CHAPTER 1

Translight Software: Manual.

This section explains some of the alterations that have been made to Transfer Matrix code as distributed by Imperial College London. All alterations have been made with a level of generality; that is to say the majority are not structure specific and can be applied or utilised in either two or three-dimensional systems. The examples included are for trivial two-dimensional systems for ease of visualisation and explanation but the methodologies can be extended to three dimensional systems subject to any limitations listed.

Before using the code read the terms and conditions of the “Licence” on page 6. Utilisation of the code is stipulates agreement with these terms and conditions.

27 August 2000 2:04 pm

1.1: Licence

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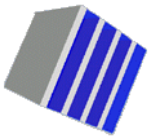
This code has been developed by Andrew L. Reynolds in the University of Glasgow. This code formulates part of the submission for the degree of Doctor of Philosophy for Andrew L. Reynolds, under the supervision of Professor John Arnold. Utilization of this code stipulates that any resultant publication or usage of results will acknowledge Andrew L. Reynolds, the Photonic Band Gap Materials Research Group within the Optoelectronics Research Group of the Department of Electronics & Electrical Engineering, the University of Glasgow and the transfer matrix method, T.M.M., and the initial program originators from Imperial College, London, Professor J. Pendry, Professor P.M. Bell, Dr. A.J. Ward and Dr. L. Martin Moreno.

This license file may be subject to change. Version Pre-Beta 09/02/2000.

A. L. Reynolds, February 2000.

1.2: Pre-defined Systems

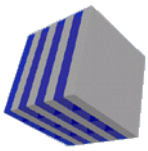
The following systems have been set up as default systems within the code. Many of the lattices also have generic settings so that the user can change the parameters of the lattice but preserve the lattice geometry.



1D Bragg Stack:

Calculating photonic Green's functions using a non orthogonal finite difference time domain method.

Ward A.J., Pendry J.B., Phys Rev B 58: (11) 7252-7259 Sep 15 1998.



1D Omni-directional Bragg Stack

Omnidirectional reflection from a one-dimensional photonic crystal,

Winn J.N., Fink Y, Fan S.H., Joannopoulos J.D.,

Opt Lett. 23: (20) 1573-1575 Oct 15 1998

2D perfect crystal & 2D crystal with planar cavity:

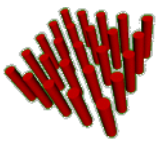
Microcavities in photonic crystals: Mode symmetry, tenability, and coupling efficiency,

Villeneuve, P. R., Fan, S.; and Joannopoulos, J. D., Phys. Rev. B 54, 7837 (1996).

2D Hexagonal Crystal ΓM and ΓK directions:

Quantitative measurement of transmission, reflection, and diffraction of two-dimensional photonic band gap structures at near-infrared wavelengths.

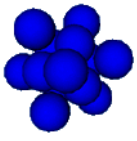
Labilloy, D.; Benisty, H.; Weisbuch, C.; Krauss, T. F.; De La Rue, R. M.; Bardinal,V.; Houdre, R.; Oesterle, U.; Cassagne, D.; and Jouanin; C., Phys. Rev. Lett. 79, 4147 (1997).



2D Metallic Photonic Band Gap Crystal

Metallic photonic band-gap materials,

Sigalas, M. M., et al., Phys. Rev. B 52, 11744 (1995).

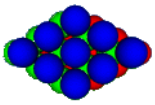


3D Opal Photonic Crystal <001>

Spectral Properties of Opal-based photonic crystal with Si02 matrix.

A.L.Reynolds, F. Lopez-Tejeira, D. Cassagne, F. J. Garcia-Vidal, C. Jouanin. J. Sanchez-Dehesa.

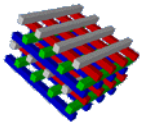
Physical Review B, 15th October 1999.



3D Opal Photonic Crystal <111>

Spectral Properties of Opal-based photonic crystal with Si02 matrix.

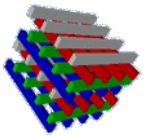
A.L.Reynolds, F. Lopez-Tejeira, D. Cassagne, F. J. Garcia-Vidal, C. Jouanin. J. Sanchez-Dehesa.
Physical Review B, 15th October 1999.



3D 94GHz Woodpile Structure

Micromachined millimeter-wave photonic band-gap crystals.

Ozbay, E., et al., Appl. Phys. Lett. 64, 2059 (1994).



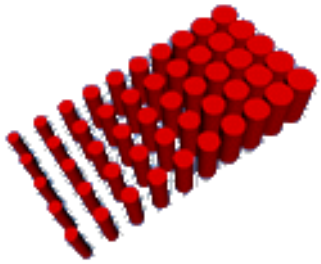
3D 500GHz Woodpile Structure

Terahertz spectroscopy of three-dimensional photonic band-gap crystals,

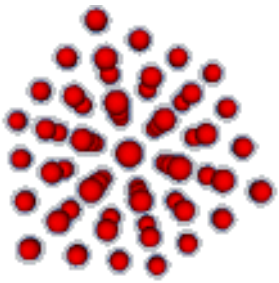
Ozbay, E., et al., Opt. Lett. 19, 1155 (1994)

There are many different crystals that can be defined with Translight. Some of the other crystals that may be of interest are shown below.

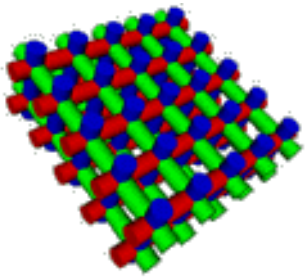
VCSEL



Chirped PBG



Simple Sphere Structure



Scaffold System

1.3: Setting up for the first time.

Once you have down loaded the code place the executable file in new folder. All file handling, generation and manipulation will take place within this directory. As the code is self contained all sub directories that are required by the code will be automatically generated without user intervention. In the event of strange behaviour, hangs, or crashes at any stage follow these instructions again before reporting errors as file corruption may have occurred. Ensure that any systems that you have developed are placed in back up directory before initialising.

Running the code.

The code is run by double-clicking on the distributed executable file. The executable will then establish whether it is being run for the first time or in a new location and generate the files and directories that it requires. Any errors and output generated by the code are placed in the runtimerrs.dat and output.dat files within the same directory location as the executable.

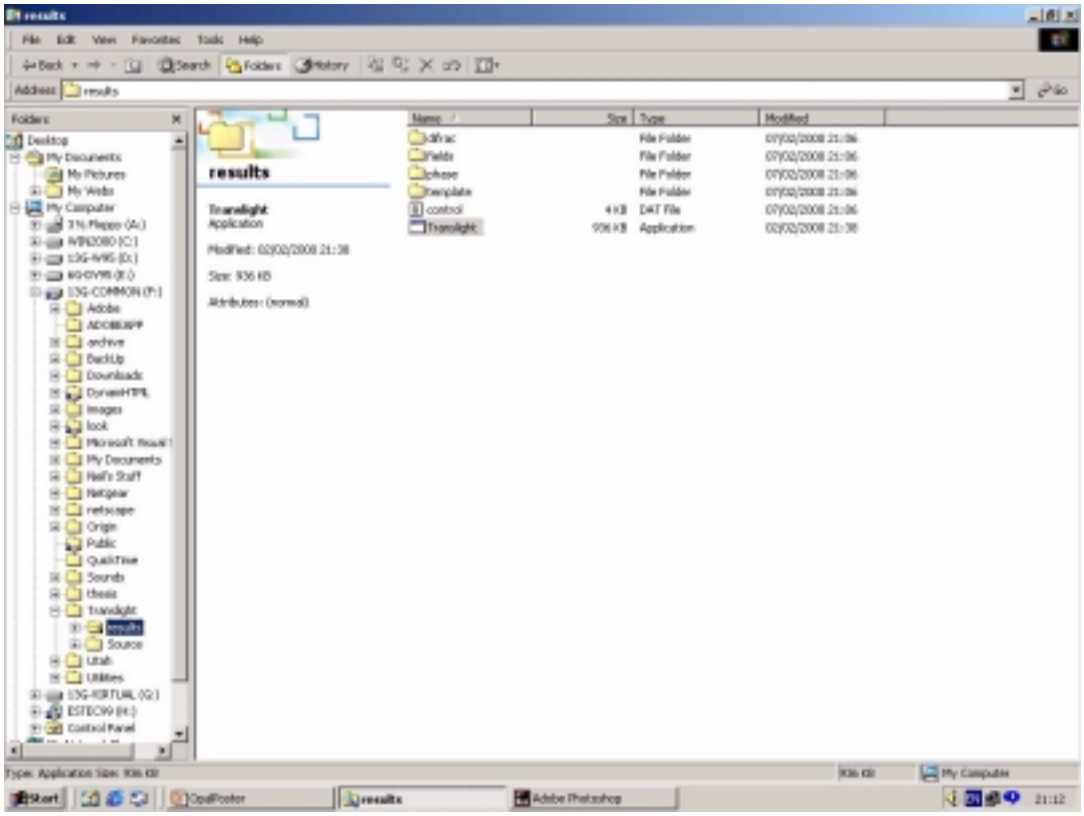


Figure 1.1 Directory Screen shot showing the executable Translight.

Upon execution a graphical user interface, herein referred to as GUI, will be presented. From this window most elements of the calculation can be controlled. A discussion and explanation of the different windows and element function is presented elsewhere within this document. It is recommended that for first time use that the user simply run the calculation for the default system so that required files and directories are then created. The default calculation has been deliberately set such that the calculation time is minimum, under a minute for most present day

personal computers. The code must be run with the default system once so that files and directories can be created.

An estimation of the time for calculation will be written to the screen and to the file timeestimate.dat. Due to the heavy numerical processing within the code there can be a difference in the estimated time and actual run time. Generally the estimation reported within the file is conservative in so far as the program calculation runs faster than the reported estimate.The on screen estimate is recursive and will adapt as the program progresses.

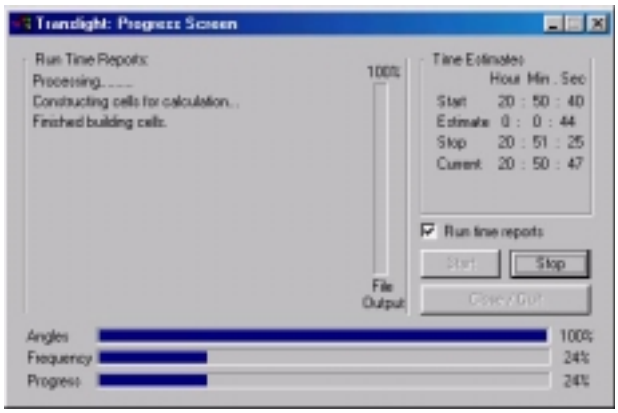


Figure 1.2 Program Running Dialog Screen

The time taken will vary for each machine due to specification and will alter on screen as the calculation progresses.

During program execution the user can start and stop the calculation to recover CPU if required for other calculations. For 3D structures the dialog screen may become unresponsive for several minutes as the refresh rate is dependent on one internal interation of the code. For 1D and 2D systems this is not normally a problem but for 3D systems some patience may be required. Once the program has finished then the screen shown in Figure 1.3 is displayed.When the calcualtion has finished the final set of results are written to the hard drive, the start and stop buttons are disabled and the dialog window should be closed using the activated Close / Quit button.

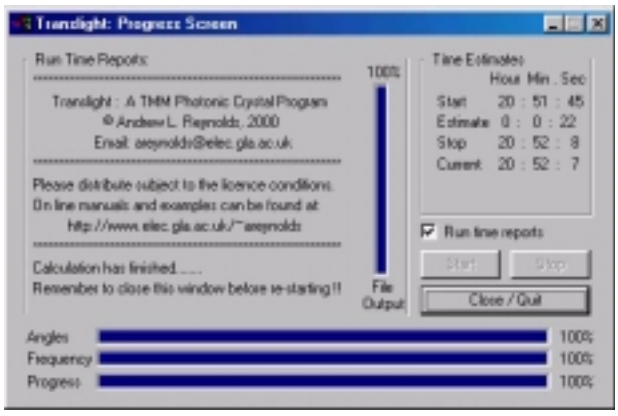


Figure 1.3 Program has finished.

1.4: Modifications

The code has been altered to run automatically from an Input File <control.dat> allowing the user to set up the run time parameters for the code. Prior to this the code used a menu system before commencing operation which was incompatible with supercomputer necessitating its removal. The graphical user interface uses the control file to keep the runtime settings, within the control file it is possible to switch off the GUI which is discussed later, see “Advanced / Help Menu” on page 20.

In the process of these changes several other features were added into the capability of the code. These new features allow coatings and relatively complex crystal definition allowing the study of defects. This can be achieved in either one, two or three dimensions.

The code also allows the user complete control over the total number of layers propagated through in the system, a feature that was previously not available. The code also automatically writes Virtual Reality Files v2.0 for the crystal under study which can be used with the <CELLONLY> switch to verify the correct definition of a crystal before embarking on a complex or time consuming calculation. VMRL files can be viewed by installing the relevant plug in with most current web browsers.

NOTE:
The VRML file that is created uses the basic shape building blocks, i.e. the box, cylinder and sphere. Therefore for crystals that are actually air cylinders in dielectric the VRML file will appear as solid cylinders in air. The VRML file can still be used to check the geometry of the crystal. Coatings will appear as semi transparent around sphere elements.

In order to understand the control file <control.dat> each parameter found within the file is discussed after the description of the GUI, see “Defining the structure through the control file.” on page 23.

1.5: Graphical User Interface, G.U.I.

The GUI has been developed to simplify the parameter input used to control the code. The GUI has several tabs at the top of the interface grouping together the main elements under each tab heading. Several controls are shared between different tabs, changing between tabs will keep any changes that have been made. Any information that is changed in a text box, i.e. a number as opposed to a push button or check box requires that you push the refresh button before running the calculation. At present it is recommended that the refresh button is pushed to ensure that all parameters are correctly initialised into the program before running the program. The refresh button flushes areas of memory and reloads parameters, re-initialises dynamic arrays and performs minor checks on the current settings. Any encountered errors will be either written to the screen, written into the <output.dat> or <runtimerrs.dat> file.

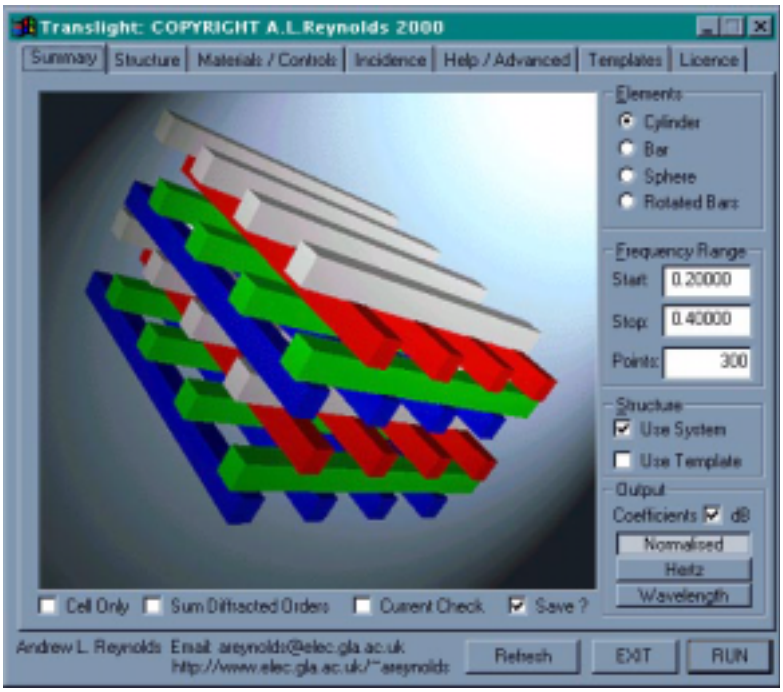


Figure 1.4 Summary / Start Up Screen.

This is the screen that is presented each time the program is executed. It summarises some of the main elements that describe the calculation, the different tab heading are located at the top of the window, Summary, Structure, Controls, Incidence, Advanced / Help, Templates and licence. The refresh, exit and run controls located in the bottom right of the window are shared between all of the different tab menus and can be used at any time to refresh the window elements, exit the calculation immediately or run the program. Once the program is running execution can be stopped by closing the console application hosting it.The summary tab has a few controls which summarise the intended calculation settings.

The elements used to build the crystal are found in the top right of the window, one element will always be selected. The material properties of the feature are found in the structure tab, see “Structure Menu” on page 15.

The frequency range for the calculation is controlled by a start and stop frequency and a number of points. The start and stop frequency displayed in the box is normalised through the relation $f_{norm}=fa/c$ where a is the lattice constant, f is frequency in Hertz and c is the speed of light in vacuum. The two push buttons below the frequency parameters determine whether the output files are written in normalised frequency of in Hertz. If the output dB box is checked then the transmission and reflection co-efficients will be written in decibels.

Finally the system and template check boxes indicate whether a pre-defined system within the code is being used or whether a user defined template is to be used. These options are mutually exclusive and the code can also run without either checked.

Structure Menu

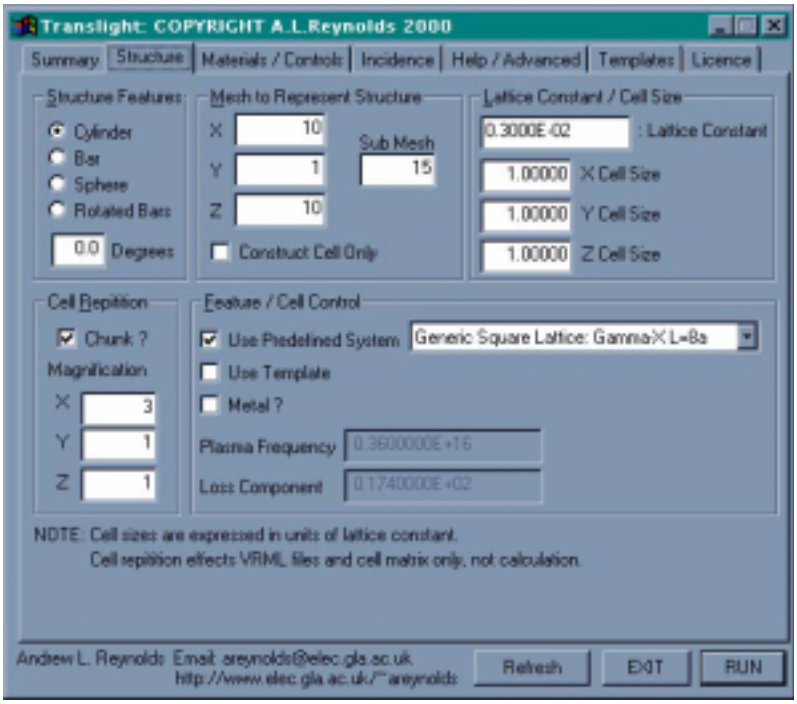


Figure 1.5 Structure Menu

Features

As discussed in “Structure Menu” on page 15 with the added control of the degrees box for the rotated bars option. If rotated bars is chosen then enter the non zero degree of rotation required into the box. The bar is rotated along its own axis.

Discretisation mesh used to represent structure

The discretisation mesh is used to represent the structure under study. The larger the discretisation mesh the more accurately the structure is represented but the longer the code takes to run. The mesh is a sensitive parameter and requires careful though. The code corrects for differences in the inter-mesh spacing but best results are obtained when the number of points in the mesh in each dimension is chosen such that the inter-mesh point spacing is as similar as possible.

Lattice constant & cell size

Most crystals have an associated lattice constant which is expressed in metres. As these calculations are theoretical and Maxwell’s equations scale, the lattice constant can be adjusted without altering the results of the calculation if normalised frequency is used. For a more in depth explanation of the scaling properties of Maxwell’s equations see Photonic Crystals: Molding the flow of Light []. The cell sizes are expressed in terms of the lattice constant. A cubic cell will therefore have each entry set to unity. Depending on the crystal under study theses parameters may not initialise.

Chunk / Cell Magnification

For multiple cells when the chunk parameter is checked the code will output a “chunk” of crystal rather than the individual cells. The magnification factors repeat the crystal in the x,y,z directions. If multiple cells are used then the magnification in the z-direction will have no effect although the x and y magnification factors remain functional. The crystal that is output into the VRML file, vrml.wrl and gnet.dat does not reflect the layer repitition that is used to control the crystal thickness. For example if the first cell is repeated three times a total of 3 “units” before encountering the second cell, 1 “unit” the total crystal thickness for the calculation is “4 units”. The VRML file and gnet.file will have only a representation of the first and second cells bolted together, i,e. 2 “units”. Cell magnification and chunk parameters do not alter the actual crystal calculation thickness, the crystal thickness is controlled with the layer and block control, see “Defining the crystal.” on page 28.

Controls Menu

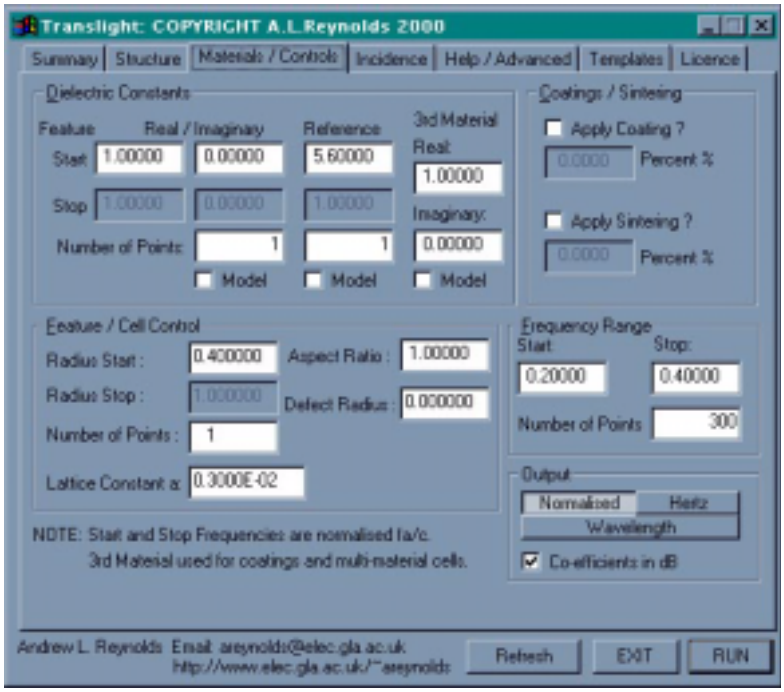


Figure 1.6 Controls Menu

Dielectric Constants.

For simple photonic crystals it is normally sufficient to define the dielectric constant of the features to be used in the crystal, the reference medium, and in this program another third material. For Chigrin's Bragg stack the third material is used as one of the materials of the stack so that the reference medium can be defined independently. For some of the other predefined lattice the third material is used in different ways, i.e. for coatings. In Chigrin's Bragg stack the materials that were chose have dielectric constants of $\varepsilon_1 = 11.56$ $\varepsilon_2 = 1.96$. The structure has been embedded in the higher dielectric constant medium, $\varepsilon_{reference} = 11.56$.

Frequency Range.

The start and stop frequencies of the calculation can be selected and altered along with the number of frequency points. Both the start and stop frequencies are expressed in normalised units which is related to the lattice constant through the Equation 1.1

$$\text{Normalised Frequency} = \frac{\text{Frequency (Hz) x Lattice Constant (m)}}{\text{Speed of Light(ms-1)}}$$

Equation 1.1 Normalised Frequency

Under the frequency start and stop edit boxes there are two push button boxes labelled ‘Normalised’ and ‘Hertz’, and a check box labelled ‘Coefficients dB’. These boxes relate to the output that will be generated in analysis of the program. If the Hertz box is pushed then the output files will relate the transmission and reflection coefficients to frequency expressed in Hertz, similarly if the Normalised button is selected then the files will be expressed in normalised frequency. The check box ‘Coefficients dB’ will change the coefficients from a linear scale to a logarithmic scale if checked.

Feature / Cell Control.

Within this group control of the features can be achieved and loops can be introduced if required. The radius start and stop values are again normalised to the lattice constant such that the values displayed are r/a where r=radius and a=lattice constant.

The ‘Aspect’ control and defect radius are used for particular lattices and are discussed elsewhere. The lattice constant value is also shown within the Feature / Cell Control box. Many of the menus have parameters repeated between them, changing the value in one menu will alter the values across all the tab menus.

Coating / Sintering.

These parameters are used in conjunction with Opal photonic crystals and in certain cases can be applied to to crystals that use either cylinders or sphere as their constituent features.

Incidence Menu

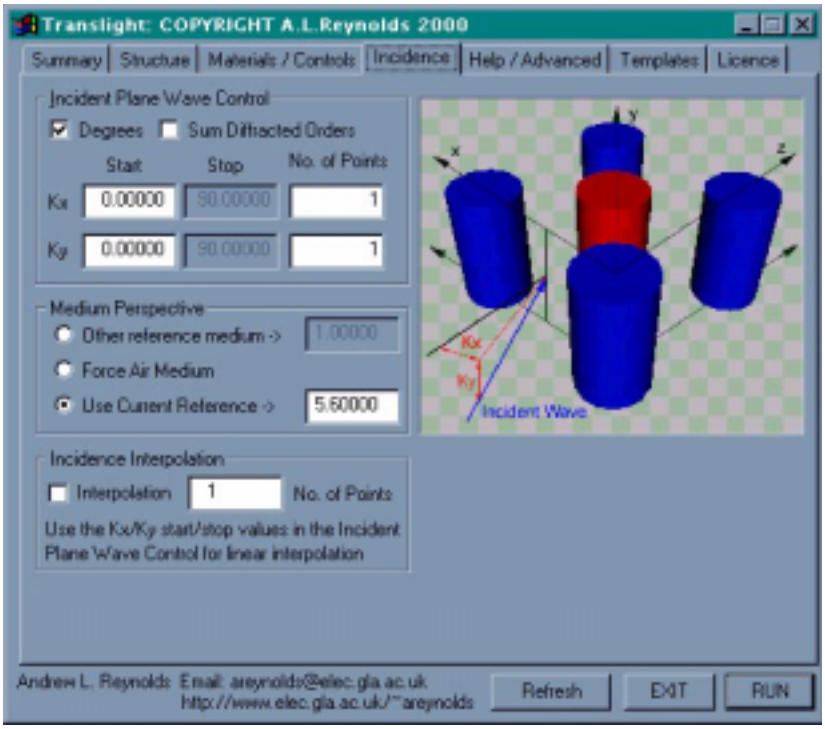


Figure 1.7

Advanced / Help Menu

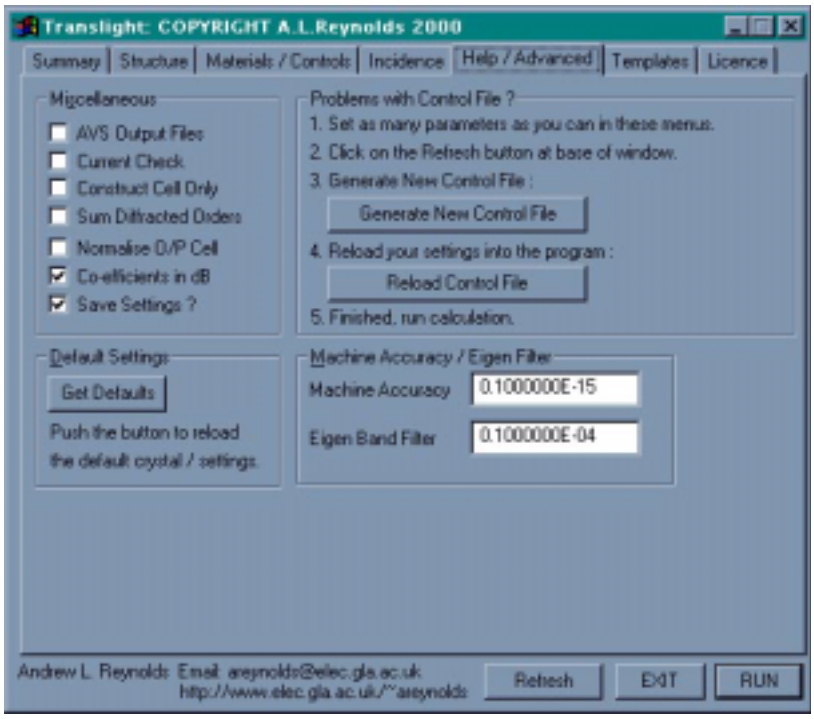


Figure 1.8 Advanced / Help Menu

Input File Generation / Reload

If the input file becomes corrupted or starts to cause problems after editing these two buttons can be used to generate a new control file and then reload the file. If the program has startup problems delete the current control file completely and re-run the code. The code will then default to the test system which you should run once before editing the control file or regenerating the control file from the menu.

Miscellaneous

Templates Menu

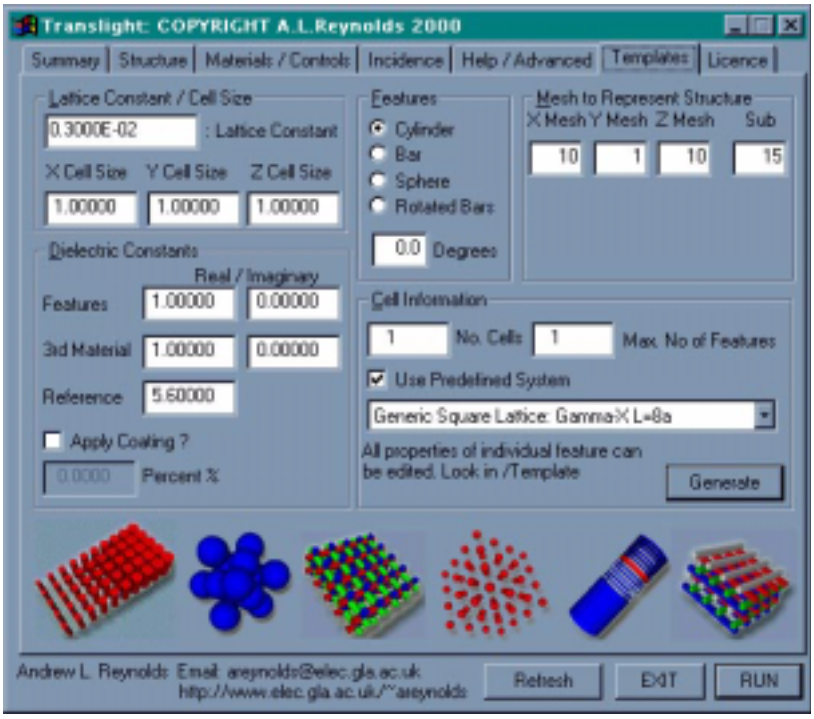


Figure 1.9 Template Menu

Licence Menu

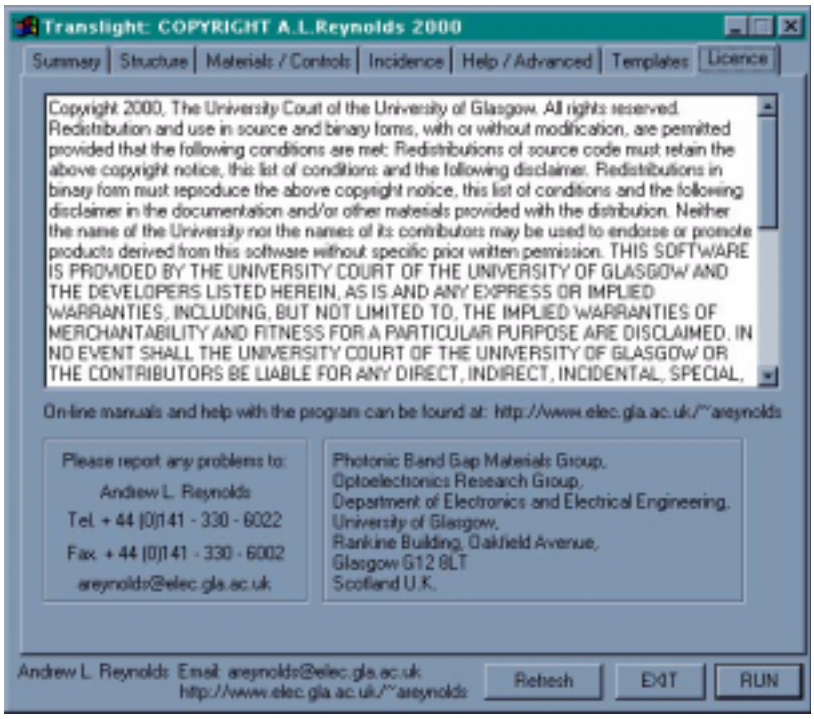


Figure 1.10 Licence Menu.

Terms and conditions for using the code. Usage of the code implies agreement of these conditions.

1.6: Defining the structure through the control file.

DEBUG: Debugging Option.

Used to generate narrative for the program to aid debugging. Unless a problem is encountered this should be set 'off' ('0'), The user should decrease the number of points in the calculation if debugging otherwise a huge run time report of the code will be generated.

Related Parameters: None

AVS: Advanced Visual Systems File Output (AVS)

If true (1) will generate the files required by Advanced Visual Systems, AVS, to visualise cell and transmission data. The files will be deposited in the same directory as the data output files negating the necessity to include path names within the AVS files. If GNU-plot or any other visualisation package is to be used then set false ('0').

Related Parameters: CELLSTRUCT,BUILDBLOCK,XMAG,YMAG,ZMAG

READONCE: Reads parameters once.

If true recovers the parameters for the cell one time only, thereafter the main program can be coded to alter them, i.e. nested sweeps of the radius of a cylinder can be achieved to obtain optimal response for a system. Usage of this parameter necessitates good knowledge of the main code, if in doubt set true ('1').

Related Parameters: None

DEFECTS: Defects.

If a cell has been set to be a defect cell, it can take one of two values, either completely filled with the dielectric constant of the reference (embedding) medium (DEFECT=0) or the dielectric constant of the features (DEFECTS=1). More complex defects can be achieved through super cells (blocks) and multi-cell structures; which are discussed in the section: Controlling the structure under study.

Related Parameters: None

Features: ANYBAR, ANYROTBAR, ANYCYL, ANYSPHERE

Feature with which to build cell, only one can be chosen. Chosen structure has value of (‘1’), all others must be set to (‘0’)

ANYBAR: Bars, square or rectangular cross-section,

ANYROTBAR: Rotated Bars, in plane angular rotation of bar, (under development)

ANYCYL: Cylinders,

ANYSPHERE: Spheres.

CELLSTRUCT: Cell Structure Creation.

When set ‘TRUE’ (‘1’) program will generate and output the structure of the unit cell and then stop. Used for visually checking the contents of the representational matrix prior to large calculations.

Related Parameters: BUILBLOCK,AVS,XMAG,YMAG,ZMAG

BUILDBLOCK: Builds a large representative matrix.

If set ‘TRUE’ (‘1’) then the multi cell crystal under study will be written into the output file as one large piece of crystal, in effect adding together all sub cells of a crystal into one large matrix. Especially useful if used in conjunction with AVS switch. If ‘FALSE’ (‘0’) each cell will be written sequentially to the output file. If the multi cell crystal under study contains either layer doubling or single layer additions within a block then at present these will be ignored. To understand cells and blocks see the section: Controlling the structure under study.

Related Parameters: CELLSTRUCT,AVS,XMAG,YMAG,ZMAG

XMAG,YMAG,ZMAG Expansion factors.

Used to repeat pieces of crystal in the X,Y, & Z directions to obtain build a bulk piece of the crystal. These parameters do not effect the calculation in any other way.

Related Parameters: BUILBLOCK,CELLSTRUCT,AVS

COEFF: Transmission Coefficient / Band Structure Calculation

If set ‘TRUE’ (‘1’) then the code will perform a transmission / reflection calculation, otherwise the band structure for a cell will be calculated.

Related Parameters: None

XSIZE,YSIZE,ZSIZE Global Discretisation Mesh

The discretisation mesh is used to represent the structure under study. Integration (propagation) is carried out through the structure in the Z-direction, therefore for two-dimensional PBG's the Y mesh size should be set to unity.

Related Parameters: ISUB

ISUB: Sub Mesh Size

Each mesh point as defined by the global discretisation mesh is sub divided into a sub mesh points on which the structure under study is formed. The sub mesh is used to provide an average value for the dielectric constant to the global mesh point.

Related Parameters: XSIZE,YSIZE,ZSIZE

EMACH: Machine Accuracy

Self-explanatory; used to determine the accuracy of the calculations.

CIKVAL: Filter on Eigen Values

Used to filter the imaginary values of the K-Values when the band structure calculation is utilised.

Dielectric Constant related parameters.

- *Dielectric Constant of Shape:*

ERSTARTR	*Start Value, real part*
ERSTOPR	*Stop Value, real part*
ERSTARTJ	*Start Value, imaginary part*
ERSTOPJ	*Stop Value, imaginary part*

TABLE 1 : Element Materials

- *Reference Medium*

REFSTARTR	*Start Value, real part*
REFSTOPR	*Stop Value, real part*

TABLE 2 : Reference Medium Material

- *Frequency of Interest:*

FSTART	*Start Frequency*
FSTOP	*Stop Frequency*
NOP	*Number of Points*

TABLE 3 : Frequency range controls

For example, to calculate the response of a structure from 4.5GHz to 9GHz using 450 points requires the following:

FSTART	4.5	*Start Frequency*
FSTOP	9.0	*Stop Frequency*
NOP	450	*Number of Points*

TABLE 4 : Frequency range controls: Example

Controlling the plane wave incidence.

The user can choose the incidence angle of the plane wave onto the structure through the AKX and AKY parameters. The parameters are normalised to the unit cell and consequently range from 0 to +/-1. Normal incidence to the structure is achieved by setting both AKX and AKY components of the light to zero; oblique incidence is achieved when they are unity.

• *Components:*

AKXSTART	*Parallel component in X-Plane, start value*
AKYSTART	*Parallel component in Y-Plane, start value*
AKXSTOP	*Parallel component in X-Plane, stop value*
AKYSTOP	*Parallel component in Y-Plane, stop value*
AKXNOP	*Number of Points used to Scan Range in X-Plane*
AKYNOP	*Number of Points used to Scan Range in Y-Plane*

Miscellaneous Parameters

Some of the following can be structure specific and will not affect all calculations, refer to the appendix on current structure libraries and systems for further details.

FRNOP: Filling Ratio Number of Points.

Used to sweep a further aspect of the structure and can be coded in various forms. New users should leave this at the default setting of (1) as it incurs complete loops of the main program otherwise. FRNOP was originally intended as ‘Filling Ratio Number of Points’ where a range of filling ratios can be set and then set to loop to generate gap maps. It is still generally used for this purpose but requires that the user correctly code the expression for the filling ratio for a structure. This has been done for elementary square lattices with cylindrical and rectangular features and has also been done for hexagonal and FCC opal systems. Caution should be exercised in using this variable as it can lead to large data matrices.

ASPECT: Cell aspect ratio.

Used in setting up cells that do not have unitary aspect ratios. Aspect ratio is defined as XCELLSIZE / ZCELLSIZE. This is especially useful for setting up super-cell lattices for the study of localised defects. Caution: The XSIZE and ZSIZE discretisation mesh ratio should mirror the ASPECT ratio to ensure that the inter-mesh spacing in the X and Z directions remains the same. Some of the pre-defined systems code this automatically, but by no means all.

DEFECTR/A: Controlling the defects.

Ratio of the Radius to the Lattice Spacing A. (RADIUS/SPACING) This is used to set the size of the features within a unit cell. For the case of bars, ROVERA results in an evaluation of RADIUS, and the bar width is set to 2*RADIUS. Alternate shapes and defects can be achieved through alteration of template file(s).

ROVERA: Controlling the element size.

See DEFECTR/A above, the only difference being that the ROVERA parameter defines FIXERADIUS, which is applied to every feature within the shape if there are no defects present. Similar conditions hold for bars.

COATING

Expressed in fractional percentage, i.e. 0.10 is 10%, this controls the coating that is applied to the feature, be it a cylinder or sphere. The coating will only be applied if the logical switch COAT within the source routines definebar(*).f is set.true. (see “Coatings” on page 31)

SINTERING

Expressed in fractional percentage, i.e. 0.20 is 20%, this controls the coating that is applied to the feature, be it a cylinder or sphere. The effect of sintering has been introduced to facilitate the definition of Opal photonic crystals and therefore is highly structure dependent, therefore caution should be exercised as for many structures it serves no purpose.

1.7: Defining the crystal.

To control the structure under study the user first picks the type of feature that will be used to create the PBG lattice. This is done in the general program set up section where the user chooses cylinders, spheres, bars etc. Thereafter the type of lattice that is created is controlled with ‘cells’ and ‘blocks’.

The parameters that control the creation of the lattice are:

•*Cell Parameters:*
NOOFCELLS,
NOOFBLOCKS,
STARTBAR,
NOOFBARS,
NOOFSINGLES, for the cell,
NOOFDOUBLES, for the cell,

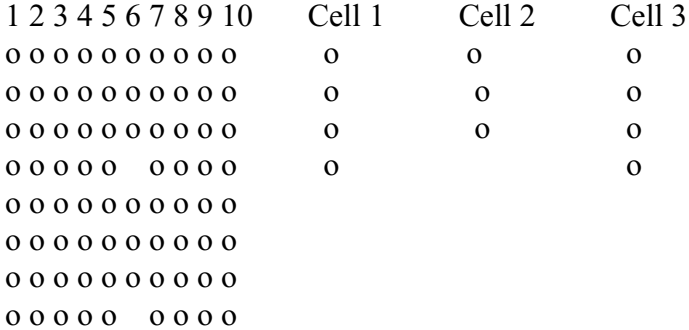
•*Block Parameters:*
BLOCKSTART,
BLOCKSTOP,
NOOFSINGLES, for the block,
NOOFDOUBLES, for the block.

The response of a crystal is obtained by propagating through the cells and blocks that make up the crystal. The system of cells and blocks is powerful, allowing relatively complex crystals to be generated with a relative amount of ease.

Terminology

A ‘cell’ defines a unit cell, within the unit cell there can be any number of features or none at all, the only limitation on the number of cells being dictated through numerical stability or computer memory. For each cell we define a start feature (STARTBAR) and the number of features to be placed in that cell, (NOOFBARS). For each cell we can choose how many times it is to be repeated within the crystal before the next cell is encountered. This repetition, or number of layers, is controlled through two parameters, NOOFSINGLES and NOOFDOUBLES for each cell. In a two-dimensional lattice these layers can be thought of as vertical strips or columns.

For example, consider the following:



The above system can be built with three cells, to create the above crystal the configuration within control file <control.dat> would be as follows:

```
NOOFCELLS =  3
NOOFBLOCKS =      0
c
STARTBAR(1)   =     38 (arbitrary choice, example only)
NOOFBARS(1)  =      4
NOOFSINGLES =       1
NOOFDOUBLES=        2
c
STARTBAR(2)   =     38 (arbitrary choice, example only)
NOOFBARS(2)  =      3  (one less than cell 1 & 3 creates defect)
NOOFSINGLES =       0
NOOFDOUBLES=        0
c
STARTBAR(3)   =     38 (arbitrary choice, example only)
NOOFBARS(3)  =      4
NOOFSINGLES =       0
NOOFDOUBLES=        2
```

NOTE: Only four features are required per unit cell as the code automatically wraps the cells in the vertical direction.

For the first cell we require five layers. This is achieved by a two layer doubling and then the addition of a single layer. The layer doubling system works to the power of two, i.e., two layer doublings means 2**2=4, three 2**3=8 etc. The number of singles simply adds an extra layer. Therefore for five layers 2**2+1=5.

For the second cell we do not want to add any extra layers or double the response for the cell, therefore both NOOFDOUBLES and NOOFSINGLES for cell number two are set to zero.

For the third and final cell we require four layers; NOOFDOUBLES = 2, NOOFSINGLES = 0.

Using BLOCKS

Blocks allow more complex crystals to be made from constituent sub cells. A block requires a minimum of two cells in the crystal, otherwise a block cannot be built. The following example demonstrates the power of blocks in conjunction with cells to create coupled defects.

```
1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1   Cell 1Cell 2Cell 3Cell 4Cell 5
o o o o o o o o o o o o o o o o o o o o o    o      o     o     o     o
o o   o o   o o   o o   o o   o o   o o o    o      o           o     o
o o o o o o o o o o o o o o o o o o o o o
o o   o o   o o   o o   o o   o o   o o o
o o o o o o o o o o o o o o o o o o o o o
```

Would be represented within the <control.dat> file as follows:

```
   NOOFCELLS =     5
NOOFBLOCKS  =      1
c
STARTBAR(1)   =    38 (arbitrary choice, example only)
NOOFBARS(1)  =     2
NOOFSINGLES =      0
NOOFDOUBLES=       0
c
STARTBAR(2)   =    38 (arbitrary choice, example only)
NOOFBARS(2)  =     2
NOOFSINGLES =      0
NOOFDOUBLES=0
c
STARTBAR(3)   =    38 (arbitrary choice, example only)
NOOFBARS(3)  =     1 (one less than others creates defect)
NOOFSINGLES =      0
NOOFDOUBLES=       0
c
STARTBAR(4)   =    38 (arbitrary choice, example only)
NOOFBARS(4)  =     2
NOOFSINGLES =      0
NOOFDOUBLES=       0
c
STARTBAR(5)   =    38 (arbitrary choice, example only)
NOOFBARS(5)  =     2
NOOFSINGLES =      0
NOOFDOUBLES=       0
c
1BLOCKSTART =      2  Cell number to define start of block.
1BLOCKSTOP   =     4  Cell number to define end of block.
NOOFSINGLES =      2  No. of times to double block.
NOOFDOUBLES=       2  No. of times to add a single block.
```

Coatings

For the Opal systems coatings play a major part in the performance of the system. The addition of a layer or 'coating' of semiconductor or other material is not difficult to achieve for a single feature or element within a cell, however multi feature cells with overlapping elements provide more of a challenge. This has been tackled successfully within the code allowing the user to define complex cells, elements that are coated and those that are not within the same cell. Merging of features is also possible and the coating algorithm ensures that it appears as a post processing application after merging. This is of great value for partially infiltrated Opal systems, as well as inverted Opal systems which can also partially infiltrated prior to the inversion process.

At present the coating control is kept at a structure definition level. At present the user must edit the <definebar(*).f> sections of code to apply the coating settings. This is due to the fact that a coating can be applied to a particular feature of a cell, global control of this aspect of the code would result in all features being coated. The dielectric constant, thickness of the coating upon the original feature, actual dimensions and position of the feature within the cell can all be controlled to ease the fabrication of complex cells. Over time a powerful library of cells will be available covering most commonly used lattices and structures while facilitating the simple addition of new cells and their features. At present there are many features defined within the libraries, defining elementary square lattices, hexagonal lattices, woodpile systems and two approaches for modelling the FCC lattice for cylinders bars and spheres.

The following visualisation is for a simple two dimensional cylindrical structure. It shows a set

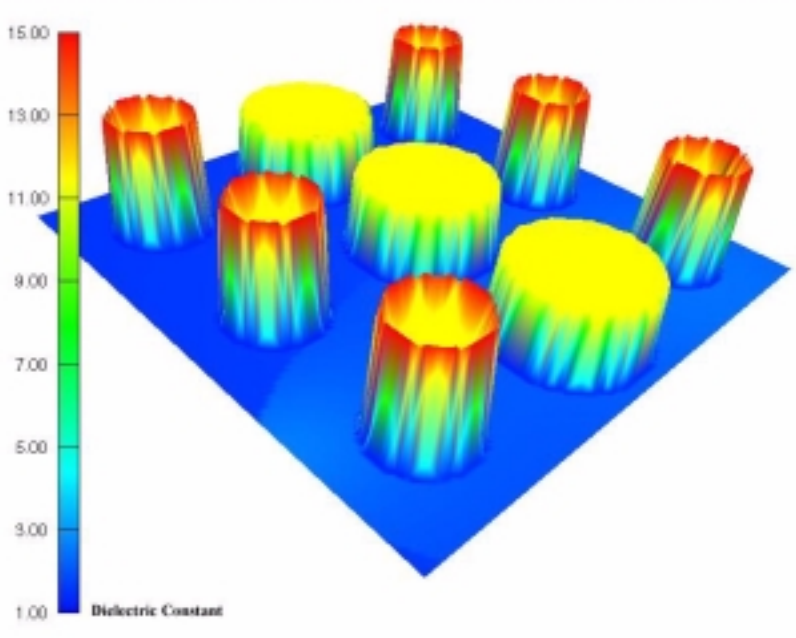


Figure 1.11 Cylinders achieved with Coating Routines

of cylinders that have no overlapping areas, the centre column of cylinders have different dimensions to the others. For this example shown in Figure 1.11 the cylinders have a dielectric

constant of $\varepsilon_r = 10$ and have been coated with a dielectric material $\varepsilon_r = 15$. While these systems maybe hard to fabricate in reality the visualisation demonstrate the capability of the code.

Sintering

The effect of sintering was introduced as a requirement for the Opal photonic crystals. Sintering causes a slight merging of constituent spheres within an Opal crystal. We illustrate the effect of sintering with spheres.

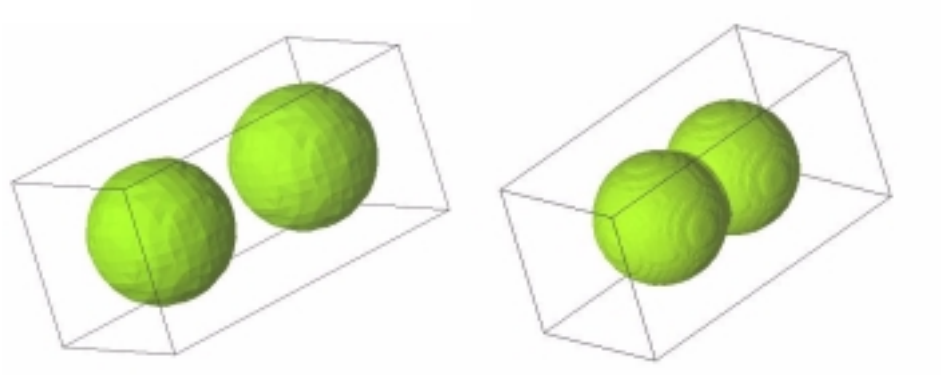


Figure 1.12 Non sintered and sintered spheres.
The non sintered spheres are shown on the left. The sintered spheres are shown on the right, the sintering effect is set at a large value to highlight the effect. The overlapping volume of the spheres is evident, the level of sintering can be controlled within the input file <control.dat>.

1.8: Output Files

The main files of interest are held in subdirectories located in the same directory location as the program executable. The transmission and reflection coefficients are sorted by polarization and placed into the sub-directory ‘Coeff’ in the files Tmtrans.dat, Tetrans.dat, Tmreflec.dat, Terelfec.dat files. In the ‘Reports’ sub-directory you will also find a runtime errors file, runtimerrs.dat, an output file output.dat, and the time estimation file. Some other directories are also created, ‘Crystal’ where the matrix representing the structure is written into the file gnet.dat, and the VRML file relating to the crystal is also kept, vrml.wrl.

The data in the transmission and reflection files are written in data files in the format illustrated in Table 5: on page 34.

Table 5: Sample Output File

Frequency	1 Layer	2 Layers	4 Layers	Kx Angle	Ky Angle	Filling Ratio	Counter
0.0100000	-0.9623395727E-01	-0.3646502536E+00	-0.1657559262E+01	0.00000	0.00000	0.33300E+00	1
0.0124500	-0.1475769739E+00	-0.5438863961E+00	-0.2160867201E+01	0.00000	0.00000	0.33300E+00	1
0.0149000	-0.2086666737E+00	-0.7446836336E+00	-0.2561814898E+01	0.00000	0.00000	0.33300E+00	1
0.0173500	-0.2787171905E+00	-0.9596262147E+00	-0.2833547142E+01	0.00000	0.00000	0.33300E+00	1
0.0198000	-0.3568626772E+00	-0.1181763281E+01	-0.2962723003E+01	0.00000	0.00000	0.33300E+00	1
0.0222500	-0.4421801540E+00	-0.1404873259E+01	-0.2944199615E+01	0.00000	0.00000	0.33300E+00	1
0.0247000	-0.5337115887E+00	-0.1623585178E+01	-0.2778708134E+01	0.00000	0.00000	0.33300E+00	1
0.0271500	-0.6304843260E+00	-0.1833393859E+01	-0.2473181549E+01	0.00000	0.00000	0.33300E+00	1
0.0296000	-0.7315292273E+00	-0.2030607041E+01	-0.2043786728E+01	0.00000	0.00000	0.33300E+00	1
0.0320500	-0.8358961302E+00	-0.2212256050E+01	-0.1522003548E+01	0.00000	0.00000	0.33300E+00	1

In the example a simple crystal with either one cell or one block has been analysed for a finite thickness. The transmission and reflection coefficients have been set to output in dB. The output file lists the frequency in the first column, either normalized, in Hertz, or in wavelength depending on the code settings. There after there can be a variable number of columns related to the crystal thickness. The pattern is always the same 1,2,4,8,16,32.... until the last column which has the total crystal thickness. For example if you want 10 periods of your crystal you would set up the layer doublings to 3, 2**3=8 and then the singles to be 2 such that 8+2=10. The output file would then have the data related to 1,2,4,10 layers in the file.

The Kx and Ky angle are expressed either in degrees or in k-vector. Note that the k-vector scales with the reference medium settings which is the technique used to observe omnidirectional reflectance in Bragg stacks, see “Controlling / Scanning the Incidence Angle.” on page 42 in the Bragg Stack tutorial for further explanation. The filling ratio is not always defined, it depends on whether one has been set for a particular lattice structure. Finally the counter is used when loops are introduced into the code in either the radius or the lattice feature materials.

Photonic Band Gap Materials Research Group, Department of Electronics & Electrical Engineering,
The University of Glasgow, Rankine Building G12 8LT
Tel.+44(0)141-330-6022 Fax.+44(0)141-330-6002: Email:areynolds@elec.gla.ac.uk