**Electron – Crystal Excitations**

Here’s the periodic table from before,

Table

Description automatically generated

I’ll talk about Si, C, and GaAs again, although our discussion is more broadly applicable than to just these guys. So the band structure of Si, C, GaAs can be calculated. Might use the tight-binding model, especially for the p-bands, since these guys are covalently bonded, and so we don’t expect the valence electrons to be roaming around too much. In the Metals/Excitations folder, we did tight-binding calculations for s and p bands of a cubic lattice, with one atom per basis (and dropped the third p-band ‘cause went to 2D for simplicity’s sake). Note that an unfilled s ‘conduction band’, corresponding to the next n-level, would lie above the green p-band, and look like the blue band.

Chart, surface chart

Description automatically generated

Si, C, and GaAs have an fcc structure with 2 atoms per basis. So their bands are expected to be different (b/c different lattice structure of course, and also we don’t expect the single particle eigenstates of the unit cell molecular Hamiltonian to necessarily resemble the single particle eigenstates of a unit cell atomic Hamiltonian). But in the plots below, you can see some similarity between the three valence bands above (one s and two p’s), and the first three valence bands of those guys below. Here’s actual result for Si, C, and GaAs.

Chart, radar chart

Description automatically generated Diagram

Description automatically generated Chart, radar chart

Description automatically generated

And the letters refer to the following points in the 1st BZ.

Chart, radar chart

Description automatically generated

Okay so can see that for each of these guys, the first four 4 bands are segregated from the 5th band. In Si, C, and GaAs, we have two atoms/basis, and four valence electrons/atom, which makes eight valence electrons/basis. And that happens to be precisely the number that the first four bands can accommodate. For visualilzation, might recall the qualitative picture we drew of GaAs bands in the Metals / Free Day / Electrons / Excitations / Tight Binding file,

A diagram of mathematical equations

Description automatically generated

So can see there is an energy gap between these 4 (valence) bands and the 5th (conduction) band. So that’s what makes these guys semiconductors/insulators, because at T = 0, we have full bands, and so no possible current. C is actually classified as an insulator because this bandgap is large ~ 5.5eV (anything over 5eV is considered insulator-ish). Si and GaAs have smaller band gaps, and so they are classified as semiconductors. But either way, note:



If the maximum of the valence band and minimum of the conduction band occur at the same spot. Then this is called a ‘direct band gap’. GaAs has a direct band gap. The max of valence band and min of conduction band occur at the center, Γ, of the bcc Brillouin zone. Otherwise, if the conduction min and valence max occur at different points, it’s called an indirect band gap, of which Si and C are exemplars. Their valence max’s occur at Γ, but the conduction min’s occur near X, the edge of the BZ face, about 80% of the way along the line Δ. And it should be noted that we’ll get the same conduction band minimum at all six of those smaller hexagonal faces.

**Density of States**

I think I’d like to calculate the density of states near a band minimum or maximum. So these band minima/maxima will frequently not be spherically symmetric, but rather ellipsoidal – meaning we’ll have an actual mass tensor to deal with. So recall from the Metals/Free Day/Electrons/Excitations/Properties file that we can approximate the energy spectrum near a minimum/maximum as:



And the density of states associated with this is:



where we change coordinates **k** → **k** + **k**0. Now let’s make another coordinate transformation. Say we find the unitary matrix which diagonalizes the inverse mass tensor **M**-1.



Given this U, let a new set of coordinates be given by ki = ΣjUijk´j, or more succinctly:



Filling this into our dispersion relation, we have:



And now let’s see how the differential volumen element changes. Well,



since the determinant of a unitary matrix is 1. So our new expression is:



Then we could change variables to k´1 = x√m1, k´2 = y√m2, k´3 = z√m3. The Jacobian of transformation would be √(m1m2m3). And we’d have:



This calculation we’ve done before in the Metals file. We found,



So replacing m with 1, ε with ε – ε0, and assuming 3D, we have:



Since |**M**-1| = m1-1m2-1m3-1, we could write this as (det and | | are synonymous):

