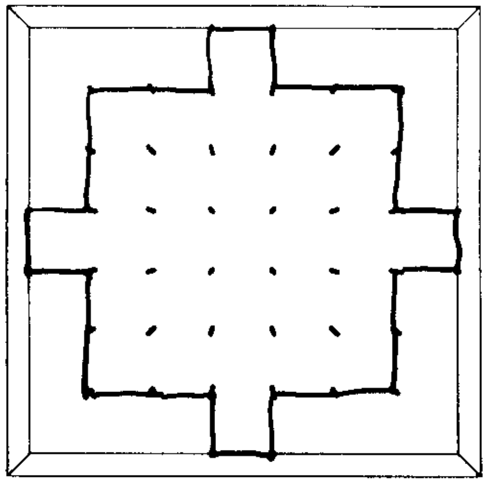

As the interparticle distance increases, the position of the resonance peak approaches the isolated-sphere result.

Resonances occur for any shape of the diel. object (not necessarily spherical)

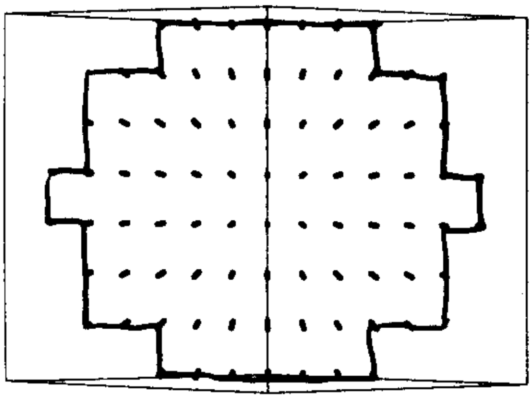
**11 11 11 ; view (10 0 0)**



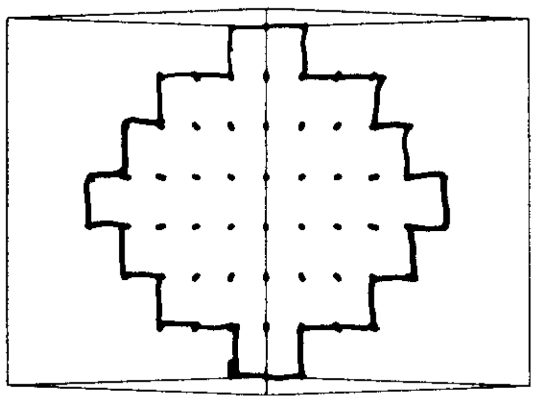
**9 9 9 ; view (10 0 0)**



**11 11 11 ; view (10 10 0)**



**9 9 9 ; view (10 10 0)**



So far studied one layer: $\cdots \bigcirc\bigcirc\bigcirc\bigcirc \cdots$

Now increase sample thickness

$\Rightarrow$ level splitting

Number of peaks = number of layers

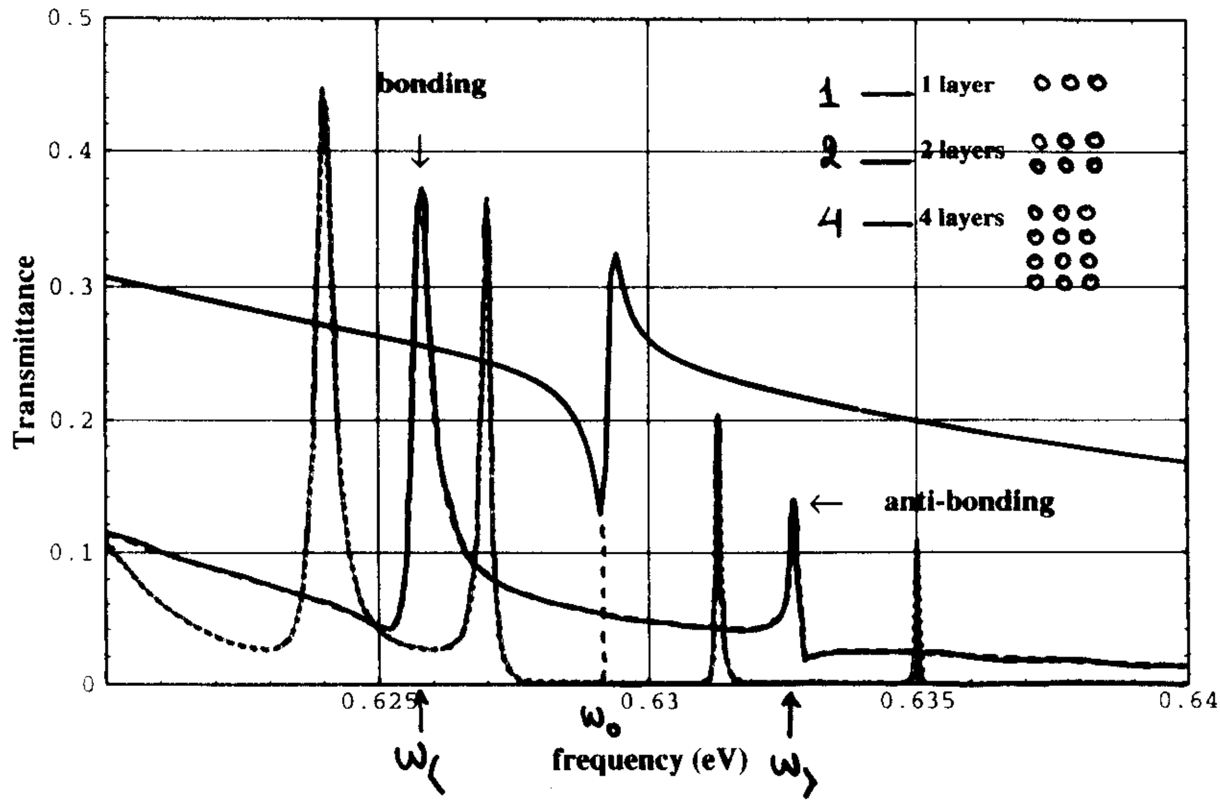
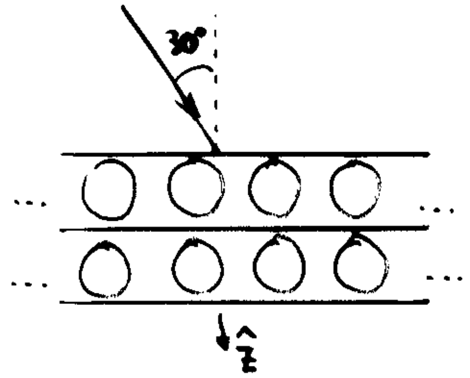


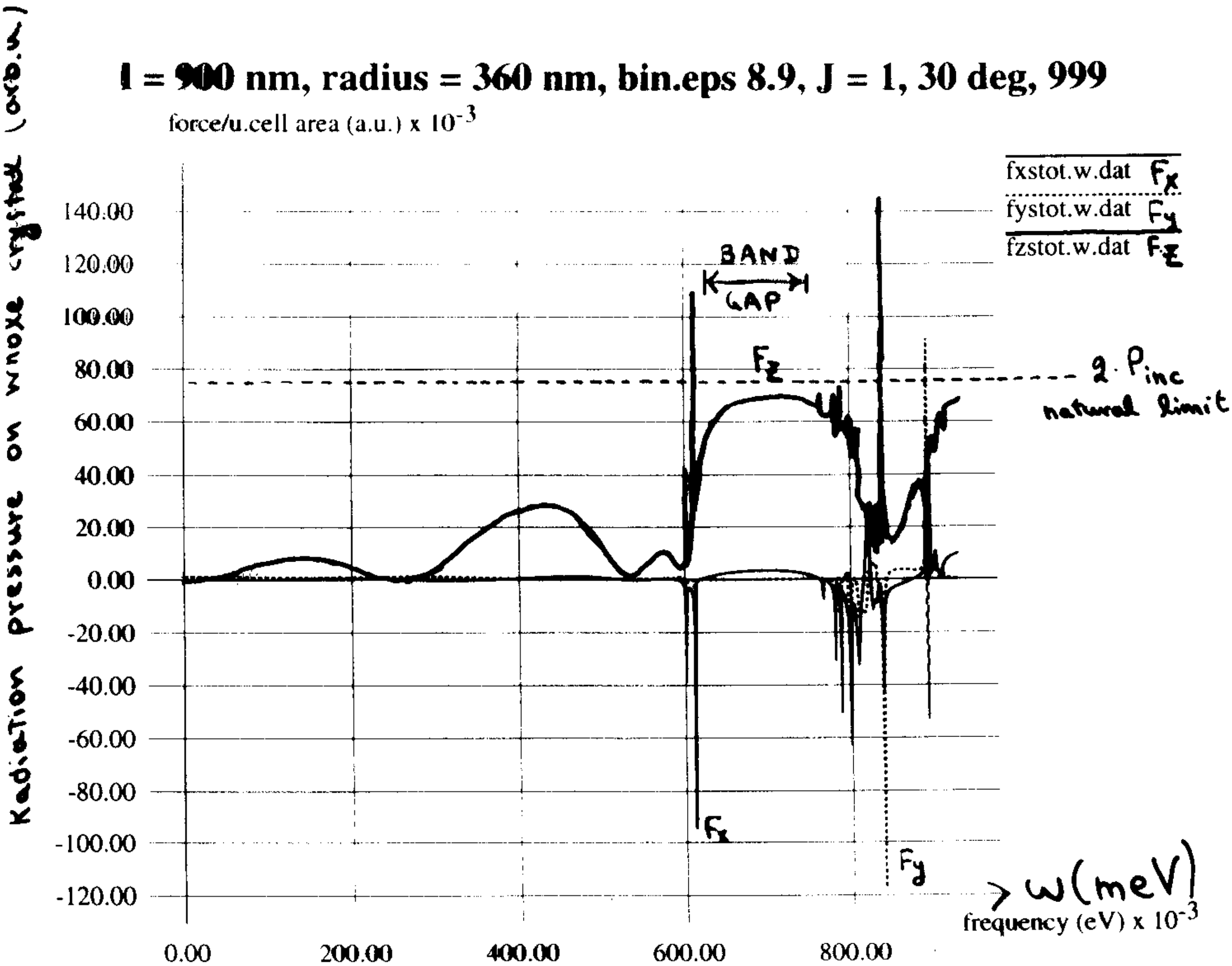

Fig5: Transmittance for three crystal samples of increasing thickness from one to ~~three~~ four unit cells in the $z$ direction. Normal incidence.

Magnitude of radiation force




$\epsilon = 8.9$ (GaP)

**l = 900 nm, radius = 360 nm, bin.eps 8.9, J = 1, 30 deg, 999**




Strength: At 0.7 eV $F_z \sim 10^{-12}$ Nt for $I_0 \sim 3.5 \times 10^8$ W/m

Compare VdW: sphere-sphere $F < 10^{-13}$ Nt

gravitational: $mg \sim 8 \times 10^{-15}$ Nt

thermal $\sim$ $10^{-15}$ Nt

So the photo-induced (i.e. radiation) forces dominate.

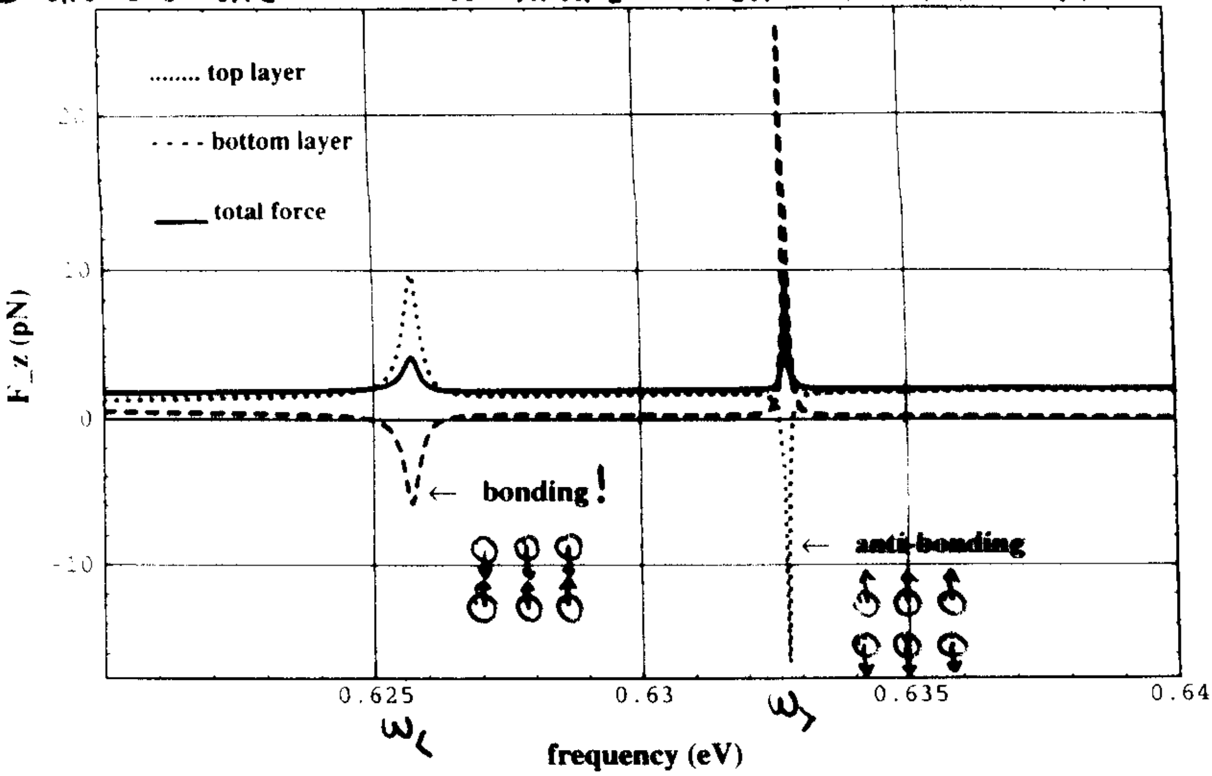



Fig.6: Normal force ($F_z$) *per unit cell* on each layer in a two-layer system and on the whole crystal for $s$ polarisation, normal incidence. Light is incident along the $+z$ direction, so $F_z > 0 (< 0)$ means positive (negative) pressure. Note that at the lower frequency forces act to push the two layers together, at the higher frequency to pull them apart.

Nature of attraction (repulsion) is that magnetic dipoles are parallel (antiparallel)

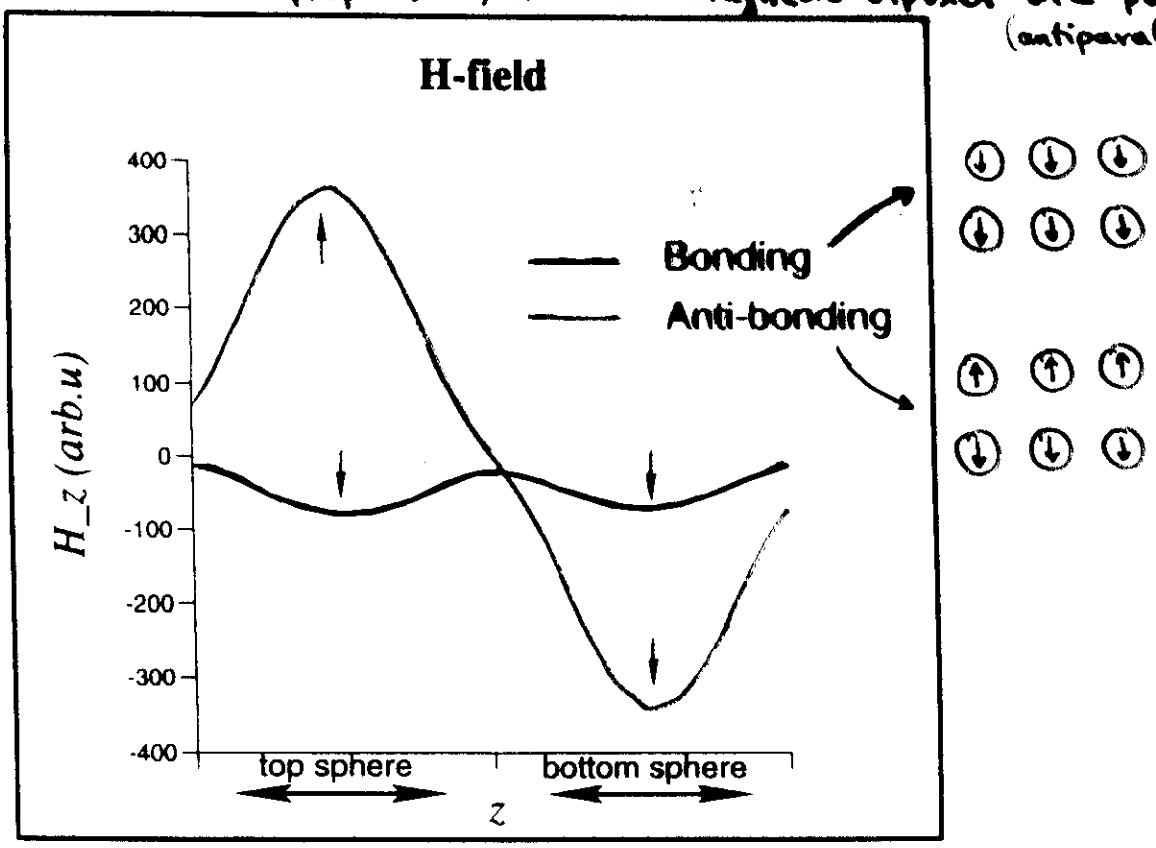
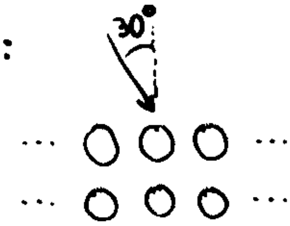
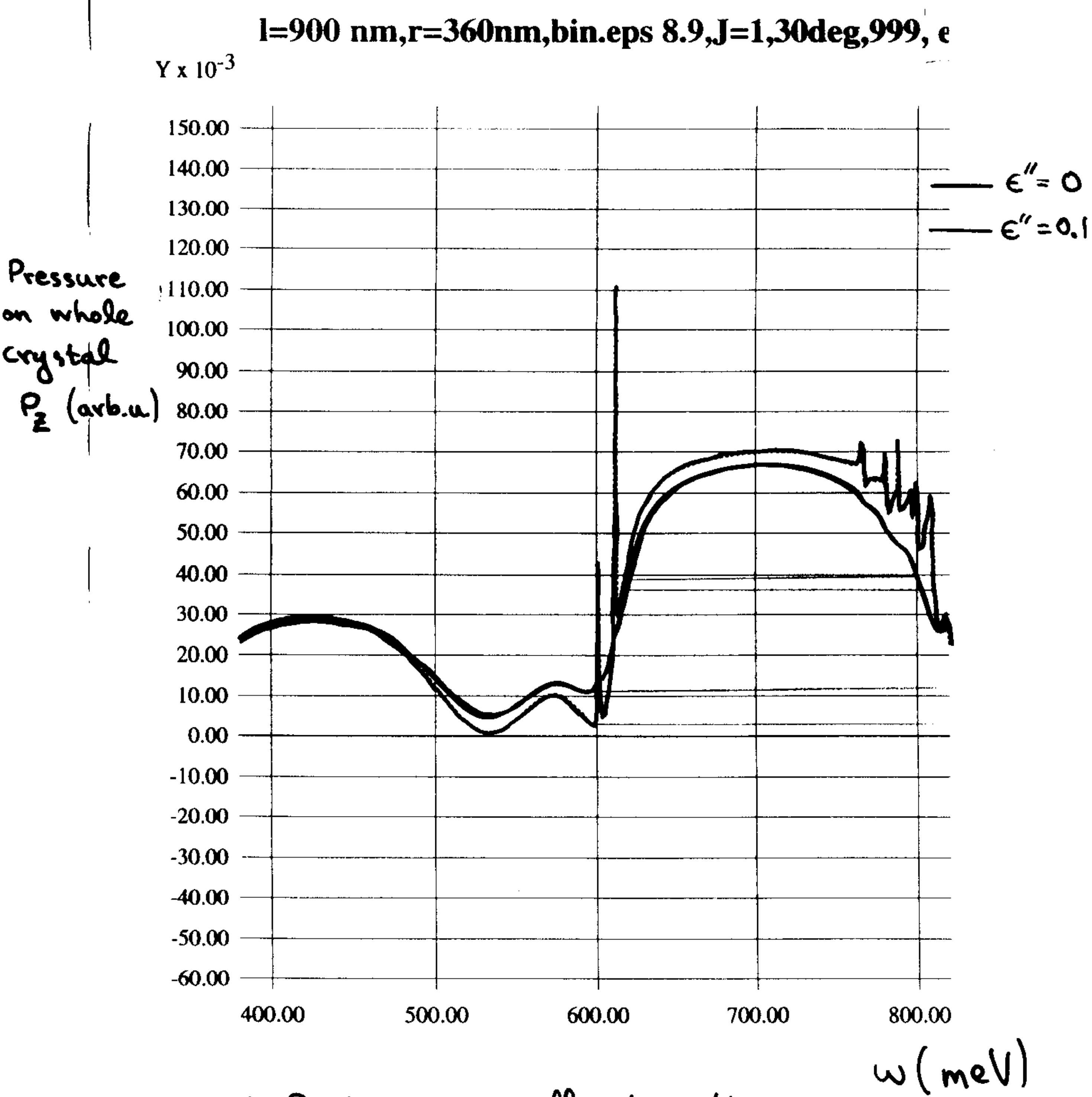



Fig.7: Magnetic fields plotted along the $z$ axis through the centre of the spheres. Light is $s$ polarised, normally incident from the $z$ direction at frequency $\omega_<$ (bonding, dipoles parallel). $\omega_>$ (anti-bonding, dipoles anti-parallel). For $p$ polarisation the directions of the fields are reversed.

Sharp resonances are sensitive to absorption:




However, GaP has very small absorption between 0.1 - 1.2 eV: $\epsilon'' \lesssim 0.0001$

So the bonding/anti-bonding effect must be observable!

Two relevant experiments :

Au nanoparticles
($r \sim 10$ nm)

white light or
laser beam

$\Downarrow$

rate of aggregates
formation increases
by $10^3$

K. Kimura, Bull. Chem.
Soc. Jpn 69, 321 (1996)

Dielectric spheres
($r \sim 10^2$ nm)

laser beam, $I_0 \sim 10^{10}$ W/m$^2$

$\Downarrow$

attractive interactions
and binding into
2D crystal planes

M.M. Burns et al,
Phys. Rev. Lett. 63, 1233 (1989)
M.M. Burns et al, 1994

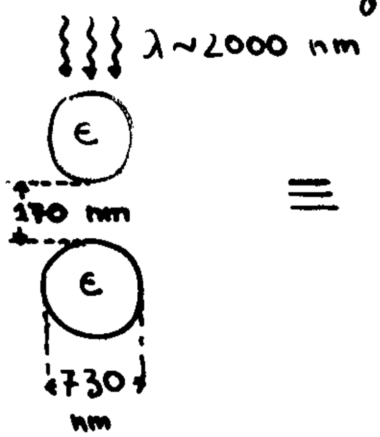
# CONCLUSIONS

- We have developed a numerical methodology for studying EM forces on nanostructures, based on the Maxwell Stress Tensor.

- We have confirmed the alternative ways of viewing forces, namely the momentum-balance and the energy-gradient methods.

- In dielectric crystals, we have studied the influence of Mie-modes on forces.

  Lowest mode : magnetic dipole




$\equiv$ Electromagnetic analogue of two H atoms in ground state being brought close together

$\Rightarrow$ hybridisation
splitting of levels into two,
one bonding ($\omega_<$), one anti-bonding ($\omega_>$)

dipoles $\downarrow\downarrow$     dipoles $\downarrow\uparrow$

- Magnitude of photo-induced forces can exceed other forces present depending on laser power and $\epsilon$.

$$\Downarrow$$

  - facilitation of 3D photonic crystals fabrication by tuning into binding mode & allowing self-organisation
  - novel non-linear phenomena arising from application of laser light fields in nanostructures

This work: M I Antonoyiannakis & J B Pendry, Europhys Lett (to appear)