Chapter 1

Lecture 1a: Introduction

- https://ocw.mit.edu/courses/materials-science-and-engineering/3-60-symmetry-structure-and-tensor-properties-of-materials-fall-2005/
- I'm reading this so I can gain intuition for semidirect products of crystallographic groups, stress-energy tensors, and tensegrity.
- In the early part of the term, we're going to use plain old geometry.
- Halfway through, we'll switch to linear algebra and eigenvalue problems. The first half of the course is one long process of synthesis.
- "It will blossom like an elegant filigreed structure".
- Textbook: Martin J Burger: "Elementary crystallography". Out of print for 15 years!
- "International tables for X-ray crystallography": Published by international union for crystallography. Volume I is symmetry tables. Everything we will derive is tabulated here.

1.1 Syllabus: Whirlwind tour

Crystallography is divided into X-ray crystallography and optical crystallography. Optical crystallography studies crystals using polarized light. We're going to be talking about geometrical crystallography / symmetry theory. This is the first month and a half.

A thing in a pattern is called as a motif.

A **translation** is given by a vector, has magnitude and direction, but no origin. We can think of it as a rubber stamp. Rather, we think of operations that act on all of space.

Definition 1. An object or a space possesses symmetry when there is an operation or a set of operations that maps it into congruence wit itself.

For **rotation**, we need to know the point about which the rotation takes place, call it A, which is the location of the axis. Then, we need to know the angle, which will denote with a subscript θ. So the full notation for a rotation is A_θ.

For **reflection**, we use the symbol M for mirror.

And this is all that we have in 2D: translation, rotation, reflection.

Chapter 2

Lecture 1b: Introduction

Definition 2. a Symmetry Element is the locus of points that's left invariant/unmoved by the operation. What is the net consequence of a sequence of transformations? We can answer by describing the symmetry element of a sequence of transformations.

We now make a profound conclusion: Translation, Rotation, and reflection are the only ones that can exist as single step transformations. A translation performs $(x, y) \mapsto (x + a, y + b)$. A mirror plane moves (x, y) to $(-x, y)$ if the mirror line is perpendicular to the x-axis and passes through the origin. If we do this again, $(-x, y) \mapsto (x, y)$: we're left with the identity. If we now rotate by 180 degrees through the origin, the point $(x, y) \mapsto (-x, -y)$. If we perform it again, it would go to (x, y).

In more general terms, if we change the sense no coordinate, that's translation. If we change the sense of one coordinate, we get reflection. If we change the sense of both coordinate, it's going to be a rotation.

We chose special cases to make it easy. But a mirror plane will always translate one coordiate, while a rotation will translate one coordinate.

Extrapolating, in 1D, we can change the sense of no coordinate, that's translation, or we change the sense of 1 coordinate, that's reflection. So we don't have rotation in 1D.

Now extrapolating in 3D, we're going to have 4 distinct one step operations.

Are there are infinitely many operations on composition of operations? We'll see what happens when we compose two operations next lecture.

2.1 Patterns in 2D

2.1.1 Translation

Translation has magnitude and direction, but it has no origin. We can summarize the periodicity by taking some feducial points P, by saying that something

hung on one of the point p will be hung on all of the other points $p' \in P$. This kind of a point is called as a **lattice point**. This array of ficticious point is called as a lattice. It is the array of ficticious point that represents the translational symmetry of the crystal is the lattice.

If we put atoms on the lattice, then it's called as a **structure**.

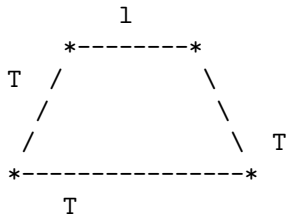
We can add another translational symmetry, let's say T_2 which is not along T_1. So we have two non-collinear translations which give us a 2D space lattice, at which motifs will be hung at $nT_1 + mT_2$ where $n, m \in \mathbb{Z}$. It's something called as a lattice net.

How can we now define the area that is unique to one lattice point? We can draw a parallelogram starting from one lattice point. This gives us the unique part that is hung at a lattice point. This is called as the **unit cell** or as the **cell**.

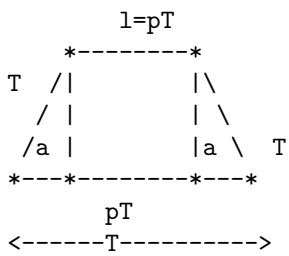
The existence of T_1, T_2 give us an array of lattice points, which define a cell. But if you pick a cell, there are many T_1, T_2 that define the exact same lattice! These are called **conjugate translations**.

So the implication is that we're going to need rules. We could pick ridiculous cells that are long thin translations. We want to talk 'fat', short(est) translations. The second rule is to pick T_1, T_2 that displays the symmetry (if any) of the lattice. The translational periodicity and the symmetry of the lattice go together. These are the only two rules we need to pick what's called as the standard cell.

What happens if we start with a translatory lattice, with a rotation A_α. We can put the rotation at our designated lattice point.



If our lattice looks like this, we need l to be a multiple of T, because we need the lattice to have translational symmetry of T. So let's set $l = pT$



From the horizational line at the bottom we get $2T\cos\alpha + pT = T$, which gives us the equation $1 - 2\cos\alpha = p$, which makes sense because nothing

in the construction depended on the size of what we took. This says that $\cos\alpha = (1-p)/2$. This gives us something we can plug and chug.

If we set $p = 3$, then we get $\cos\alpha = (3-1)/2 = -1$, which means $\alpha = 180^\circ$. We can try this. We start with:

```
*----T-->*
O         O'
```

now let's rotate by 180 degrees counter clockwise about O, giving us O_1

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*<--T---*----T-->*
O1       O         O'
```

Next we can rotate it 180 degrees clockwise about O', giving us O_2:

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*<--T---*----T-->*<------*
O1       O         O'       O2
```

Now it's indeed true that the distance between O_1 and O_2 is $3T$, as we picked $p = 3$. Only a small number of rotations will be compatible. We'll pick up on that from the next lecture.