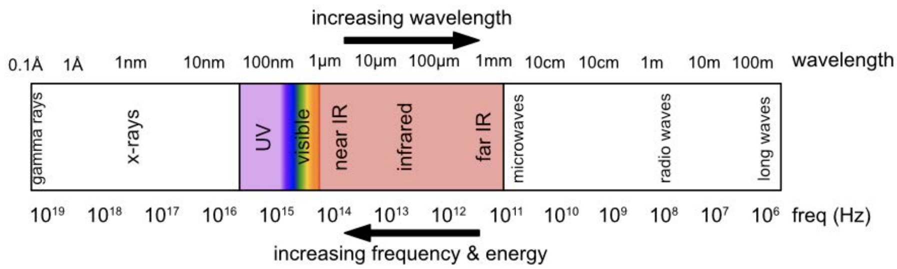
1 X-ray generation

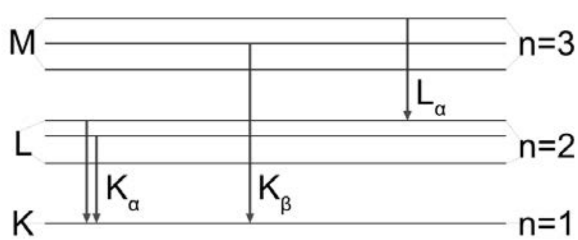
X-rays are a form of high-energy electromagnetic radiation. We have talked about ways to generate EM



radiation before: think back to semiconductors. The visible light emitted from LEDs has energy on the order of a few eVs. X-rays are much more energetic! They can range from hundreds to hundreds of thousands of eVs. Therefore, to generate x-rays, we need a much higher energy differential than the band gap of even an insulator.

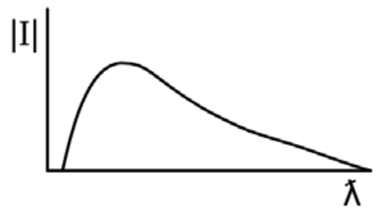
To achieve such a massive ΔE, we turn to another old friend: interatomic transitions! When we first went quantum, we talked about Bohr's model of quantization in the hydrogen atom. Though the Bohr model really only applies to the hydrogen atom, atoms with higher Z are roughly proportional to the Bohr model prediction by a factor of $(Z-1)^2$. Though the ionization energy of hydrogen was only 13.1 eV, with the intra-atomic energy transitions even lower in energy, larger elements can have energy states separated by massive amounts of energy: enough to produce x-rays.

To actually generate x-rays, we need to excite an electron between two atomic energy levels within an atom. For historical reasons, the atomic transitions that produce x-rays are denoted in Siegbahn notation: the familiar our n=1, n=2, and n=3 shells are called K, L, and M, respectively.



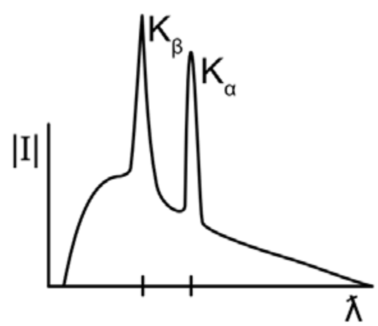
The x-rays that are emitted are named by a letter with a subscript: the letter tells us which shell the electron *ended* in, and the subscript tells us which shell the electron *started* in. For example, K_α radiation ends in the K shell (n=1), and the α tells us it started one shell higher, in the n=2, or L shell. Similarly, K_β ends in the n=1 shell, but comes from two shells up (β), or the M shell. Don't worry about the subshells; we'll just focus on transitions between principal energy levels. These x-rays are called characteristic x-rays, because their character (properties) are atom-specific.

Finally, we need to consider how this energy transition is excited. This is done with high energy electrons: the electrons are accelerated by applying high voltages. When they crash into a heavy element, x-rays are produced (if the electrons are energetic enough). The act of high-energy electrons colliding into a solid is enough to produce some x-rays: these are called Bremsstrahlung.



When the electrons collide with the solid target, they rapidly decelerate as they interact with the charged nuclei. Above all else, energy must be conserved: the excess kinetic energy dissipated through deceleration is emitted as a photon. These photons have a continuous spectrum, as shown in the plot above. However, there is a hard lower bound on the wavelength that can be emitted: since energy and wavelength are inversely proportional, this lower bound is determined by the energy of the incoming electrons (you can also think of it as an upper bound on energy/frequency).

In addition to the Bremsstrahlung, characteristic x-rays are emitted. They show up at specific wavelengths in the x-ray spectrum. We can determine which intraatomic transition the peaks correspond to by referencing the diagram above, and recalling that the energy levels get closer together as n increases.



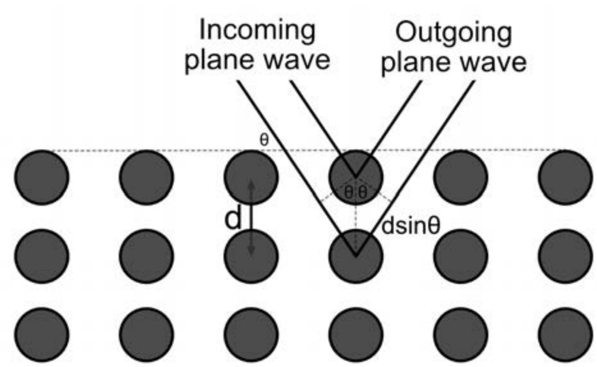
The K_β transition is larger in energy than K_α, so it occurs at a lower wavelength. The L_α would be the lowest energy (highest wavelength) of the three, and would appear to the right on this plot.

2 Diffraction and Bragg's law

Next time we'll talk about what we can do with x-rays, but for now, we need to brush up on Bragg's law. The basic idea is that when light that is incident on a periodic structure satisfies the *Bragg condition*, it scatters coherently. The Bragg condition gives the angle at which coherent scattering occurs as a function of the wavelength of the incident light and the periodicity of the lattice:

$$n\lambda = 2dsin\theta$$

This equation is the condition for constructive interference, and n is an integer (n=1 dominates for most lattices), λ is the wavelength of the x-rays, θ is an experimental knob, and d is the interplanar spacing, d_{hkl}.



From the figure above, we can see that when the Bragg condition is fulfilled, what is actually happening is that the extra path length traveled by neighboring photons that scatter coherently is exactly $dsin\theta$ as it comes in and again as it comes out. Therefore the incoming and outgoing waves constructively interfere, and light registers as bouncing off the crystal.