18.369 Problem Set 6

Due Monday, 30 April 2005.

Problem 1: Brillouin zones and band diagrams

In class, we derived the irreducible Brillouin zone for a lattice of cylindrical dielectric rods in air with lattice constant a: either a square lattice, where the lattice vectors differ by $90°$, or a triangular lattice, where the lattice vectors differ by $60°$ (in class we used $120°$, but you can get $60°$ just by flipping the sign of one of the lattice vectors).

(a) If you look in the MPB tutorial (http://ab-initio.mit.edu/mpb/doc/user-tutorial.html), it shows you how to compute the TM band diagrams in these two cases. Repeat these calculations, but use rods with radius $r = 0.2a$ and $\varepsilon = 8.9$ rather than the $\varepsilon = 12$ in the tutorial, and find the size of the first TM gap for both the square and triangular lattices. (See also the sq-rods.ctl and tri-rods.ctl files posted on the course web page, from the MPB examples.)

(b) Now, consider an intermediate case: a lattice of the same circular rods in air where the primitive lattice vectors both have length a but the angle between them is $75°$. Figure out what the Brillouin is zone in this case, and the irreducible Brillouin zone, and then run MPB to compute the size of the first TM gap.

Be careful about units (see the note on units in the MPB tutorial): in MPB, the $\mathbf{k}$ points are specified in the basis of the reciprocal lattice vectors. If you work out the Brillouin zone in Cartesian coordinates, you can convert to the reciprocal basis by dividing by 2π and calling the (cartesian->reciprocal (vector3 x y z)) function in MPB as described in the reference section of the manual.

Problem 2: Line-defect modes

For this problem, you should make use of the file line-defect.ctl on the course web page, which computes the bands of a line defect formed by a missing row of rods in a triangular lattice of rods.

(a) Change ε to 8.9 to match problem 1. Compute and plot the TM projected band diagram of this mode. By increasing the supercell size (which folds more and more bands in the continuum regions but leaves the defect mode unchanged), identify the continuum regions on your plot (the projection of the bands of the perfect crystal).

(b) Sketch the Brillouin zone of the triangular lattice of rods, and show how it is projected for the line defect. *Careful:* for the line defect, we have to project this onto the $\Gamma - K$ direction (the nearest-neighbor direction), but the edge of the new 1d Brillouin zone is *not* K. Where is the edge of the projected 1d Brillouin zone?

Problem 3: Meep!

For this problem, you will use the *Meep* finite-difference time-domain code, which is installed on the Athena Linux/Intel machines in the meep locker (add meep); see also the Meep manual at http://ab-initio.mit.edu/meep. As your starting point, you should use the rod-transmission.ctl example file, which is posted on the course web page, which computes the transmission spectrum of TM planewave source in the x direction through nx layers of the square-lattice rod crystal from problem 1.

(a) Compute the transmission spectrum as a function of nx, for nx=1, 2, 3, 4, 5, 6, and plot them (on a single plot). The transmission spectrum should be normalized by dividing by the transmission for nx=0 (no holes). Relate the features of this transmission spectrum to the band diagram of problem 1.

(b) Compute the *TE* transmission spectrum for nx=10 layers, and relate it to the TE band diagram (which you can compute yourself with MPB, or you can look up from the band diagram in the course notes). Careful: you need to change *three* places in the control file. (What happens to the symmetry?)

(c) Try making the pulse frequency spectrum very broad, e.g. df=2 (computing the flux in a correspondingly wide frequency range), and plotting the TM transmission spectrum; in the original range from (a), does the new transmission spectrum match what you had before?

(d) Predict analytically at what frequency ω_0 you should start to see additional diffracted orders in the reflected wave (i.e. reflected waves at angles in *addition* to the normal 0° reflection). Now, modify the simulation to use a TM *continuous-wave* (CW) source and output E_z at the end, as in the Meep tutorial, and show that there is a qualitative change in the reflected field pattern if you put in a frequency *just* below ω_0 versus a frequency *just* above ω_0. If you look *just* below ω_0, then you will have to increase the "pad" parameter in order to see an undisturbed 0° reflection pattern far from the crystal—why?