Lecture 8

- **Elastic strains, compliance, and stiffness**
- **Review for exam**

Stress: force applied to a unit area

Strain: deformation resulting from stress

Purpose of today's derivations: Generalize Hooke's law to a 3D body that may be subjected to any arbitrary force.

We imagine 3 orthogonal vectors $\hat{x}, \hat{y}, \hat{z}$ embedded in a solid before we have deformed it. After we have deformed the solid, these vectors might be of different length and they might be pointing in different directions. We describe these deformed vectors x', y', z' in the following way:

$$x' = (1 + \epsilon_{xx})\hat{x} + \epsilon_{xy}\hat{y} + \epsilon_{xz}\hat{z}$$

$$y' = \epsilon_{yx}\hat{x} + (1 + \epsilon_{yy})\hat{y} + \epsilon_{yz}\hat{z}$$

$$z' = \epsilon_{zx}\hat{x} + \epsilon_{zy}\hat{y} + (1 + \epsilon_{zz})\hat{z}$$

The components $\epsilon_{\alpha\beta}$ define the deformation. They are dimensionless and have values much smaller than 1 in most instances in solid state physics. How one 'reads' these vectors is (for example) ϵ_{xx}➔force along x, deformation along x; ϵ_{xy}➔shear xy-plane along x or y direction (depending which unit vector it is next to)

The new axes have new lengths given by (for example):

$$x' \cdot x' = 1 + 2\epsilon_{xx} + \epsilon_{xx}^2 + \epsilon_{xy}^2 + \epsilon_{xz}^2$$

Usually we are dealing with tiny deformations so 2nd order terms are often dropped.

Deformation also changes the volume of a solid. Considering our unit cube, originally it had a volume of 1. After distortion, it has volume

$$V' = x' \cdot y' \times z' = \begin{vmatrix} 1 + \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & 1 + \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & 1 + \epsilon_{zz} \end{vmatrix} \approx 1 + \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$$

Dilation (δ) is given by:

$$\delta \equiv \frac{V - V'}{V} \cong \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$$

(2nd order terms have been dropped because we are working in a regime of small distortion which is almost always the appropriate one for solid state physics. This expression also gives us the intuition that sheer stresses, to first order, do not change volume)

Now we temporarily go back to considering atoms by writing down the effect that a generic 3D deformation will have on an atom originally located at $\boldsymbol{r} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}$

After the deformation, the atom will be located at $\boldsymbol{r'} = x\boldsymbol{x'} + y\boldsymbol{y'} + z\boldsymbol{z'}$

$$\boldsymbol{R} \equiv \boldsymbol{r'} - \boldsymbol{r} = x(\boldsymbol{x'} - \hat{\boldsymbol{x}}) + y(\boldsymbol{y'} - \hat{\boldsymbol{y}}) + z(\boldsymbol{z'} - \hat{\boldsymbol{z}})$$

Rather than plugging in expressions for **x',y',z'** at this point, we define new variables u, v, w.

$$\boldsymbol{R}(\boldsymbol{r}) = u(\boldsymbol{r})\hat{\boldsymbol{x}} + v(\boldsymbol{r})\hat{\boldsymbol{y}} + w(\boldsymbol{r})\hat{\boldsymbol{z}}$$

In the limit of very small deformations we define new **scalar** strain components:

$$\epsilon_{xx} \rightarrow e_{xx} \equiv \frac{\partial u}{\partial x}$$

$$\epsilon_{yy} \rightarrow e_{yy} \equiv \frac{\partial v}{\partial y}$$

$$\epsilon_{zz} \rightarrow e_{zz} \equiv \frac{\partial w}{\partial z}$$

The other **strain** components are defined in terms of changes in angle between axes

$$e_{xy} \equiv \boldsymbol{x'} \cdot \boldsymbol{y'} \cong \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$$

$$e_{yz} \equiv \boldsymbol{y'} \cdot \boldsymbol{z'} \cong \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}$$

$$e_{zx} \equiv \boldsymbol{z'} \cdot \boldsymbol{x'} \cong \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}$$

Stress components

We have been discussing strains thus far, and now we move on to stresses (effect before cause…).

Stress=force per unit area

Strain=change in length (dimensionless, by convention)

There are 9 stress components, which we now write with different letters: $X_x, X_y, X_z, Y_x, Y_y, Y_z, Z_x, Z_y, Z_z$

The capital letter is the **direction of the force**, and the subscript is the **normal of the plane that the force is being applied to**. For example, the Y_z stress component is a sheer stress in the y direction, applied to the xy plane (to which the z axis is normal).

The number of stress components can be reduced to 6 by noticing that when you sheer one plane, you simultaneously sheer another plane: $X_y = Y_x, X_z = Z_x, Y_z = Z_y$

Use these stress components to make a 3D 6x6 generalization of Hooke's law:

$$X_x = C_{11}e_{xx} + C_{12}e_{yy} + C_{13}e_{zz} + C_{14}e_{yz} + C_{15}e_{zx} + C_{16}e_{xy}$$
$$Y_y = C_{21}e_{xx} + C_{22}e_{yy} + C_{23}e_{zz} + C_{24}e_{yz} + C_{25}e_{zx} + C_{26}e_{xy}$$

$$Z_z = C_{31}e_{xx} + C_{32}e_{yy} + C_{33}e_{zz} + C_{34}e_{yz} + C_{35}e_{zx} + C_{36}e_{xy}$$

$$Y_z = C_{41}e_{xx} + C_{42}e_{yy} + C_{43}e_{zz} + C_{44}e_{yz} + C_{45}e_{zx} + C_{46}e_{xy}$$

$$Z_x = C_{51}e_{xx} + C_{52}e_{yy} + C_{53}e_{zz} + C_{54}e_{yz} + C_{55}e_{zx} + C_{56}e_{xy}$$

$$X_y = C_{61}e_{xx} + C_{62}e_{yy} + C_{63}e_{zz} + C_{64}e_{yz} + C_{65}e_{zx} + C_{66}e_{xy}$$

Or:

$$X = Ce$$

Where C is a 6x6 matrix and e is a column vector.

Key points:

- Stress that is purely compressive/stretching can generically produce strain in the orthogonal direction, as if a sheer stress was applied
- The components of C are **elastic stiffness constants or elastic moduli**. They have units of F/A (same as stress) because strain is dimensionless.
- There are ways to reduce from 36 components of elastic stiffness to a much fewer number using symmetry.

Simplification applicable to all crystal systems:

Remember Hooke's law: $U = \frac{1}{2}kx^2$

Generalize to this case. Elastic energy density:

$$U = \frac{1}{2}\sum_{\lambda=1}^{6}\sum_{\mu=1}^{6} \tilde{C}_{\lambda\mu}e_\lambda e_\mu$$

The indices 1-6 are defined as: $1 \equiv xx, 2 \equiv yy$ ... (same order as eqns for X_i above); twiddle is used over C's because we will refine our definition of them further in a little bit.

Or $U = e'Ce$

$$X_x = \frac{\partial U}{\partial e_{xx}} \equiv \frac{\partial U}{\partial e_1} = \tilde{C}e_1 + \frac{1}{2}\sum_{\beta=2}^{6}(\tilde{C}_{1\beta} + \tilde{C}_{\beta 1})e_\beta$$

(first step comes because Force is spatial derivative of potential energy; on the right side, first term doesn't have factor of ½ because it is a derivative of something like 1/2Cx^2; the term inside the summation come from the fact that each strain component shows up twice in the sum for U)

Note that the second term on the right side of the equation above is always symmetric:

$$\frac{1}{2}(\tilde{C}_{\alpha\beta} + \tilde{C}_{\beta\alpha})$$

Thus, off-diagonal components are symmetric and there are only 21 independent components of elastic stiffness:

$$C_{\alpha\beta} = C_{\beta\alpha} = \frac{1}{2}(\tilde{C}_{\alpha\beta} + \tilde{C}_{\beta\alpha})$$

We can make further simplifications using **symmetry** for specific crystal systems.

Example: cubic crystals

In cubic crystals, the number of unique components in the stiffness matrix is reduced to 3.   I will first write down the result, then explain in words why it is correct:

$$\begin{pmatrix} X_x \\ Y_y \\ Z_z \\ Y_z \\ Z_x \\ X_y \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix}$$

C_{11}: these terms are on the diagonal in the top left quadrant, and they denote elastic constants relevant when one pushed on one face and considers displacement in the same direction as the force. For a cubic crystal, this 'spring constant' is clearly the same whether the force is applied along x, y, z.

C_{12}: these terms are off diagonal in the top left quadrant. They are the elastic constants involved, for example, when you push/pull the cube in the x direction, and the cube bulges in the y and z direction. Clearly, the amount of bulging in that direction will be the same in both y and z (because it is a cube), and when an identical force is applied along the y or z direction, the other two dimensions will bulge or contract in the same way.

The zero terms in the top right quadrant: in a cube (and other orthogonal systems), when you push down on a face, there will not be a sheer deformation.

The zero terms in the bottom left quadrant: when you sheer a cube, you will not produce a compressive deformation

C_{44}: these are the components of sheer moduli. They are the same because sheering one plane in a cube is equivalent to sheering an orthogonal plane.

Bulk modulus of a cubic crystal

Elastic constant to convert between hydrostatic pressures and volume changes

Consider uniform dilation, which is expected for a cube: $e_{xx} = e_{yy} = e_{zz} = \frac{1}{3}\delta$

Potential energy from this deformation:

$U = \frac{1}{2}B\delta^2$ (B is defined as the bulk modulus)

Comparing this to the general expression for U given earlier, and dropping all C terms that are 0 or sheer:

$$U = \frac{1}{6}(C_{11} + 2C_{12})\delta^2$$

Putting it together:

$$B = \frac{1}{3}(C_{11} + 2C_{12})$$

Review for exam

- **Lattice and basis**
- **Miller indices, especially in terms of primitive vs conventional lattice vectors**
- **Structure factor**
- **Bragg's law**
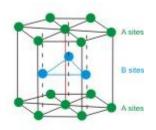
Lattice and basis:

Vocabulary:

Lattice: any regular repetition of points in space. This is a mathematical construct

Primitive lattice: a lattice in which all of the points can be reached by D translation vectors (D=dimension—1,2, or 3) of the form $r = \sum_{i=1}^{D} u_i a_i$; when these primitive translation vectors are used to construct a parallelogram or parallelepiped cell, there will be one lattice point per cell. There are only 5 unique primitive lattices in 2D and 14 in 3D

Basis: a group of one or more atoms which is attached to each point in a lattice which are repeated infinitely in space

Unit cell: Lattice+basis attached to each lattice point; this object repeats infinitely in space to form a crystal
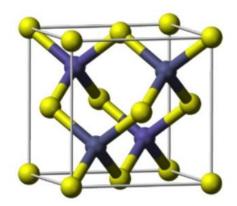
Primitive vs conventional cell: for a subset of primitive lattices, there is a way to visualize them within a rectangular, cubic, or otherwise orthogonal structure. These conventional cells are often easier to work with because cross products are easy with orthogonal vectors, but they have more than one lattice point per cell which can make other calculations (e.g. structure factor) more difficult.

Hexagonal-close packed structure: identify lattice and basis

HCP Structure

ZincBlende structure: identify lattice and basis

ZincBlende structure is based on the FCC lattice and it is almost like the diamond structure except the internal atoms are different from the FCC atoms. Internal atoms located at $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ and three equivalent positions with alternating corners.
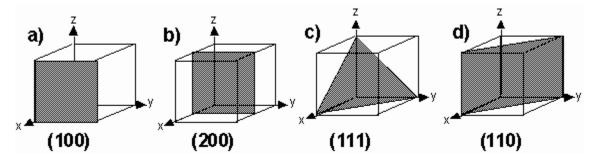
Miller indices:

Procedure for extracting them in textbook:

1."Find the intercepts of the axes in terms of the lattice constants a1, a2, and a3. The axes may be those of a primitive or non-primitive cell
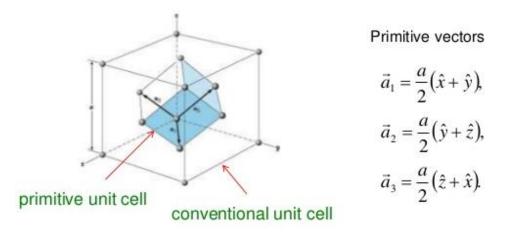
2. Take reciprocals and reduce to three integers

Example FCC lattice:

Conventional cell (cubic): find 200 plane

Primitive lattice for FCC:

Primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}),$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z}),$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x}).$$

primitive unit cell

conventional unit cell

How to describe that same object (plane cutting cube halfway) in terms of primitive lattice vectors?

Find intersection point of each lattice vector with the plane:

$$a_1 \rightarrow 1$$
$$a_2 \rightarrow \infty$$
$$a_3 \rightarrow 1$$

Inverses→(101)

Another example: (110) plane in conventional cell is the _____ plane in primitive cell?

$$a_1 \rightarrow 1$$
$$a_2 \rightarrow 2$$
$$a_3 \rightarrow 2$$

Inverses→ (1, 1/2 , ½)

Miller indices→(122)

Another example: find (110) plane referenced to *primitive* cell

Intercepts: 1 along a1, 1 along a2 and infinity along a3

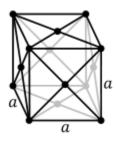This ends up being a plane parallel to the xz plane, intersecting halfway into the cube→the (020) plane.

Structure factor

Name of the game (usually): find when it is zero

$$S_G = \sum_{j=1}^{s} f_j e^{-i G \cdot r_j}$$

$$S_G(v_1 v_2 v_3) = \sum_{j=1}^{s} f_j e^{-2\pi i(v_1 x_j + v_2 y_j + v_3 z_j)}$$

Example: FCC (use conventional cell)

Putting the origin at the back left corner and having z point up and y to the right, we have atoms at the following fractional coordinates (factor of a is omitted):

$$(0,0,0); \left(\frac{1}{2}, 0, \frac{1}{2}\right); \left(0, \frac{1}{2}, \frac{1}{2}\right); \left(\frac{1}{2}, \frac{1}{2}, 0\right)$$

(When atoms are shared with adjacent cells we count only enough of those atoms to get the total number contained in one cell. For example, we counted all of the back corner atom (0,0,0) and left the other 7 to other unit cells because there are 8*1/8=1 corner atoms; ditto for the face-centered atoms which are each shared with 2 other cells, only count 3 of them)

The structure factor for the conventional FCC cell is given by:

$$S_G(v_1 v_2 v_3) = \sum_{j=1}^{s} f_j e^{-2\pi i (v_1 x_j + v_2 y_j + v_3 z_j)}$$

$$= f[1 + e^{-i\pi(v_1+v_3)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_2)}$$

$$= \begin{cases} 0 \text{ if one index is odd and other two even or if two are odd and one is even} \\ 4f \text{ if all indices are odd or all are even} \end{cases}$$

When is the structure factor zero when we use the *primitive* cell: (ans: never)

Why? For FCC structure, there is only one atom in the primitive cell (if we considered the diamond structure, there would be 2 and we would have cancelation)

What would happen if the face-centered atoms were a different species from corner ones?

$$S_G = [f_{corner} + f_{face} e^{-i\pi(v_1+v_3)} + f_{face} e^{-i\pi(v_2+v_3)} + f_{face} e^{-i\pi(v_1+v_2)}]$$

This would not be zero except for some great coincidence, but it is possible for some diffraction peaks for be *reduced*. Note that for x-rays, the atomic form factor, f, is proportional to the number of electrons in that type of atom/ion.

Bragg law:

$$2d\sin\theta = n\lambda$$

We derived this in two ways in class, via path length difference for 2 planes and via phase difference for an infinite crystal. In the latter case, the angle and wavelength is encoded in the wavevector of the plane wave $e^{ik \cdot r}$. In the second derivation, we found that the difference between wavevector of

incoming and outgoing beams needs to be a vector of the reciprocal lattice for there to be constructive interference and a diffraction peak: $\mathbf{k'} - \mathbf{k} = \Delta\mathbf{k} = \mathbf{G}$

The way you use that information is $d_{hkl} = 2\pi/|\mathbf{G_{hkl}}|$

Were $\mathbf{G_{hkl}} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is a specific vector of the reciprocal lattice which you showed in your homework to be perpendicular to the hkl plane. The equation above makes it very easy to calculate the spacing between crystallographic planes that have complicated orientations.

Once d_{hkl} is known, one can calculate the predicted diffraction angle that type of plane will produce for a known wavelength of radiation. Also, one can (and often does) work the other way: they are given a diffraction angle (usually powder diffraction) and they know they wavelength, and they are asked to calculate d_{hkl} and also figure out what planes they are looking at.