CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES
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Lecture 09(B): Weiss Zone Law

In this lecture, I'm going to discuss a rule known as the Weiss zone law. Let me begin with a cubic unit cell. Suppose we have a (hkl) plane and a [u v w] direction that lies within this plane. As we saw in the previous lecture, for the direction [u v w] to lie in the plane, its dot product with the plane normal must be zero.

From the earlier discussion, we know that the normal to the (hkl) plane is simply the direction with indices [h k l]. This means the vector [u v w] dotted with [h k l] must equal zero. Taking their dot product just involves multiplying the corresponding components, giving us:

$$hu + kv + lw = 0$$

Although I demonstrated this using a cubic unit cell, this relationship is actually quite general and holds for other unit cells as well. My goal now is to derive this expression in a more general way, rather than relying on the special case of the cubic lattice.

So, let's consider an arbitrary (hkl) plane in any unit cell. The intercepts of this plane will again be $\frac{a}{h}$ on the x-axis, $\frac{b}{k}$ on the y-axis, and $\frac{c}{l}$ on the z-axis.

Now, let's take two vectors that lie in the plane ABC, specifically, the vectors $\overline{AB}$ and $\overline{AC}$. We'll start by writing their expressions.

For the vector $\overline{AB}$, we can break it into two segments: $\overline{AO}$ and $\overline{OB}$. Starting at point A, we move to the origin O using a vector $\overline{AO}$, and then travel from O to B using a vector $\overline{OB}$. So,

$$\overline{AB} = \overline{AO} + \overline{OB}$$

From earlier discussions, we know how to express these in terms of the unit cell vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$. Therefore,

$$\overline{AB} = \frac{\bar{b}}{k} - \frac{\bar{a}}{h}$$

Next, let's write the vector $\overline{AC}$. Again, we go from A to O using $\overline{AO}$ (which is the same as $-\overline{OA}$) and then from O to C using $\overline{OC}$. So,

$$\overline{AC} = \overline{AO} + \overline{OC} = \frac{\bar{c}}{l} - \frac{\bar{a}}{h}$$

Now, consider another direction lying in the same plane ABC, with Miller indices [uvw]. Let's represent this direction as a vector r. We can write r in terms of the unit cell vectors as:

$$r = u\bar{a} + v\bar{b} + w\bar{c}$$

Now, consider the three vectors $\overline{AB}$, $\overline{AC}$, and r. If we take their *Triple scalar product*, it can be written as:

$$r.(\overline{AB} \times \overline{AC})$$

Here, $\overline{AB} \times \overline{AC}$ gives a vector that is perpendicular to the plane ABC. Since r also lies in that same plane, it must be perpendicular to this cross-product vector. Therefore, the dot product between r and $\overline{AB} \times \overline{AC}$ must be zero.

This condition implies that the three vectors can be written in a linear combination that sums to zero. In other words, we can write:

$$s \cdot \overline{AB} + t \cdot \overline{AC} + z \cdot r = 0$$

for some scalar constants $s,\ t,$ and z.

Rearranging the terms and dividing by z, we get:

$$r = p\,\overline{AB} + q\,\overline{AC}$$

where $p =- \frac{s}{z}$ and $q =- \frac{t}{z}$.

So, effectively, the vector r can be expressed as a linear combination of the vectors $\overline{AB}$ and $\overline{AC}$.

Now, let's go one step further. We will substitute the expressions for $\overline{AB}$ and $\overline{AC}$ written in terms of the unit cell vectors $\overline{a},\ \overline{b},\ \overline{c}$ into the equation for the vector r.

First, write **r** explicitly as:

$$r = u\overline{a} + v\overline{b} + w\overline{c}$$

Now substitute the expressions for the vectors $\overline{AB}$ and $\overline{AC}$ on the right-hand side.
Using the forms established earlier:

$$\overline{AB} = \frac{\overline{b}}{k} \cdot \overline{b} - \frac{\overline{a}}{h} \cdot \overline{a}$$

$$\overline{AC} = \frac{\overline{c}}{l} \cdot \overline{c} - \frac{\overline{a}}{h} \cdot \overline{a}$$

Substituting these into
$r = p\,\overline{AB} + q\,\overline{AC}$,
 we get:

$$r =- p\frac{\overline{a}}{h} \cdot \overline{a} + p\frac{\overline{b}}{k} \cdot \overline{b} - q\frac{\overline{a}}{h} \cdot \overline{a} + q\frac{\overline{c}}{l} \cdot \overline{c}$$

Now, collect like terms. The coefficients of $\overline{a},\ \overline{b},$ and $\overline{c}$ become:

- For $\bar{a}$: $\dfrac{-p-q}{h}$

- For $\bar{b}$: $\dfrac{p}{k}$

- For $\bar{c}$: $\dfrac{q}{l}$

So we can rewrite the right-hand side as:

$$r = \frac{-p-q}{h}\,\bar{a} + \frac{p}{k}\,\bar{b} + \frac{q}{l}\,\bar{c}$$

But we already wrote:

$$r = u\bar{a} + v\bar{b} + w\bar{c}$$

Comparing the coefficients of the basis vectors $\bar{a},\ \bar{b},\ \bar{c}$ we obtain:

- $u = \dfrac{-p-q}{h}$

- $v = \dfrac{p}{k}$

- $w = \dfrac{q}{l}$

Now evaluate the expression $hu + kv + lw$ by substituting these values of $u,\ v,$ and w:

$$hu + kv + lw = h\left(\frac{-p-q}{h}\right) + k\left(\frac{p}{k}\right) + l\left(\frac{q}{l}\right)$$

This simplifies to: $-p - q + p + q = 0$

So the result is zero, and importantly, nowhere did we assume any specific crystal system. Thus, the result is fully general, applicable to any unit cell.

Therefore, we have the general relation, $hu + kv + lw = 0$

which holds for any unit cell (the lattice vectors a, b, c and the interaxial angles α, β, γ may be arbitrary). This relation is known as the Weiss zone law.

As an application, we can use this law to find a common direction (the line of intersection) of two planes. For example, consider the planes $(1\,1\,1)$ and $(1\,1\,\bar{2})$. Let $[u\,v\,w]$ denote the common direction; then $[u\,v\,w]$ must lie in both planes and therefore satisfy the Weiss condition for each plane.

For $(1\,1\,1)$: $1 \cdot u + 1 \cdot v + 1 \cdot w = 0 \Rightarrow u + v + w = 0$

For $(1\,1,\bar{2})$: $1 \cdot u + 1 \cdot v - 2 \cdot w = 0 \Rightarrow u + v - 2w = 0$

Let's call these Equation 1 and Equation 2.

Subtracting the second equation from the first gives

$u + v + w - (u + v - 2w) = 0 \Rightarrow 3w = 0 \Rightarrow w = 0$

Next, multiply equation (1) by 2 and add it to equation (2). Multiplying (1) by 2 gives $2u + 2v + 2w = 0$. Adding equation (2) (which is $u + v - 2w = 0$) causes the w-terms to cancel, yielding $3u + 3v = 0$.

This implies $u =- v$. Therefore the indices are $[u\bar{u}0]$. Dividing through by u gives the common direction as $[1\,\bar{1}\,0]$. Of course, since we already found $w = 0$, we could have substituted directly into either equation to get $u =- v$ without the extra multiplication step.

WEISS ZONE LAW

Cubic unit cell

(hkl) and [uvw] in the plane (hkl)

Normal to (hkl) → [hkl]

$\Rightarrow [uvw].[hkl] = 0$

$\Rightarrow \boxed{hu + kv + lw = 0}$

General Expression
valid for other unit cells

$\overline{AB} = \overline{AO} + \overline{OB} = \dfrac{\overline{b}}{k} - \dfrac{\overline{a}}{h}$

$\overline{AC} = \overline{AO} + \overline{OC} = \dfrac{\overline{c}}{l} - \dfrac{\overline{a}}{h}$

$\overline{r} = u\overline{a} + v\overline{b} + w\overline{c}$

Triple Scalar Product:

$\overline{r}.(\overline{AB} \times \overline{AC}) = 0$

$\Downarrow$

$s.\overline{AB} + t.\overline{AC} + z\overline{r} = 0$

$\Downarrow$

$\overline{r} = p\,\overline{AB} + q\,\overline{AC}$

$\hookrightarrow$ Linear Combination
of $\overline{AB}$ and $\overline{AC}$

$\overline{r} = u\overline{a} + v\overline{b} + w\overline{c}$

$= p\left(\dfrac{\overline{b}}{k} - \dfrac{\overline{a}}{h}\right) + q\left(\dfrac{\overline{c}}{l} - \dfrac{\overline{a}}{h}\right)$

$= \underbrace{-\left(\dfrac{(b+q)}{h}\right)\overline{a}}_{u} + \underbrace{\dfrac{p}{k}\,\overline{b}}_{v} + \underbrace{\dfrac{q}{l}\,\overline{c}}_{w}$

$u = \dfrac{-p+q}{h}; v = \dfrac{p}{k}; w = \dfrac{q}{l}$

$hu + kv + lw$

$= -p - q + p + q = 0$

$\boxed{hu + kv + lw = 0}$

Find a common direction
between two planes

Ex (111) and (11$\overline{2}$) planes

[uvw] be the common
direction

(111): $u + v + w = 0$ ①

(11$\overline{2}$): $u + v - 2w = 0$ ②

Subtract ② from ①:

$3w = 0 \Rightarrow w = 0$

Multiply ① by 2 and add to Eq②

$3u + 3v = 0 \Rightarrow u = -v$

$[u \overline{u} \ 0] \equiv [1\overline{1}0]$

Now let us look at this geometrically. The planes are (1 1 1) and (1 1 $\overline{2}$), and the common direction is [$u\ v\ w$]. To draw this in a unit cell (in an arbitrary cell), first mark the axes **a, b,** and **c**. The (1 1 1) plane would be drawn so that it intersects the **a, b,** and **c** axes at $\frac{a}{1}, \frac{b}{1}, \frac{c}{1}$, respectively.

So, its intersections are 1 along x, 1 along y, and 1 along z in fractional coordinates. Now consider the plane (1 1 $\overline{2}$). Instead of drawing (1 1 $\overline{2}$), let me negate all the indices and consider ($\overline{1}\,\overline{1}$ 2). Using the Miller-index definition (take reciprocals), the intercepts become -1 along x, −1 along y, and $\frac{1}{2}$ along z.

I can change the origin so that this new origin gives axes **a,b,c** as shown. The intersection at −1 along the **a**-axis is here, the intersection at −1 along the **b**-axis is here, and the ($\bar{1}\,\bar{1}\,2$) plane then appears like this in the figure, while (1 1 1) is the other plane.

In this same figure it is clear that the common direction is along the face diagonal. If I shift the origin (for example, move the origin to this lower corner), the intercepts become 1 along **a**, −1 along **b**, and 0 along **c**, so the common direction becomes [1 $\bar{1}$ 0], which is the same result obtained earlier.

Thus, negating the indices gives the same plane; alternatively, if I keep the indices as (1 1 $\bar{2}$) I can shift the origin appropriately and represent the same geometry.

So, this plane intersects at 1 along the x-axis, 1 along the y-axis, and $-\frac{1}{2}$ along the z-axis, giving the plane shown. Remember, the two planes are not different; they belong to the same set of parallel planes.

Now, what is the intersection (common direction) of the planes (1 1 $\bar{2}$) and (1 1 1)? In the figure, there is a point on the left face and another on the rear face; if I draw a vector between them (shown in a different color), call it r. Careful inspection shows that r is parallel to [$\bar{1}$ 1 0], and hence its Miller indices are equivalent to that direction. Depending on how I draw or orient the vector, the same direction may also be written as [1 $\bar{1}$ 0].

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