**Scattering**

**Photon Scattering**

We could talk about photon scattering processes. Typically, we’d be doing this in the context of shining a laser into a crystal and looking to see what light we got back out. Normally we look at a process whereby a single phonon is created or destroyed. These would be described by conservation of momentum/energy equations:

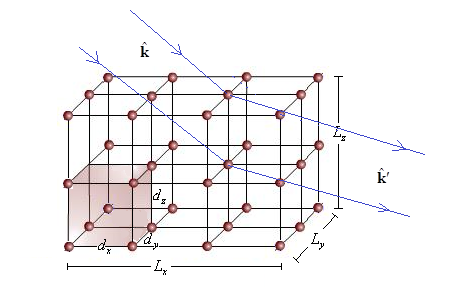
respectively. Or if we allow Umklapp processes, then,

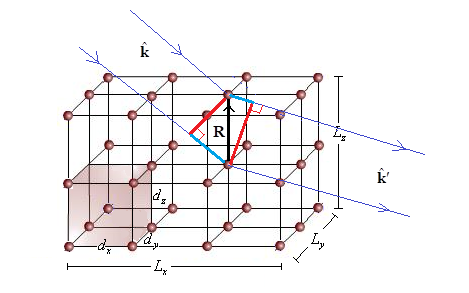
If we’re at low T’s, then both q and ωq will be small. Energy conservation then requires ωk ~ ωk´. But this means k ~ k´, and so momentum conservation means we shouldn’t have any solutions with non-zero **G**. Thus at low T’s, Umklapp processes are frozen out.

**Neutron Scattering and Crystal Structure**

One can determine the RLV’s (and from these the BLV’s) from scattering experiments. Consider sending radiation into a crystal. The radiation source (typically neutrons, as these would have wavelengths around a lattice spacing) is presumed far enough away that the incident beam is in phase and headed along direction , and presume that each molecule specularly reflects the radiation – equally in all directions (perhaps we must assume that the incoming radiation is close to a resonant frequency?). Let’s consider one particular direction ´.



Let’s work out the condition for constructive interference of these waves when they hit the detector. To do so, we must isolate the path length difference,



The difference (highlighted in bold blue) is:



And they’ll be in phase if:



In order to make a distinctive bright spot on the detector we need more than just two coherent waves. Preferably all waves scattering off the atoms/molecules would be in phase. This would require:



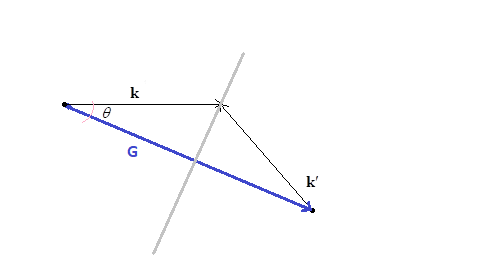
for all **R** ∈ LV, though with presumably different n’s. It suffices to make this true for all primive cell basis vectors, as all others are linear combinations of such, and so would consequently automatically satisfy our condition. Exponentiating this expression we have:



Of course it is the reciprocal lattice vectors that satisfy this equation. So we must have:



Note how this is just expresses crystal momentum conservation presuming our neutron didn’t excite any phonons, and we could’ve just started from here. For elastic scattering, as we’re presuming, **k** and **k**´ must have the same magnitude. So geometrically, our equation looks like this:



So I suppose it isn’t a given that for any given **k**, there will be a **k**´ which satisifes this equality (for some **G** in that set). We can write this another way, which tells us which incident **k** vectors will give us constructive interference scattering. For some **G**, we have **k** - **k**´ = **G**. Now **k** and **k**´ have the same magnitude, since the scattering is elastic, so



which is:



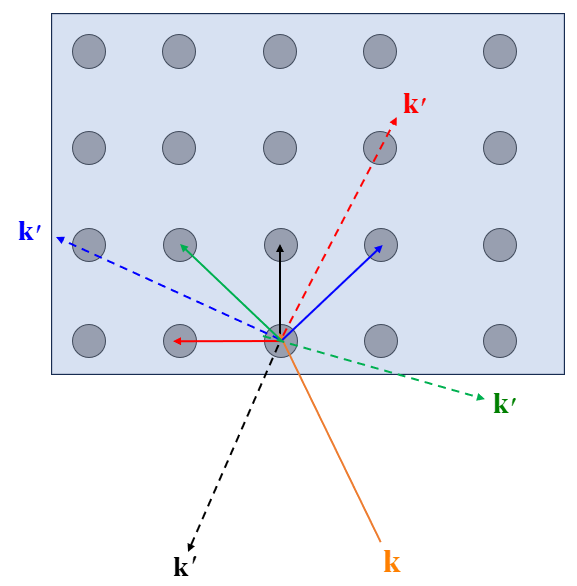
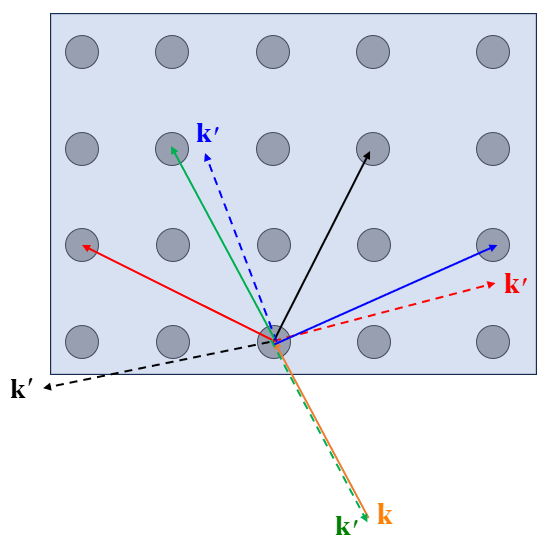
this is the Von Laue condition. It says that we only get constructive interference scattering for **k** vectors which, when projected against some **G**, are equal to G/2. And the scattered vector, **k**´, will be the vector reflected about **G**. Can see this directly from the geometrical picture above. Now let’s write this another way, and get the Bragg condition. So consider that angle θ. We have:



where **G**smallest is the smallest RLV parallel to **G**. Let this be called Gsmallest = 2π/d. And let k = 2π/λ. Then we can write:

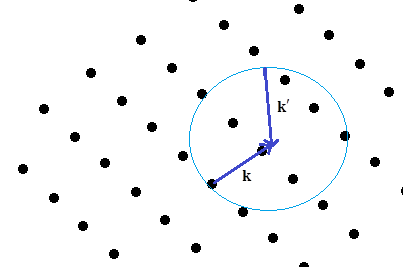


This is the Bragg scattering condition. So basically, for every reciprocal lattice vector **G** = n1**b**1 + n2**b**2 + n3**b**3, there is a smallest vector, **G**smallest pointing in the same direction (basically have to find all common factors of n1, n2, n3, and take them out). Or another way to think about it is that {**G**smallest} is the set of **G** = n1**b**1 + n2**b**2 + n3**b**3, where the n1,2,3 have no common factors. This Gsmallest is usually written as: **G**smallest = h**b**1 + k**b**2 + ℓ**b**3, or just (h,k,ℓ) for short, where h, k, ℓ are called the *Miller Indices*. As just discussed, h, k, and ℓ must have no common factors. Anyway, the Bragg condition tells us the angles that **k** will reflect about that RLV. And remember this reflection will be in the plane formed by the incident vector **k**, and **G**smallest. Below I drew a couple Gsmallest RLV’s in black, green, red and blue. I drew the incident **k** wave in orange, and a possible reflected wave **k**´ about the RLV as a dotted arrow in the same color as the RLV. Note that on the left, RLV’s are, using Miller Indices for our 2D lattice: black = (0,1), red = (-1,0), green = (-1,1), blue = (1,1). And on the right, we have: black = (1,2), red = (-2,1), green = (-1,2), and blue = (2,1).

Now if, say, the incident ray happens to be at a magic angle for one of those RLV’s so that we get Bragg reflection, it isn’t likely that it would also be at a magic incident angle w/r to any of the others, to also get Bragg reflection from one of them. So I’d think we’d be getting Bragg reflection from basically one **G**smallest at a time? Or just a few? Another thing is, if we are likely to get Bragg reflection from the first set of {**G**smallest} (the ones on the left), we are less and less likely to get Bragg reflection from the larger {**G**smallest} (the ones on the right, and others even larger, not displayed). This is because our d = 2π/Gsmallest, and the larger Gsmallest is, the smaller d is, and at some point d will be too small for there to be solutions to the Bragg equation. So even though there are technically probably millions of **G**smallest candidates, only the very smallest will be able to accommodate solutions to the Bragg equation.

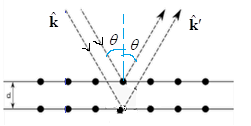
I guess the easiest way to get the reciprocal lattice is by the Ewald construction.



You start with a given small **k** (it looks like **k** is lying on a RLV point, but it’s not meant to be per se´) and then rotate your detector to pick up all, if any, **k**´. Then you increase **k** a little and do it again. With the **k**´, you have **k**-**k**´, and so the **G**’s.Then you can work out the **G**primitive’s, and thence, **R**primitives.

**Example**

Let us have two incident plane waves, making angle θ with the plane. And suppose they exit at the same angle, reflecting, so to speak, off the two planes (angle θ is the angle w/r to the normal, not the more typical angle w/r to the plane).



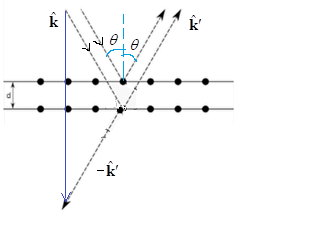
Then of course the path length difference between them must be equal to nλ in order to get constructive interference, as we asserted above. And equivalently, we require



The difference of the two vectors lies in the direction perpendicular to the planes. The reciprocal lattice basis vector in this direction is (2π/d)(letting the normal vector point along the z-direction). And so we must have:



The difference of the two vectors is illustrated below:



Using law of cosines, say, to get the magnitude of the difference, we have:



and this reduces to:



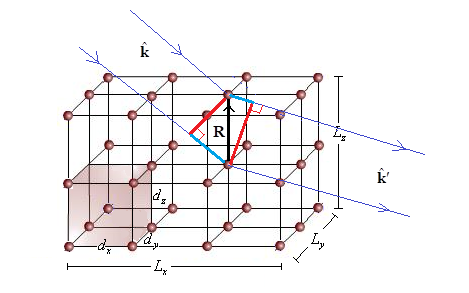
just as the Bragg condition says it must. If we solve for θ, we’d have:



This formula tells us that if λ << d, then there would be lots of angles at which we’d get constructive interference – too many to resolve if λ << d in the extreme. On the other hand, if λ >> d, then we may fail to get any angles – because nλ/2d > 1 for all n, and so we’d get no angles with constructive interference. This illustrates the fact that we need to use λ ~ d if we are to practically probe the structure of the crystal.

**Scattering in a Lattice with a Basis**

In order to add in a basis, it’s easiest to go back to the beginning and look at it a different way. So we revisit our lattice and look at the two incoming and exiting waves.



Now let’s write down an expression for the scattered electric field of these two waves. This would be something like,



The phase difference φR of the top wave is the basically the amount of phase that it has/or doesn’t have, relative to the bottom wave. We can see this is φR = **k**∙**R**. So we can write,



Now let’s put all the waves, coming from all the atoms, together,



This guy in parentheses is called the structure factor (well, sometimes |S(q)|2 = S(q)S(-q) is called the structure factor instead),



So we can write,



We will get constructive interference when we have:



and this ill happen if,



for all **R**, which would happen if,



as we found before. And so we have recovered our earlier result, and all that follows from it. Now if we have a basis, we would amend our result for **E**, to include as well, a sum over all position vectors within the basis, **d**j. But not only this. Each different atom in the basis will reradiate the field with a different amplitude. We have to account for this by putting in a so-called form factor *f(j), which depends on the identity of the atom, but not the atom’s location.*



Defining the structure factor again, now accounting for the extra atoms in the basis,



we have, again:



Considering SR(q) by itself for the moment, we can say that we’ll recover all of our old results for **k** and **k**´. Adding Sd(q) back into the mix, we see that if the pair **k** and **k**´ is such as to make Sd(**k**-**k**´) = 0, then that pair will be disallowed. How can we tell if a pair that we solve for from the Bragg condition will be one for which Sd = 0? Well, we will know **G**smallest = h**b**1 + k**b**2 + ℓ**b**3 by presumption. And **G** will just be **G** = n**G**smallest. And **k** - **k**´ = **G**. So basically, the nth order result is eliminated if Sd(n**G**smallest) = 0.

**Example**

Consider a crystal of CsCl with a simple cubic lattice that has a unit cell of a = 4.12A˚ .  
A beam of electrons of energy E=128 eV is incident on the crystal. At what angles will there be Bragg reflection, perpendicular to the planes **G**smallest = (0,1,1)? Assume for the sake of discussion that the form factors of the two atoms are identical, so f(Cs) = f(Cl) = 1.

CsCl is a simple cubic lattice, with a basis. The Cesium atom sits in the middle of the cube. If the basis vectors are,



then since **G**smallest = (0,1,1), we have:



which points at a 45o angle in the y-z plane. This gives us an effective d of a/√2. So now the Bragg condition yields,



Let’s get λ,



So, for n = 1, 2, 3, 4, 5, we have:



Now not all of these will be allowed, possibly. So we have to work out Sd(q). So the basis consists of a Choride atom at the origin, and a Cesium atom in the middle of the cube. So Sd is:



Now gotta work out,



Since this doesn’t equal 0 for any n, none of the reflections we found are disallowed.

**Intensity of Radiation**

The radiation intensity is proportional to the structure factor squared,



Filling in our result for S,



So,



**Example**

Barium Titanate, BaTiO3, crystalizes in a simple cubic Bravais lattice structure. The basis consists of one Ba atom at (0,0,0), one Ti atom at (1,1,1)a/2, and three O atoms at (1,0,1)a/2, (0,1,1)a/2, and (1,1,0)a/2, where a is the lattice constant. Given that the form factors of the atoms are fBa = 7fO, and fTi = 3fO, determine the intensity relationship between the first four Bragg reflections, I(200): I(111): I(110): I(100).

Well we’ll recall:



Constructive interference will give us that SR(k´-k) = N (since e-i(**k**´-**k**)∙**R** = 1). So,



What is Sd(q)?



Okay, so:



and,



and,



and finally,



So the ratio of intensities is:

