

Crystals, Symmetry and Tensors
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Lecture 5b

Length of G^*_{hkl} is reciprocal of interplanar spacing (d_{hkl})


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Reciprocal Lattice

$$L^* = \{ \vec{g}^* = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \mid h, k, l \in \mathbb{Z} \}$$

$\vec{g}^*_{hkl} \perp (hkl)$

reciprocal lattice vector with components h, k, l real plane with Miller indices h, k, l .




$$|\vec{g}^*| = \frac{1}{d_{hkl}}$$

Definition of d_{hkl} (Interplanar spacing d_{hkl})

Construct planes with intercepts

$n\left(\frac{a}{h}\right) \quad n\left(\frac{b}{k}\right) \quad n\left(\frac{c}{l}\right)$

These planes define a set of parallel (hkl) planes.
 The spacing between any two successive planes of this family is d_{hkl} .



So, in the last lecture we have seen an important property an interesting property of reciprocal lattice that the reciprocal lattice vector $h k l$ or $g^*_{h k l}$ as I have denoted it here is perpendicular to the plane the real lattice plane $h k l$. Now, today we will derive another interesting relationship that is the length of the reciprocal lattice vector is reciprocal of the inter

planar spacing of the $h k l$ plane. So, $d_{h k l}$ is the symbol for interplanar spacing and that also requires a definition the careful definition is not so obvious what is $d_{h k l}$ and sometimes it is left little undefined but we should define it precisely.

So, the way we will define $d_{h k l}$ is to construct planes given any $h k l$ we will construct planes with intercept n times a by h n times b by k and n times c by l $h k l$ r number $a b$ and c are length n is again an integer. So, all these are three lengths what you are having is three lengths which will vary as you will vary n . So, for n is equal to one you will have a by h b by k and c by l as intercepts and considering these as three intercepts you get a plane the next plane for n is equal to two comes at two a by h two b by k two c by l similarly three a by h three b by k three c by l .

So, you let n vary over all integers. So, n , n varies over integers that is n can be anything from minus infinity minus 2, minus 1, 0, 1, 2 and so on these are now periodically spaced planes because first plane is making intercept a by h on the x axis the next plane is making an intercept two a by h the next plane is making an intercept three a by h . So, on the x axis you can see they are going in a periodic way and same with Y and Z axis. So, in the space also they are periodically spaced with a fixed spacing that fixed spacing is what we are defining as the $d_{h k l}$ of this set of planes.

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the spacing between any two successive planes of this family is d_{hkl} .

In particular,

$n = 1$	$\frac{a}{h}$	$\frac{b}{k}$	$\frac{c}{l}$
intercepts			
$n = 0$	0	0	0

The diagram shows a 3D Cartesian coordinate system with x, y, and z axes. A plane is drawn in the first octant, intersecting the x-axis at a/h, the y-axis at b/k, and the z-axis at c/l. A normal vector is shown perpendicular to the plane. The distance between two parallel planes is labeled as d_hkl.

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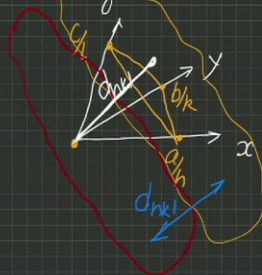
So, spacing between any two successive planes is the $d_{h k l}$. So, let us say for n is equal to 1 we have the spacing a by h , b by k , c by l intercepts not a spacing intercepts. So, if I have my axis all

I have to do is to make a plane with x axis intercept as a by h, y axis intercept as b by k and z axis intercept as c by l. So, I get a plane notice that this is only a piece of plane when we say plane actually you have to extend this in your imagination this is only part of the plane intercepted by the three axes. So, the plane is actually extended into Infinity of which this triangle is only a part.

Now, if I take n is equal to 0 you will get all three intercepts as 0. So, that means that plane will be passing through origin and we will draw that plane passing through origin but parallel to this original plane. So, which means now these two planes are spaced by some distance and that distance is what we will call the d spacing.

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$n = 1$			
intercepts	$\frac{a}{h}$	$\frac{b}{k}$	$\frac{c}{l}$
$n = 0$	0	0	0



d_{hkl} = distance from origin of the plane with intercepts $\frac{a}{h}$, $\frac{b}{k}$ and $\frac{c}{l}$.

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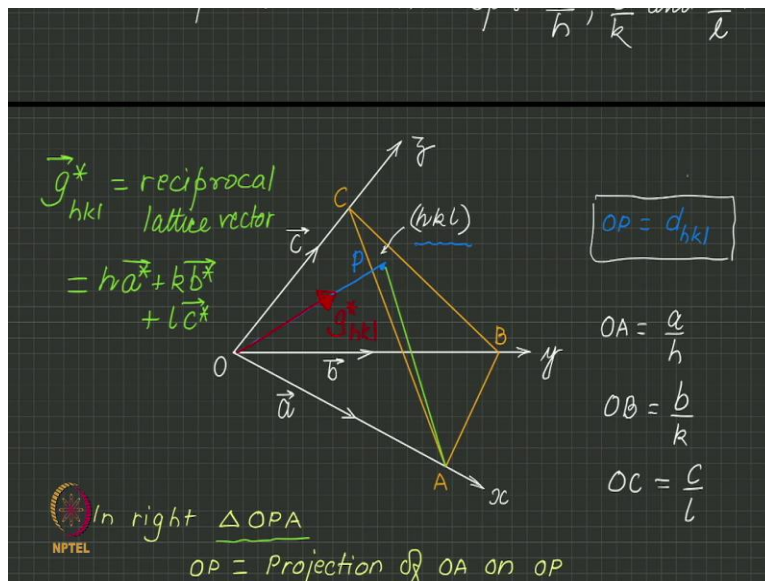
Reciprocal Lattice

$$L^* = \{ \vec{g}^* = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \mid h, k, l \in \mathbb{Z} \}$$

$\vec{g}_{hkl}^* \perp (hkl)$

reciprocal lattice vector with components h, k, l

real plane with Miller indices h, k, l .



So, we can also say that d spacing is distance from origin of the plane with intercepts a by h, b by k and c by l this will become because the distance between this plane, this plane and this plane since the red plane is passing through origin you can drop a perpendicular from the origin onto this plane that will also be same d_{hkl} .

So, now let us try to establish that relationship the relation between relation between g_{hkl}^* the reciprocal lattice vector hkl and the plane hkl . So, let us drop a perpendicular OP we are draw dropping OP a perpendicular on the plane abc plane abc is my hkl plane which means o a is hkl plane.

So, from what we have said OA the first intercept is a by h OB the second intercept is b by k and OC the third intercept is c by l that is the meaning that is the definition of Miller indices that is the meaning of hkl plane. So, we get these three intercepts and we drop a perpendicular by very definition of what we said about d_{hkl} the length OP is d_{hkl} and from what we have proved the earlier relation between g_{hkl} and the plane we know that g_{hkl} is normal to the plane. So, which means g_{hkl} is also in the direction OP .

So, g_{hkl} is in the same direction from the previous previously established relation the g_{hkl} is perpendicular to hkl OP is perpendicular to hkl . So, g_{hkl} is parallel to OP now let us join P with A , let us join P with A this green line PA and consider the triangle OPA sorry g_{hkl} is the reciprocal lattice vector which means hkl are components with respect to the reciprocal basis. So, that means it is a vector with h as it is first component with respect to a star. So, it is $h a^*$ similarly k is the second component with respect to b^* and l is the third component with respect to c^* .

So, we are showing only $a^* b^* c^*$ we are not showing you $a^* b^* c^*$ that will make my drawing too complicated but we are assuming that $a^* b^* c^*$ has been calculated and they are also existing somewhere in this space and now I am going h times a^* , k times b^* and l times c^* , if I do that then from the relationship we if the first relationship which we established last time that g_{hkl} is supposed to be perpendicular to the plane and that is why I am confident to draw my g_{hkl} vector also along OP because I said OP is perpendicular to the plane g_{hkl} is perpendicular to the plane. So, g_{hkl} is parallel to OP .

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hkl lattice vector
 $= h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

$OP = d_{hkl}$

$OA = \frac{a}{h}$
 $OB = \frac{b}{k}$
 $OC = \frac{c}{l}$

In right $\triangle OPA$
 $OP = \text{Projection of } OA \text{ on } OP$
 $= \vec{OA} \cdot \hat{n}$

$d_{hkl} =$

In right $\triangle OPA$
 $OP = \text{Projection of } OA \text{ on } OP$
 $= \vec{OA} \cdot \hat{n}$ ← unit vector along OP

$d_{hkl} = \frac{\vec{a}}{h} \cdot \frac{\vec{g}_{hkl}^*}{|\vec{g}_{hkl}^*|}$
 $= \frac{\vec{a}}{h} \cdot \frac{1}{|\vec{g}_{hkl}^*|} (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$
 $= \frac{1}{h|\vec{g}_{hkl}^*|} h(\vec{a} \cdot \vec{a}^* + k\vec{a} \cdot \vec{b}^* + l\vec{a} \cdot \vec{c}^*)$

Then g^*_{hkl} is in the same direction as OP . So, now since OP is perpendicular to PA . So, we have this as our right angle this is our right angle. So, you can say that OP is projection of OA on OP in this direction in the normal direction. So, OA is being projected because if you draw this triangle let us say we draw it like this we are going to P this is OA and this is AP and the angle APO is 90 degree because in this orientation sometimes it is little disturbing to see we usually like to draw it this way.

So, you can see that OP is projection of OA in the Triangle in the right triangle AOP in right triangle each of the either the base or perpendicular both of them are projection of the

hypotenuse because you go by perpendicular lines. So, OP is projection of OA on OP. Now, projection how can you write in terms of the vector, yeah dot product of OA with unit vector along that direction. So, unit vector along g^*_{hkl} . So, $OA \cdot n$ where n is the unit vector along OP. So, which means this is O now OA, OA is what vector, OA length is a by h . So, vector is vector a by h .

So, OA is a by h and n we can write in terms of because we know one vector along that direction that is g^*_{hkl} . So, we can write this as g^*_{hkl} divided by the magnitude of g^*_{hkl} that is the unit vector n . You happy with this? Now, g^*_{hkl} as I defined is nothing but $h a^* + k b^* + l c^*$. So, now this is a dot product here. So, we can take a , a dot inside. So, we have $h a \cdot a^* + k a \cdot b^* + l a \cdot c^*$. Now, what is $a \cdot b^*$ that is 0 $a \cdot c^*$ 0 and $a \cdot a^* = 1$.

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$$\begin{aligned}
 &= \frac{\vec{a}}{h} \cdot \frac{1}{|g^*_{hkl}|} (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \\
 &= \frac{1}{h|g^*_{hkl}|} h(\vec{a} \cdot \vec{a}^* + k\vec{a} \cdot \vec{b}^* + l\vec{a} \cdot \vec{c}^*) \\
 &= \frac{1}{h|g^*_{hkl}|} (h \cdot 1)
 \end{aligned}$$

$$\boxed{d_{hkl} = \frac{1}{|g^*_{hkl}|}} \Rightarrow \boxed{|g^*_{hkl}| = \frac{1}{d_{hkl}}}$$

Units of reciprocal lattice vectors
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So, you get the very interesting result h into 1 the numerator and the denominator h cancel. So, you get d_{hkl} as 1 by g^*_{hkl} or if you want to write it in terms of g^*_{hkl} . So, length of this is what we wanted to prove length of g^*_{hkl} is nothing but just 1 by d_{hkl} . So, this actually gives you a formulation also of finding d_{hkl} if you have to determine d_{hkl} of any plane in any Crystal you should look for the corresponding reciprocal lattice vector and find its length that is the easiest way easiest mathematical way.

Otherwise if you try to actually draw the plane and do the geometry you can do without reciprocal lattice because the plane is in real space and we have already drawn the plane and we have dropped the perpendicular from the origin you can always do sufficient geometry to find the distance of that plane from the origin to get your d_{hkl} in real space itself but that is going to be a little bit more challenging if you actually try to do that than finding algebraically the length of reciprocal lattice vector.

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$$= \frac{1}{|\vec{g}_{hkl}^*|} \cdot (h \cdot k \cdot l)$$

$$\boxed{d_{hkl} = \frac{1}{|\vec{g}_{hkl}^*|}} \Rightarrow \boxed{|\vec{g}_{hkl}^*| = \frac{1}{d_{hkl}}}$$

Units of reciprocal lattice vectors

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V_p} = \frac{\text{\AA} \cdot \text{\AA}}{\text{\AA}^3} = \frac{1}{\text{\AA}^2}$$

So, the unit of reciprocal lattice vector as you have seen the very definition that a star was b cross c by the volume of the unit cell. So, if you think in terms of angstrom as the unit of b and c . So, you have angstrom into angstrom by the volume is in angstrom cube. So, you have 1 by angstrom. So, you can see that the reciprocal lattice vectors will have length which is 1 by angstrom or 1 by meter that is one of the justification of using the word reciprocal and we will keep seeing that there are many other justification for the word reciprocal just now we saw now the d_{hkl} of real space is reciprocal of g_{hkl}^* .