

## ***CrystalWave TECH NOTE***

### Modeling a photonic crystal cavity with CrystalWave

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November 2007

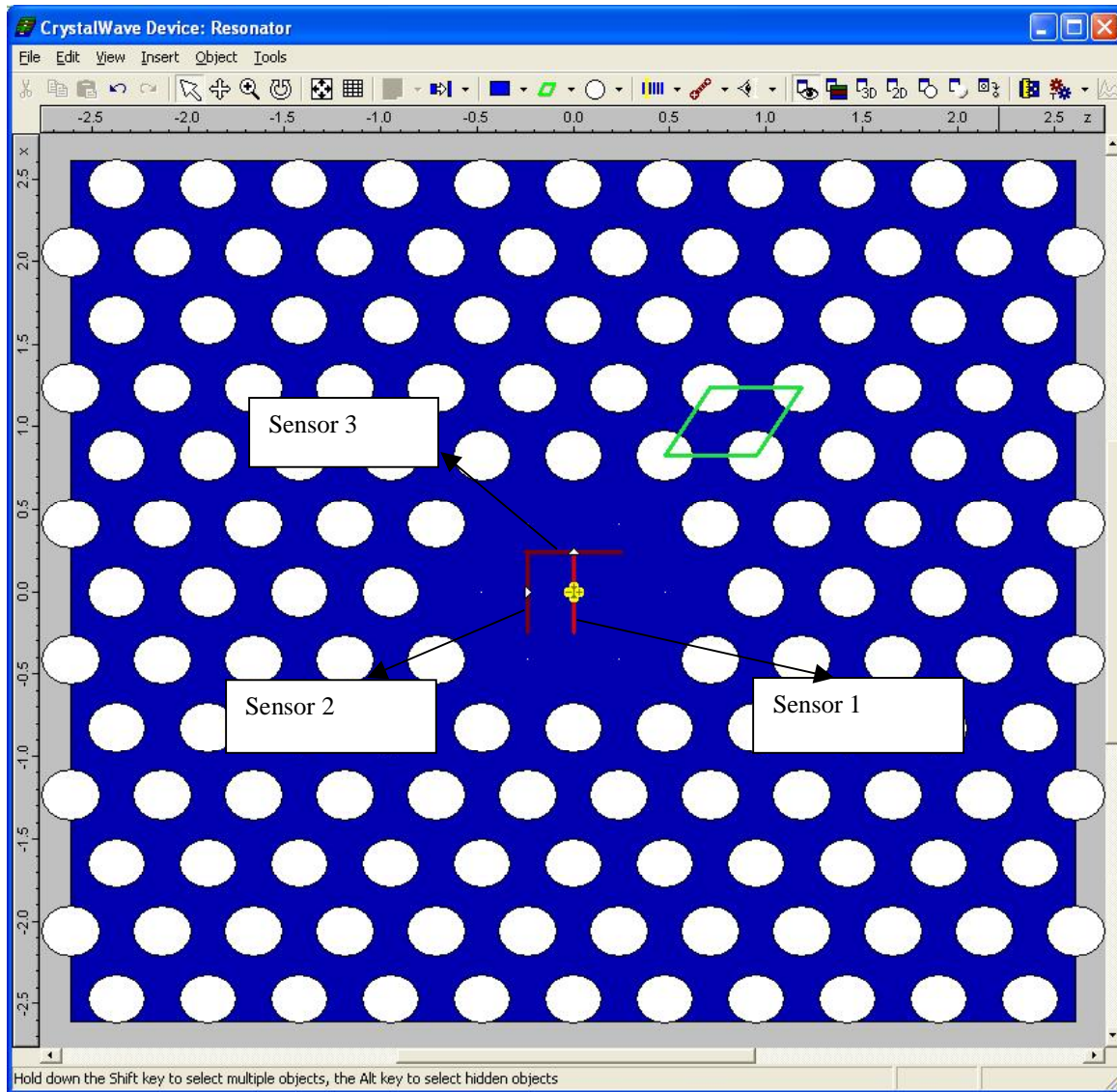
**Abstract:** We present a method for modelling a cavity in a photonic crystal. We will identify the resonant frequencies and the Q of each resonance. Then we will investigate the effect of grid size on the wavelength and the Q factor of the resonances.

## Introduction

The band gap properties of photonic crystals are well known. If we remove a few atoms in a photonic crystal, then, for wavelengths within the band gap, this region will be a cavity with perfectly reflecting walls. We will try to find the resonant frequencies, the associated Q-factors, and the resonant modes of such a cavity.

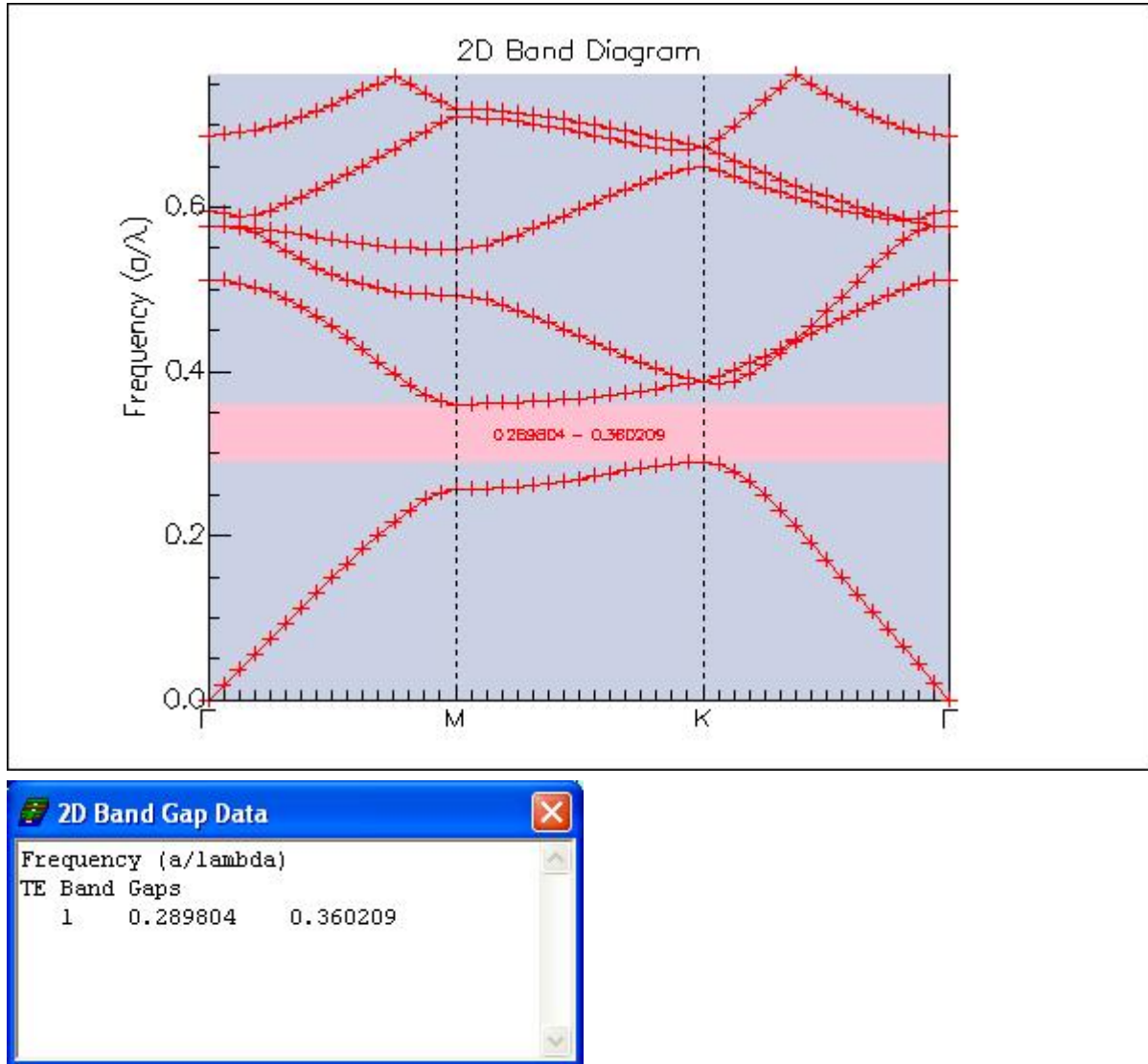
## 2D Structure

The structure we will simulate can be seen on Fig. 1. It is a hexagonal photonic crystal, made of air holes drilled in a 2.5 index material. The lattice constant is chosen to be  $0.475\mu\text{m}$ , and the atom radius  $0.15\mu\text{m}$ . Such a structure exhibits a complete band gap for the TE modes (magnetic field parallel to the axis of the holes, electric field in plane).



**Figure 1: 2D photonic crystal and photonic crystal cavity.** The cavity has a hexagonal shape, so it follows the symmetry of the crystal. The exciters are two dipole exciters polarised along x and z, so that we can excite both polarisations. Sensors are placed in different points in case a mode of the cavity has a zero in a particular position.

The band diagram of the structure can easily be computed with CrystalWave's band solver. We add the unit cell (green parallelogram in Fig 1) and we find the band diagram (Fig. 2). We see the band gap in TE modes, between 1.319 $\mu\text{m}$ -1.639 $\mu\text{m}$ .



**Figure 2: Band diagram for the TE modes of the photonic crystal in Fig. 1. We see that there is a complete band gap between wavelengths 1.319 $\mu\text{m}$ -1.639 $\mu\text{m}$ .**

## Simulation

To excite the resonant modes of the cavity we will excite with a pulse centred somewhere near the middle of the band gap, at 1.55 $\mu\text{m}$ . We will use a narrow pulse, so that all the frequencies within the band gap will get excited. In order to excite both polarisations ( $E_x$  and  $E_z$ ) we use two dipoles, polarised along  $x$  and  $z$ . If the two dipoles are in phase, they are equivalent to a dipole polarised along 45deg. So we introduce a 90deg phase shift. This way we can create something closer to a spherical wave Fig 3. The latter configuration should contain more spatial frequencies, and is therefore more likely to excite modes of different profiles and polarisations.

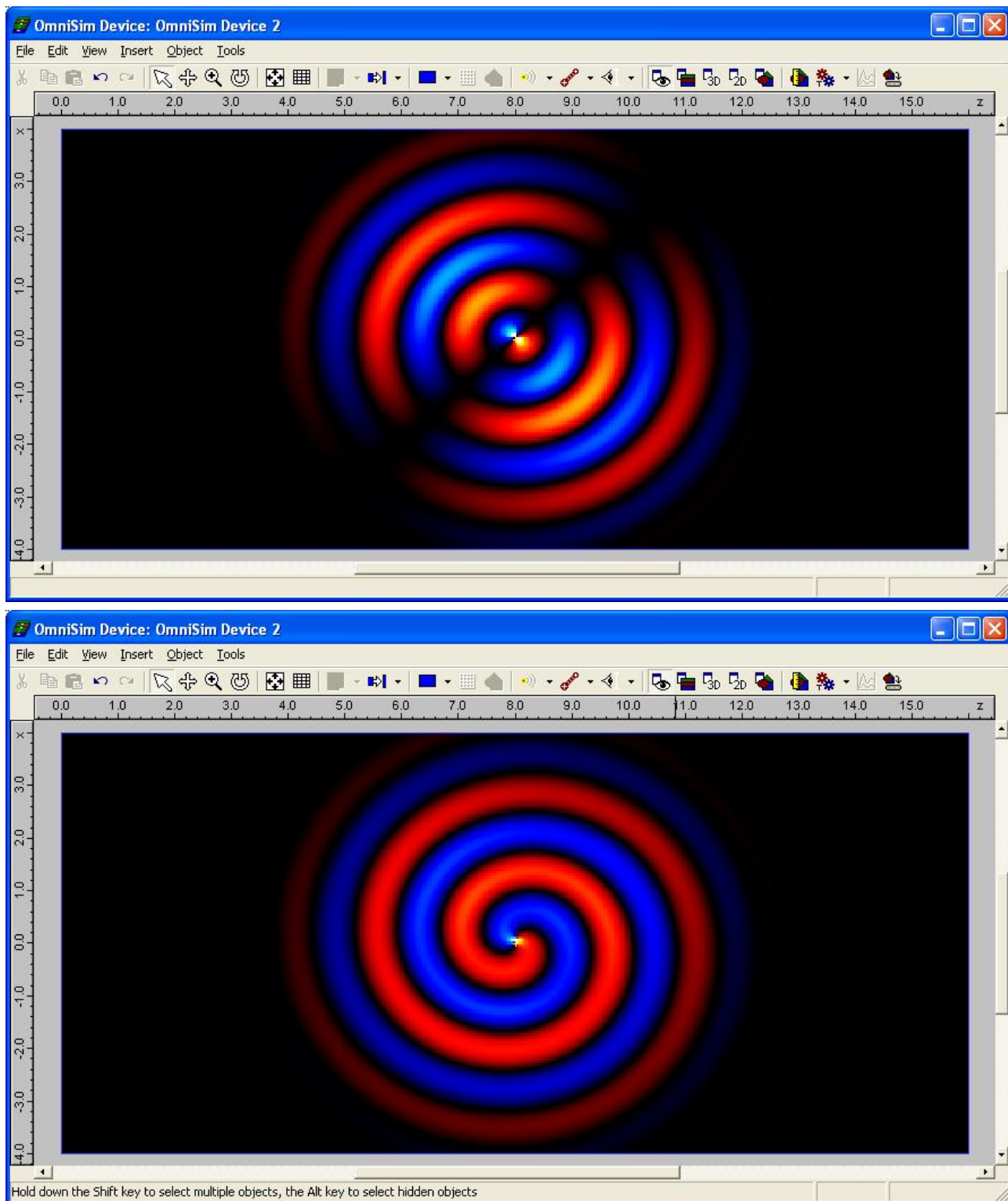
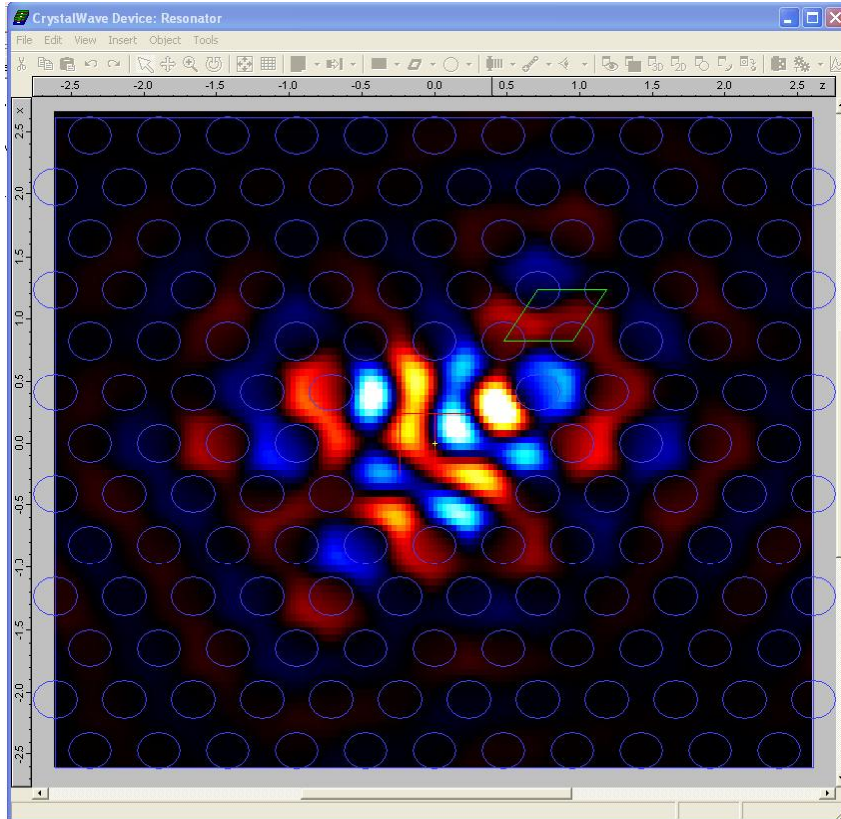


Figure 3:  $H_y$  field produced by two dipoles (top) in phase (bottom) with a 90 degrees phase difference.

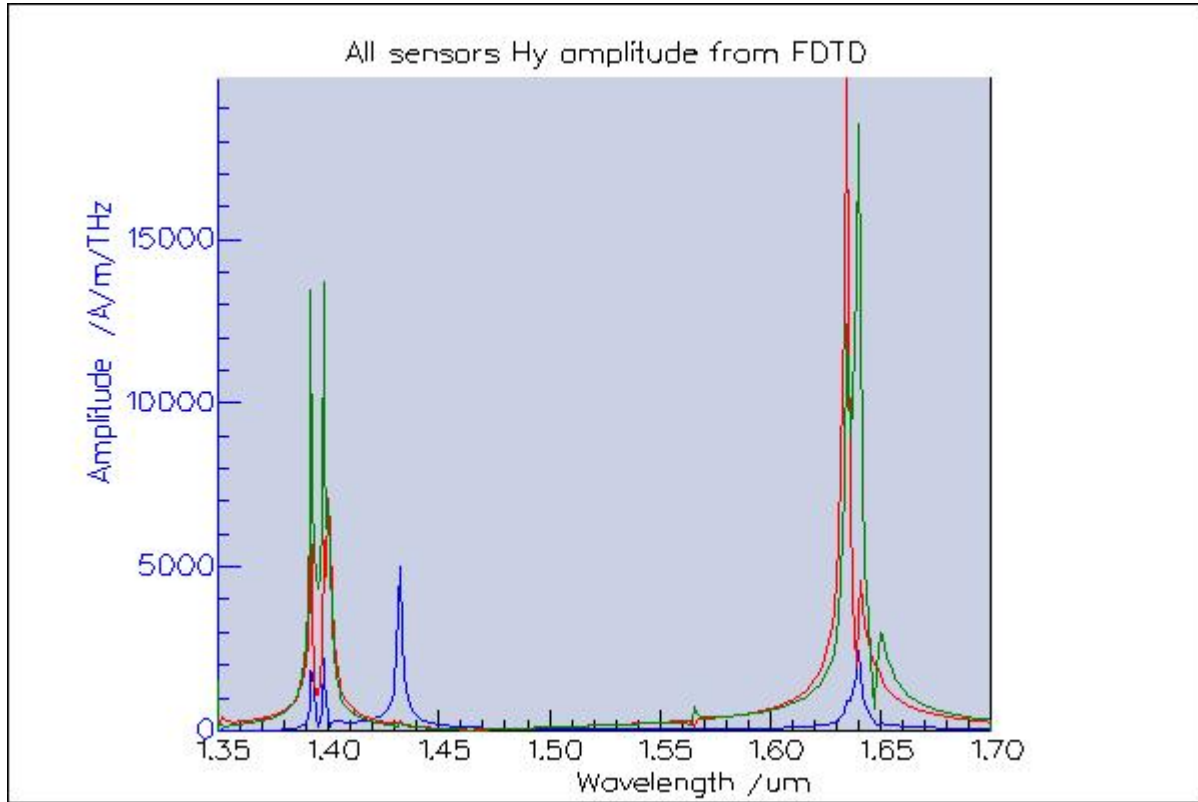


We now run the simulation. We use grid spacing equal to  $1/15^{\text{th}}$  of the lattice constant. The duration now is 120000 time steps. As the simulation progresses we see first the excitation pulse go away, leaving behind only the wavelengths that have coupled to the resonant modes. Then these slowly decay exponentially. The reason of the decay here is that the photonic crystal does not extend infinitely, so there is power leaking from the sides, despite the complete band gap.



**Figure 4:** Hy plot of the field in the cavity during the simulation. The field profile here is a superposition of the different resonant modes. We can also see the radiated power. Note also that the field is zero at the centre of the cavity. If we had used only one sensor, the one whose centre is at the centre of the cavity, we would not have obtained a good picture of the resonances. The reason is that the field at the centre of this sensor would be zero because of the spatial profile of the modes.

The sensors record the field at each time steps only at one point, at their centre. So if the field at the centre of the sensor is zero because of the spatial profile of the mode, we will not obtain good information about the resonances from this sensor. That is the reason we put more than one sensor (three in this example) at different symmetry points of the cavity. We also note that these sensors do not have to be large, as we need only the field at one point: at the centre of the sensor. So we can make them small. This can save memory in 3D calculations. If we plot the amplitude of Hy in the frequency domain for these three sensors, we have Fig. 5.



**Figure 5: Amplitude of Hy at the centres of the three sensors. We see that the sensor at the centre of the cavity shows much weaker resonances from the other two sensors. But it displays an additional resonance that the other two do not show. Sensor 1 is green, sensor 2 is red, and sensor 3 is green.**

## Q factor calculation

The spectrum in Fig 5 is wide. We will now closely zoom to one resonance and identify its resonance wavelength and Q. In fact we will do that for the two resonances near 1.4um, and we will use the data from sensor 3. We will use the Q-calculator to find the resonance spectrum and the Q factors. The Q-calculator provides the use of the Pade transform. This transform is ideal for finding the frequency spectrum of decaying resonances. Its biggest advantage is frequency resolution; it needs 4-5 times fewer time steps than the Fourier transform to achieve the same resolution. It also includes an automatic tool to find the Q factor from the spectrum.

For the Q factor calculation we used a 60000 time step window, and found the spectrum from 1.37um to 1.42um. Fig 6 shows the Q calculator window with the parameters set and the calculated Q factors written. To change the duration of the Time Window you have to click on the Time Window button.

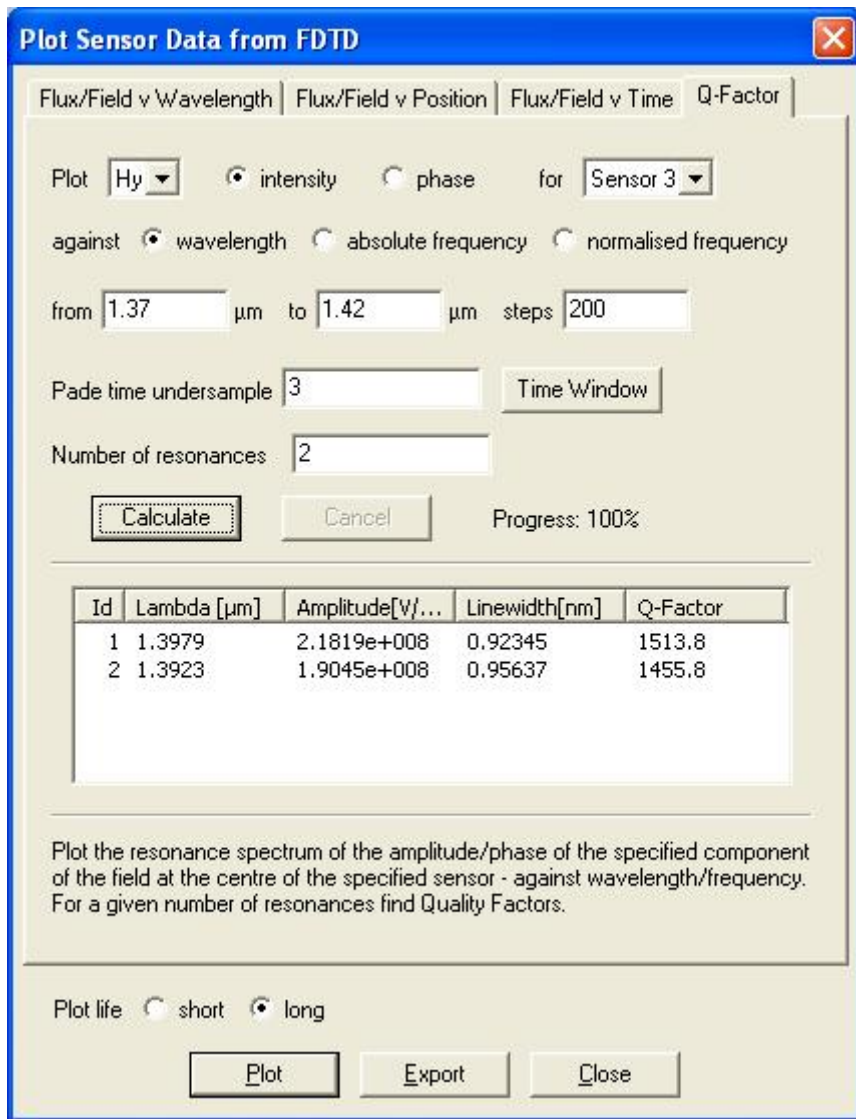


Figure 6: Q calculator window, showing the parameters used and the obtained Q-factors.

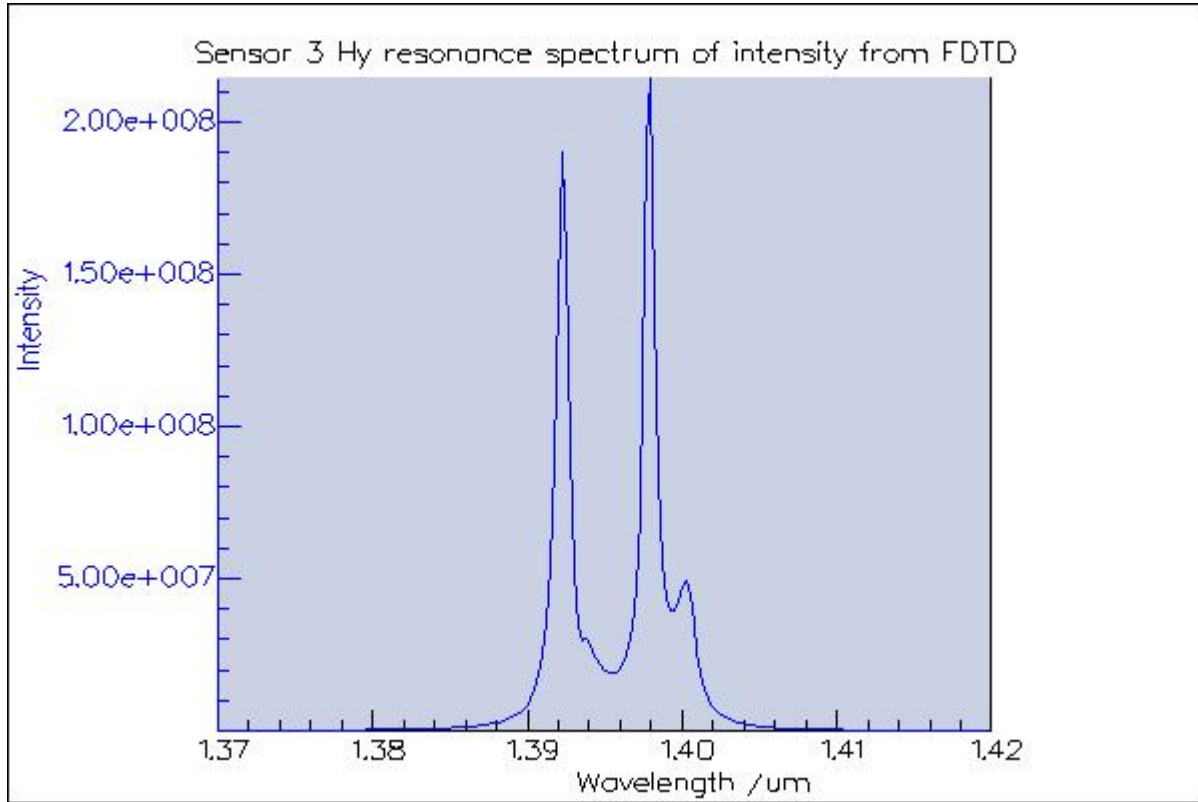


Figure 7: Spectrum obtained from the Pade Transform (Q-calculator) for the two resonances near 1.4um.

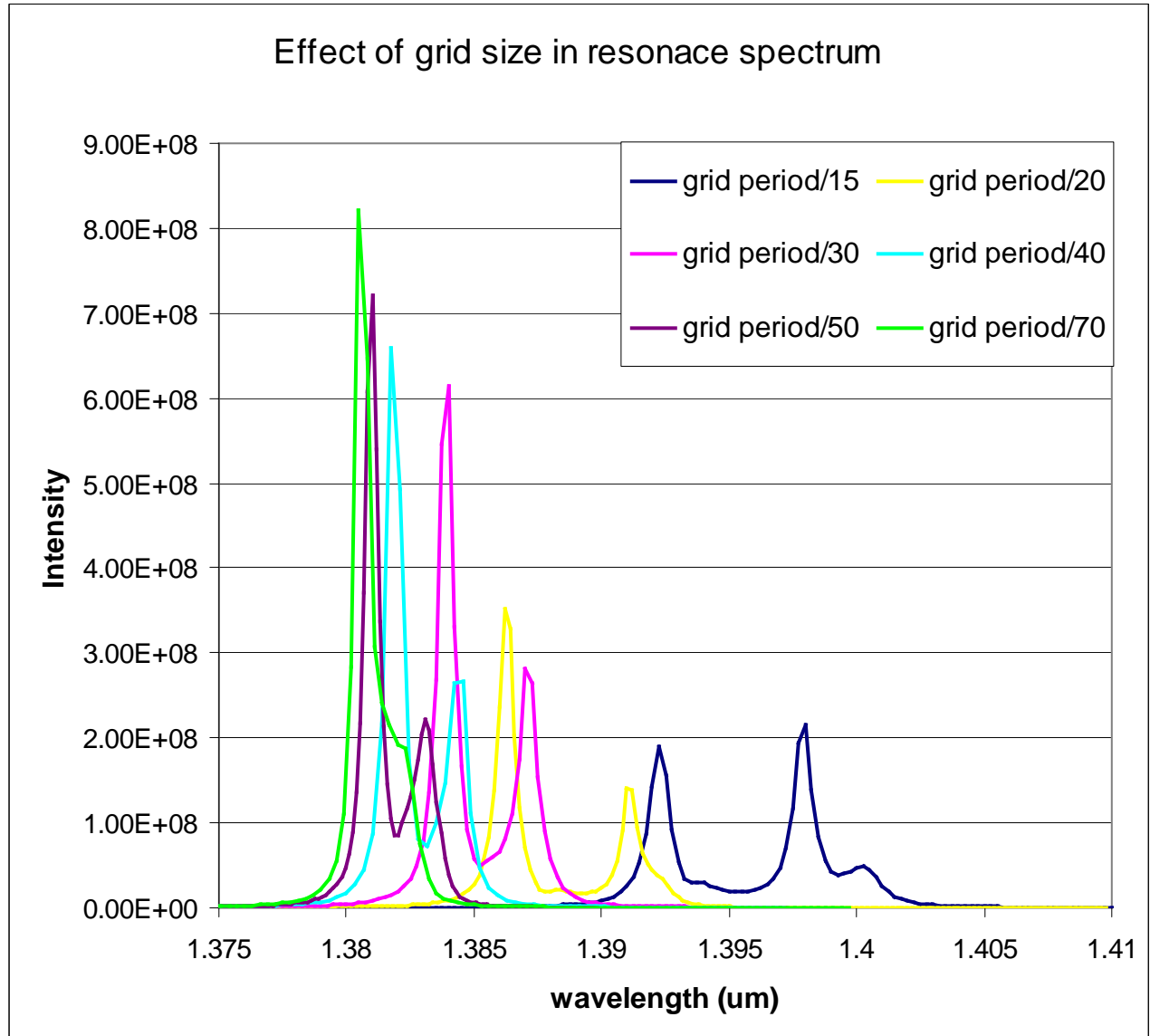
## Effect of grid size

We will now study the effect of grid size on the position (wavelength) and width (Q factor) of the resonances. We ran several simulations with different grid sizes, each time calculating the spectrum around the two resonances near 1.4um. The Pade transform was employed to calculate the spectrum and the Q calculator was used to automatically identify the resonances and calculate their Q-factors. The duration of the simulation was kept constant in time, so the number of time steps increased inversely proportionally to the grid size. The Time window of the Q-calculator was also kept constant in temporal duration, so the width in time steps increased with reducing grid spacing. The duration of the simulation and of the time window used for the Q-calculator was 4108fs. The Hy component at the centre of Sensor 3 was used for all the calculations.

Again, we will focus on the behaviour of the two closely shaped resonances near 1.4um. In Fig 8 we can see the resonance spectrum calculated from the Q calculator, for different grid spacing. We see that

- 1) The resonances move to smaller wavelength with smaller grid size
- 2) The resonances come closer with decreasing grid spacing. For 70 points per period it becomes very difficult to distinguish them
- 3) The longer wavelength resonance becomes weaker, and the shorter becomes stronger





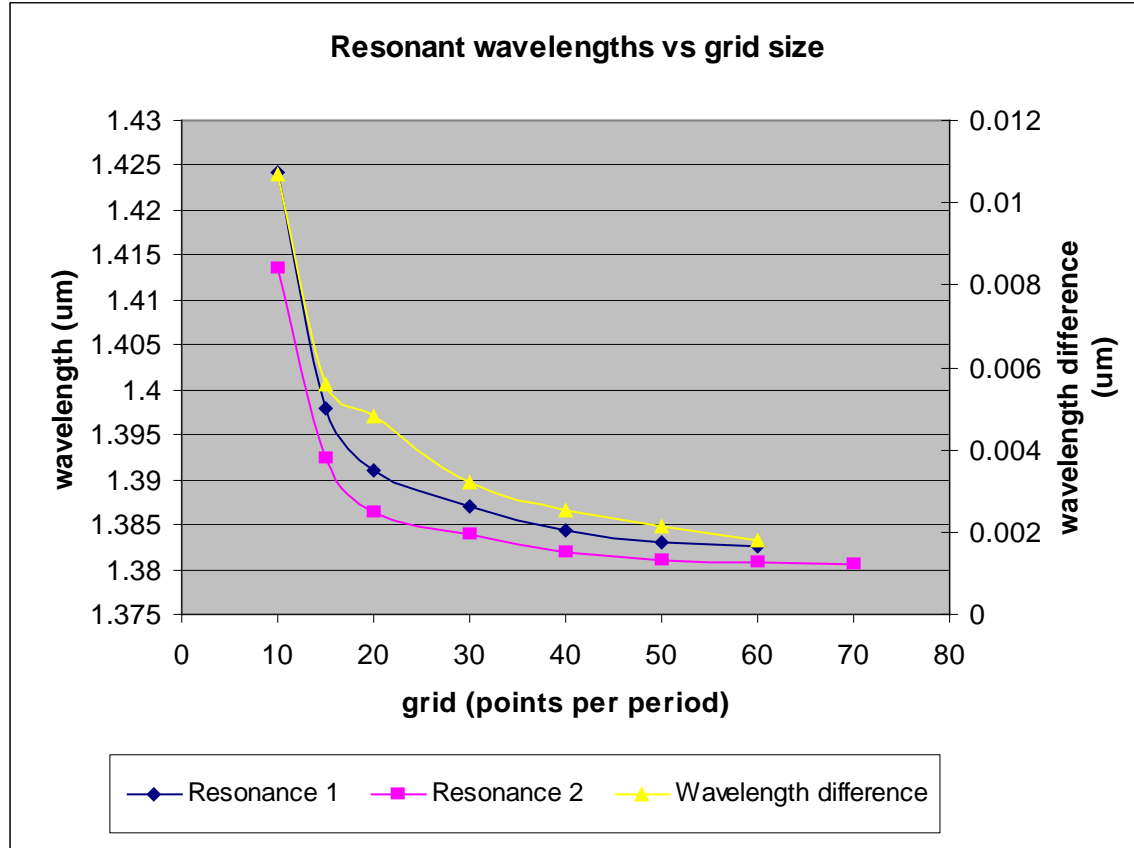
**Figure 8: Resonance spectrum for different grid spacings, The grid spacing is indicated here in the legend, as a fraction of the lattice period. We can clearly see the resonances move to shorter wavelengths and move closer to each other with decreasing grid spacing.**

We will interpret these results. The fact that the resonances move to shorter wavelengths is because the coarser grid size effectively created a different structure, which had different resonances. By different we mean slightly shifted to longer wavelengths. The resonance positions seem to converge (Fig 9) with decreasing grid spacing.

The result that the wavelength spacing between the resonances decreases is interesting. From Fig. 1, we can see that the cavity is a regular hexagon. Such a shape preserves the symmetry of the hexagonal lattice. Therefore, we would expect the resonant modes to be same whatever direction they are travelling. That means that there shouldn't be two closely spaced resonances, but only one. A good analogy of this is a square and a rectangular resonator. The rectangular resonator will have two different resonant wavelengths, for the two modes that propagate along different dimensions, while the square will have one.

What happens here is that the symmetry of the crystal and the cavity is altered by the grid. The crystal and the cavity are hexagonal, while the grid is square. Therefore the discretisation disrupts the symmetry and causes two closely spaced resonances to appear. When we decrease the grid size, the disruption of the symmetry

becomes less important, and the two resonances converge to one resonance. In Fig 9, we plot the spacing between the resonances vs grid size. The spacing is going steadily down.



**Figure 9 : Wavelength of the resonances vs grid spacing. Grid size is indicated here as a fraction of the lattice period. We can see that the wavelength position falls but seems to converge to the final value. Also the wavelength spacing steadily decreases, up to the point that the resonances become indiscernible.**

For similar arguments, the Q of the longer wavelength resonance is also falling for decreasing grid size. It seems that the shorter wavelength resonance is the real resonance of the cavity, and the longer one is the one caused by the disruption of the symmetry. The Q of the resonances is plotted against grid size in Fig. 10.

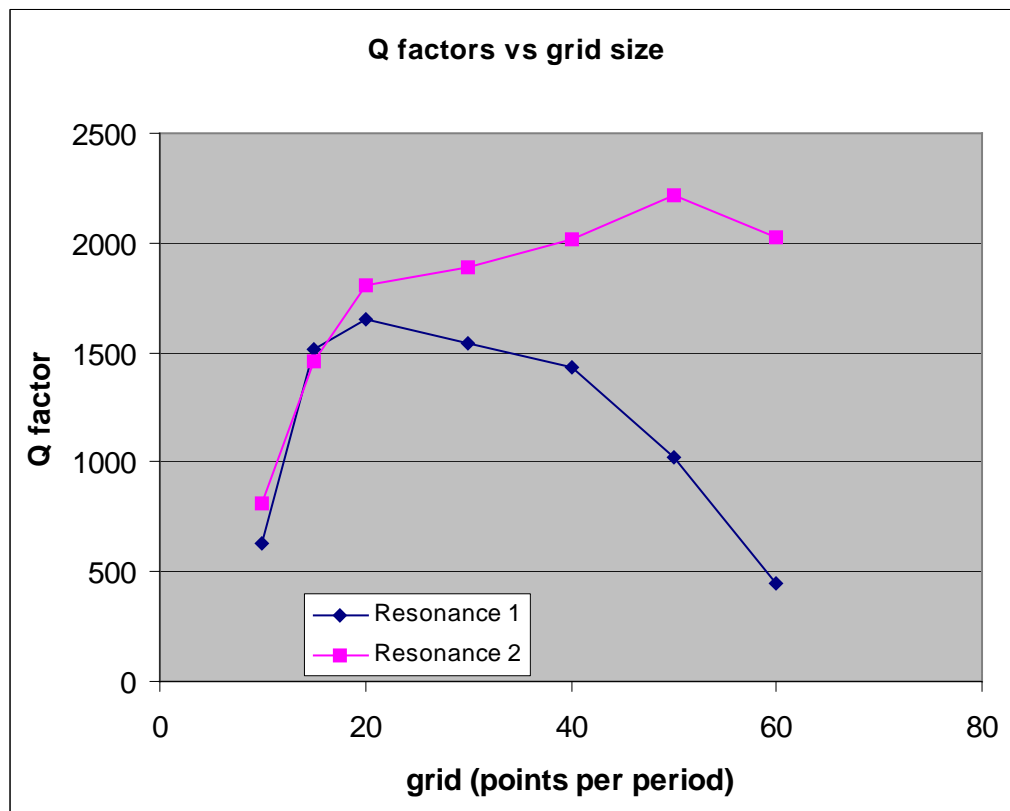


Figure 10: Q factor of the resonances for decreasing grid size