

Coarse graining (and some leftovers from last session)

1 Leftovers from last session: Some elementary notes about strain, stress, and geometry

1.1 Maximal shear/normal stress/strain

It is instructive to examine the planes on which the normal or shear stresses are maximal. As a motivation, we'll note that some materials, when stretched, tear in a plane perpendicular to the stretching direction. This is very intuitive, because the normal (dilatational) stress is highest on this plane. When compressed, however, things are not as simple. When a metal is compressed above its capability to sustain the deformation, it typically undergoes irreversible deformation in a plane at 45° to the compression, cf. Fig. 1. But why at 45° ? That's because it is much easier to perform irreversible deformation in shear than in compression (the shear strength is much smaller than the compressive hardness). Phenomena which are shear-driven occur at planes which have maximal shear.

In general, say we have a stress tensor σ . What is the normal stress on a given plane? It is given by the normal component of the force on that plane. If the normal to the plane is \hat{n} , the force is $\sigma \hat{n}$, and the normal component is $\sigma_n = \hat{n}^T \sigma \hat{n}$. Note that if \hat{t}_1, \hat{t}_2 are vectors orthogonal to \hat{n} (tangent to the plane) then the stress in the coordinate system $\{\hat{n}, \hat{t}_1, \hat{t}_2\}$ is

$$[\sigma]' = \begin{pmatrix} - & \hat{n} & - \\ - & \hat{t}_1 & - \\ - & \hat{t}_2 & - \end{pmatrix} [\sigma] \begin{pmatrix} | & | & | \\ \hat{n} & \hat{t}_1 & \hat{t}_2 \\ | & | & | \end{pmatrix},$$

so σ_n is simply the nn component of σ written in the new basis. Note that σ_n goes like $\sim n^2$, and not like $\sim n$ as one might think.

So say we apply uniaxial stress, so that the stress tensor is of the form (forget for the

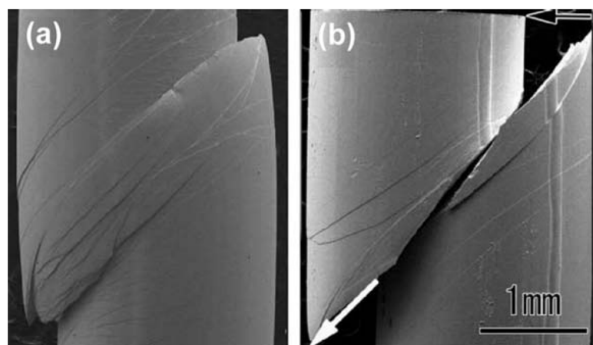


Figure 1: Compressive shear failure (shear banding) of a metallic glass. Wait, what? What does it even mean a metallic glass? can a material be both a metal and a glass? Hang on in the course to find out. From: Louzguine-Luzgin et. al., *Metals* **3** (2013).

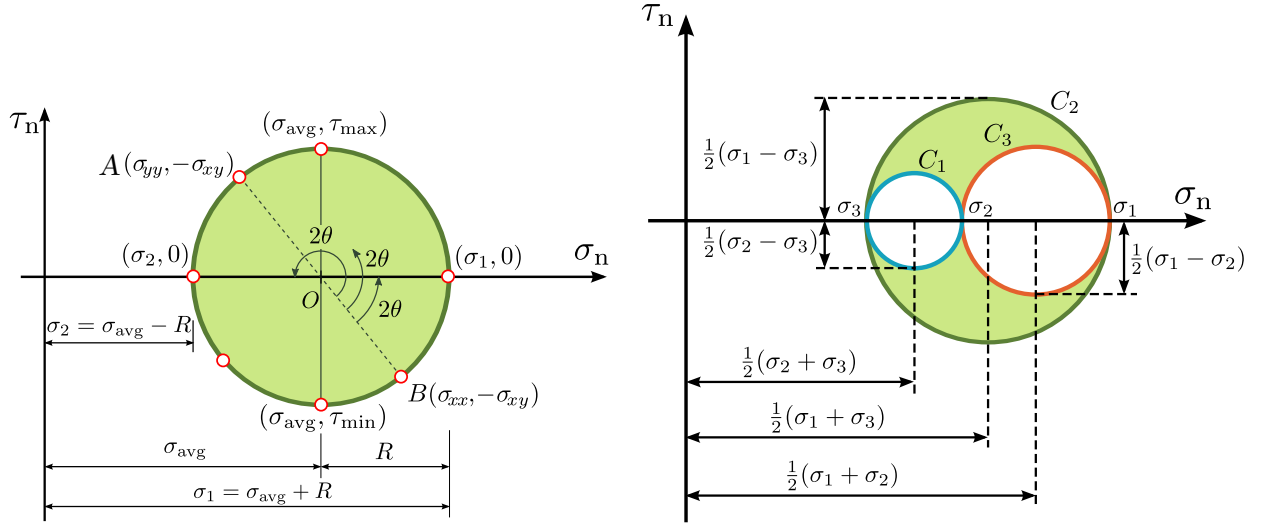


Figure 2: Illustration of Mohr's circle in 2D (left) and 3D (right), adapted from Wikipedia.

moment about the 3rd dimension):

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (1)$$

Rotating by an angle α we get

$$\boldsymbol{\sigma} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} = \sigma_1 \begin{pmatrix} \cos^2 \alpha & -\cos \alpha \sin \alpha \\ -\cos \alpha \sin \alpha & \sin^2 \alpha \end{pmatrix}$$

So you see that the maximal shear stress occurs for $\alpha = 45^\circ$.

1.2 Mohr's circle

1.2.1 2D case

We saw that different planes are subject to different shear and normal (compressive) stresses. Mohr's circle is a simple geometrical way to see all possible shear and normal stresses of a given stress state. Here we'll only consider a 2D system (later in the course we'll see exactly what we mean when we say 2D), but this concept can be generalized also to 3D.

Let's consider a general stress state,

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix}, \quad (2)$$

and ask what is the normal and shear stresses, which we'll denote by σ_n and τ_n , on a plane in an angle θ to the x axis. This means we need to rotate the stress by α , and look at the 11 and 12 components of the resulting matrix. Performing the matrix multiplication, we get

$$\sigma_n = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) + \frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \cos 2\theta + \sigma_{xy} \sin 2\theta \quad (3)$$

$$\tau_n = -\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \sin 2\theta + \sigma_{xy} \cos 2\theta \quad (4)$$

If we look in the $\sigma_n - \tau_n$ plane, what geometrical form do these equations describe? It is easy to see that the answer is a circle:

$$\begin{aligned} \tau_n^2 + \left(\sigma_n - \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) \right)^2 &= \\ \left(\sigma_{xy} \cos 2\theta - \frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \sin 2\theta \right)^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \cos 2\theta + \sigma_{xy} \sin 2\theta \right)^2 & \\ = \sigma_{xy}^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy}) \right)^2 & \end{aligned}$$

This is a circle of radius $\sqrt{\sigma_{xy}^2 + \left(\frac{1}{2}(\sigma_{xx} - \sigma_{yy})\right)^2}$, centered around $\sigma_n = \frac{1}{2}(\sigma_{xx} + \sigma_{yy})$ and $\tau_n = 0$. This circle is called Mohr's circle, and is shown in Fig. 2.

A point on the circle corresponds to an admissible pair (σ_n, τ_n) , and rotating the axes by θ corresponds to traversing an angle 2θ along the circle. This means that rotating by 180° puts you back where you started, which is not surprising. The intersections of the circle with the σ_n axis are the eigenvalues of $\boldsymbol{\sigma}$ – the principal stresses.

1.2.2 3D case

In 3D things are less simple because we have 2 angles of rotation. We denote the principal stresses (i.e. the eigenvalues of $\boldsymbol{\sigma}$) by $\sigma_1 > \sigma_2 > \sigma_3$, and start with coordinates in which $\boldsymbol{\sigma}$ is diagonal. If we choose a plane whose normal is \vec{n} , then the force (per unit area) on this plane is $\vec{T} = \boldsymbol{\sigma}\vec{n}$. As in 2D, we denote the normal pressure $\vec{T} \cdot \vec{n} = (\boldsymbol{\sigma}\vec{n}) \cdot \vec{n}$ by σ_n and the shear force by τ_n . We thus have

$$T^2 = (\boldsymbol{\sigma}\vec{n})^2 = \sigma_{ij}\sigma_{ik}n_jn_k = \sigma_n^2 + \tau_n^2 = \sigma_1^2n_1^2 + \sigma_2^2n_2^2 + \sigma_3^2n_3^2 \quad (5)$$

$$\sigma_n = \sigma_1n_1^2 + \sigma_2n_2^2 + \sigma_3n_3^2 \quad (6)$$

$$n_in_i = n_1^2 + n_2^2 + n_3^2 = 1 \quad (7)$$

These are three equations, which we can solve for the three variables n_i^2 to get

$$n_1^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_2)(\sigma_n - \sigma_3)}{(\sigma_1 - \sigma_2)(\sigma_1 - \sigma_3)} \geq 0 \quad (8)$$

$$n_2^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_3)(\sigma_n - \sigma_1)}{(\sigma_2 - \sigma_3)(\sigma_2 - \sigma_1)} \geq 0 \quad (9)$$

$$n_3^2 = \frac{\tau_n^2 + (\sigma_n - \sigma_1)(\sigma_n - \sigma_2)}{(\sigma_3 - \sigma_1)(\sigma_3 - \sigma_2)} \geq 0 \quad (10)$$

The 1st and 3rd denominators are positive, and the 2nd is negative, so we have

$$\tau_n^2 + (\sigma_n - \sigma_2)(\sigma_n - \sigma_3) \geq 0 \quad (11)$$

$$\tau_n^2 + (\sigma_n - \sigma_3)(\sigma_n - \sigma_1) \leq 0 \quad (12)$$

$$\tau_n^2 + (\sigma_n - \sigma_1)(\sigma_n - \sigma_2) \geq 0 \quad (13)$$

After some trivial algebraic manipulations, these can be re-written as

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_2 + \sigma_3) \right]^2 \geq \left(\frac{1}{2}(\sigma_2 - \sigma_3) \right)^2 \quad (14)$$

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_1 + \sigma_3) \right]^2 \leq \left(\frac{1}{2}(\sigma_1 - \sigma_3) \right)^2 \quad (15)$$

$$\tau_n^2 + \left[\sigma_n - \frac{1}{2}(\sigma_1 + \sigma_2) \right]^2 \geq \left(\frac{1}{2}(\sigma_1 - \sigma_2) \right)^2 \quad (16)$$

These are equations of three circles, which are shown in Fig. 1.

2 Coarse graining

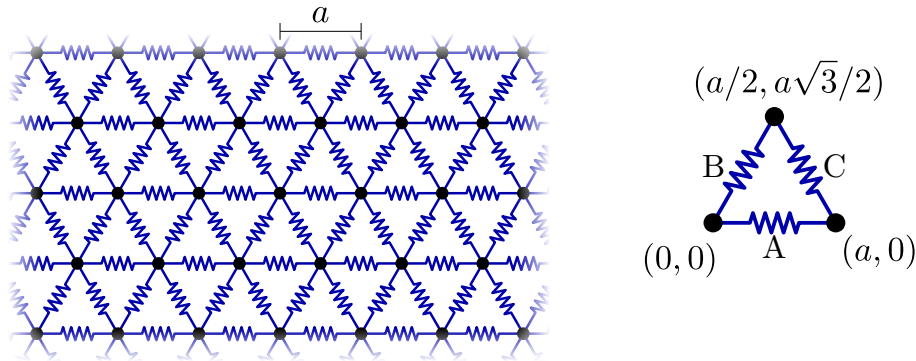


Figure 3: Left: A triangular lattice with a lattice constant a . Right: the unit cell with the coordinates of the vertices.

The purpose of this section is to see how to develop a continuum theory to describe the deformation of a discrete system, a process known as “coarse graining”. This is also the first time in the course that we’ll develop a *constitutive relation*, i.e. calculate how the stress depends on the deformation.

The system we’ll examine is a two-dimensional triangular lattice of masses and springs, shown in Fig. 3. We assume that the springs are usual linear springs with an identical spring constant k and that in the undeformed state all the springs are at their rest-lengths, which we denote by a .

The central quantity we will want to calculate is the energetic cost of deformation. As You’ll hear from Eran in the next lecture, stresses and strains are intimately related and the observable that relates the two is the energy. Formally, stress and strain are a conjugate variable pair (like many other pairs you know of: pressure-volume, magnetic field-magnetization, chemical potential-particle number etc.).

Assume the material undergoes some motion $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X})$. A crucial requirement in coarse graining is that the observables of interest vary slowly in space, much slower than the relevant microscopic degrees of freedom. Formally, this means that the Fourier decomposition of $\boldsymbol{\varphi}$ only has contributions from wavevectors \mathbf{q} satisfying $|\mathbf{q}a| \ll 1$ (you may have seen a similar requirement when you learned about the Debye model for the phonon contribution to the specific heat). Thus, we assume that we can analyze each

small portion of the lattice separately and write the energy density u as a function of the *local values* of the deformation (and its gradients)

$$u(\mathbf{r}) = u\left(\boldsymbol{\varphi}(\mathbf{r}), \mathbf{F}(\mathbf{r}), \nabla \mathbf{F}, \dots\right). \quad (17)$$

Note that in Eran's notes energy density is defined per unit mass and here I use densities per unit volume (=area). The two are simply related by a factor ρ . Finally, we can then express the total energy of the system as a volume integral $\mathcal{U} = \int u(\mathbf{r}) d^3\mathbf{r}$.

So let's calculate u defined in Eq. (17). Since we do not consider any external fields, the energy must be independent of global translation, i.e. $\boldsymbol{\varphi}$ itself. Also, we consider here only the contribution of \mathbf{F} to the energy and neglect higher gradients. This is an "extra" approximation which follows the same spirit of the coarse-graining: if $|\mathbf{q}a| \ll 1$ then two adjacent masses will experience roughly the same \mathbf{F} , and the approximation becomes better when $|\mathbf{q}a|$ becomes smaller. Note that it is perfectly "kosher" to consider also terms like $\nabla \mathbf{F}$, $\nabla^2 \mathbf{F}$, etc, but that would require the theory to include explicitly a microscopic lengthscale, something that we would like to avoid at this point.

Examine the unit cell that in the undeformed state is located at $\mathbf{X} = 0$. Its vertices are at $\mathbf{X}^{(1)} = (0, 0)$, $\mathbf{X}^{(2)} = (a, 0)$ and $\mathbf{X}^{(3)} = (a/2, a\sqrt{3}/2)$. After the deformation, their positions are

$$\mathbf{x}^{(\alpha)}(\mathbf{X}) \approx \boldsymbol{\varphi}(0) + \mathbf{F}\mathbf{X}^{(\alpha)} + \mathcal{O}(a^2) \quad (18)$$

$$\mathbf{x}^{(1)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \mathbf{x}^{(2)} = a \begin{pmatrix} F_{1,1} \\ F_{2,1} \end{pmatrix} \quad \mathbf{x}^{(3)} = a \begin{pmatrix} \frac{1}{2}F_{1,1} + \frac{\sqrt{3}}{2}F_{1,2} \\ \frac{1}{2}F_{2,1} + \frac{\sqrt{3}}{2}F_{2,2} \end{pmatrix} \quad (19)$$

The deformed lengths of the three springs denoted by A,B,C in the figure are

$$L_A = \left| \mathbf{x}^{(2)} - \mathbf{x}^{(1)} \right| = \left| (aF_{1,1}, aF_{2,1}) \right| = a\sqrt{F_{1,1}^2 + F_{2,1}^2}, \quad (20)$$

$$L_B = \left| \mathbf{x}^{(3)} - \mathbf{x}^{(1)} \right| = \frac{a}{2} \sqrt{\left(F_{1,1} + \sqrt{3}F_{1,2} \right)^2 + \left(\sqrt{3}F_{2,2} + F_{2,1} \right)^2}, \quad (21)$$

$$L_C = \left| \mathbf{x}^{(3)} - \mathbf{x}^{(2)} \right| = \frac{a}{2} \sqrt{\left(F_{1,1} - \sqrt{3}F_{1,2} \right)^2 + \left(\sqrt{3}F_{2,2} - F_{2,1} \right)^2}. \quad (22)$$

The total energy is given by

$$Su = \frac{1}{2}k(L_A - a)^2 + \frac{1}{2}k(L_B - a)^2 + \frac{1}{2}k(L_C - a)^2 \quad (23)$$

where $S = a^2\sqrt{3}/2$ is twice the area of the unit cell. It's easy to see that if $\mathbf{F} = \mathbf{I}$ then $L_i = a$ and clearly the energy will vanish, as expected.

Let us examine this energy function. The first thing we note about u is that it doesn't look like a "tensor function", i.e. it seems to depend on all the entries of \mathbf{F} in some kind of a nasty manner that cannot be written in a nice geometrical form like $f(\text{tr } \mathbf{F}, \det \mathbf{F}, \mathbf{F} : \mathbf{F}, \dots)$. Second, it seems that, unlike what we said in the last TA session, it seems to depend on both the symmetric and the antisymmetric parts of \mathbf{F} .

So let's see if we can write u in a way that makes some more sense. We'll denote the line segments that connect the vertices by $d\mathbf{X}^{(A)}$, $d\mathbf{X}^{(B)}$ and $d\mathbf{X}^{(C)}$ and their deformed counterparts as $d\mathbf{x}^{(A)} = \mathbf{F}d\mathbf{X}^{(A)}$, $d\mathbf{x}^{(B)} = \mathbf{F}d\mathbf{X}^{(B)}$ and $d\mathbf{x}^{(C)} = \mathbf{F}d\mathbf{X}^{(C)}$. The deformed lengths are

$$L_\alpha^2 = d\mathbf{x}^{(\alpha)} \cdot d\mathbf{x}^{(\alpha)} = d\mathbf{X}^{(\alpha)T} \mathbf{F}^T \mathbf{F} d\mathbf{X}^{(\alpha)} = \mathbf{F}^T \mathbf{F} : (d\mathbf{X}^{(\alpha)} \otimes d\mathbf{X}^{(\alpha)}) \quad (24)$$

Starting to look familiar? (I remind you of the definition of the Green-Lagrange strain tensor $\mathbf{E} \equiv \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{I})$). In order to write the energy, it seems that the matrices $\mathbf{M}^{(\alpha)} \equiv d\mathbf{X}^{(\alpha)} \otimes d\mathbf{X}^{(\alpha)}$ will be handy. Explicitly, they read

$$\mathbf{M}^{(A)} = a^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \mathbf{M}^{(B)} = a^2 \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} \quad \mathbf{M}^{(C)} = a^2 \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} \quad (25)$$

Note that $\text{tr} \mathbf{M}^{(\alpha)} = a^2$ and $\sum \mathbf{M}^{(\alpha)} = \frac{3}{2}a^2 \mathbf{I}$. We are now ready to write the energy:

$$Su = \frac{1}{2}k(L_A - a)^2 + \frac{1}{2}k(L_B - a)^2 + \frac{1}{2}k(L_C - a)^2 \quad (26)$$

$$= \frac{1}{2}k \left[L_A^2 + L_B^2 + L_C^2 - 2a(L_A + L_B + L_C) + 3a^2 \right] \quad (27)$$

$$= \frac{1}{2}k \left[\mathbf{F}^T \mathbf{F} : \left(\sum_\alpha \mathbf{M}^{(\alpha)} \right) - 2a \sum_\alpha \sqrt{\mathbf{F}^T \mathbf{F} : \mathbf{M}^{(\alpha)}} + 3a^2 \right] \quad (28)$$

$$= \frac{1}{2}k \left[\frac{3}{2}a^2 \text{tr}(\mathbf{F}^T \mathbf{F}) - 2a \sum_\alpha \sqrt{\mathbf{F}^T \mathbf{F} : \mathbf{M}^{(\alpha)}} + 3a^2 \right] \quad (29)$$

$$= \frac{1}{2}k \left[\frac{3}{2}a^2 \text{tr}(2\mathbf{E} + \mathbf{I}) - 2a \sum_\alpha \sqrt{(2\mathbf{E} + \mathbf{I}) : \mathbf{M}^{(\alpha)}} + 3a^2 \right] \quad (30)$$

$$u = k\sqrt{3} \left[\text{tr} \mathbf{E} - \frac{2}{3} \sum_\alpha \sqrt{1 + 2\mathbf{E} : \tilde{\mathbf{M}}^{(\alpha)}} + 2 \right] \quad (31)$$

where we defined $\tilde{\mathbf{M}}^{(\alpha)} = a^{-2} \mathbf{M}^{(\alpha)}$ and in the last transition we divided by S .

So that's about it. This is the energy function in its full glory. Two things are worth noting about this energy function: First, you can already see that it depends only on \mathbf{E} which is rotationally invariant and symmetric. That is, the continuum level quantity \mathbf{E} emerges naturally from the discrete analysis. Second, note that although we are using strictly linear springs whose energies are quadratic in their elongation the energy function is far from being a simple quadratic function. This is because the geometry itself introduces nonlinearities.

Let's take this one step further, and develop u in orders of \mathbf{E} to see if we can get understand this better. The zeroth order clearly vanishes, which is a good sign that we didn't have any mistakes. The first order should also vanish (why?), and indeed

$$u^{(1)} = k\sqrt{3} \left[\text{tr} \mathbf{E} - \frac{2}{3} \sum_\alpha \left(1 + \mathbf{E} : \tilde{\mathbf{M}}^{(\alpha)} \right) + 2 \right] = k\sqrt{3} \left[\text{tr} \mathbf{E} - \frac{2}{3} \mathbf{E} : \sum_\alpha \tilde{\mathbf{M}}^{(\alpha)} \right] = 0$$

So in all subsequent orders we can worry only about the sqrt term. To second order we have (recall that $\sqrt{1+x} \approx 1 + \frac{x}{2} - \frac{x^2}{8}$)

$$u^{(2)} = \frac{k}{\sqrt{3}} \sum_{\alpha} \left(\mathbf{E} : \tilde{\mathbf{M}}^{(\alpha)} \right)^2 = \frac{k}{\sqrt{3}} \sum_{\alpha} E_{ij} E_{kl} \tilde{M}_{ij}^{(\alpha)} \tilde{M}_{kl}^{(\alpha)} = \frac{1}{2} E_{ij} E_{kl} C_{ijkl} \quad (32)$$

$$C_{ijkl} \equiv \frac{2k}{\sqrt{3}} \sum_{\alpha} \tilde{M}_{ij}^{(\alpha)} \tilde{M}_{kl}^{(\alpha)} = \left(\frac{2k}{a^4 \sqrt{3}} \sum_{\alpha} d\mathbf{X}^{(\alpha)} \otimes d\mathbf{X}^{(\alpha)} \otimes d\mathbf{X}^{(\alpha)} \otimes d\mathbf{X}^{(\alpha)} \right)_{ijkl} \quad (33)$$

\mathbf{C} is called the stiffness tensor and you'll hear a lot about it tomorrow in Eran's lecture. Note that the fact that to quadratic order $u = E_{ij} E_{kl} C_{ijkl}$ for *some* tensor \mathbf{C} is generally true in the framework of linear elasticity. Also, the fact that C_{ijkl} is symmetric under any of the transpositions $i \leftrightarrow j$, $k \leftrightarrow l$ and $ij \leftrightarrow kl$ (and any compositions of them) also generally holds. However, our \mathbf{C} has some extra symmetries on top of that. First, note that $C_{ikjl} \propto \sum_{\alpha} dX_i^{(\alpha)} dX_j^{(\alpha)} dX_k^{(\alpha)} dX_l^{(\alpha)}$ so the tensor is fully symmetric to any permutation of $ijkl$. But there's even more than that: In fact, explicit calculation shows that

$$C_{ijkl} = \frac{\sqrt{3}k}{4} \left(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{kj} \right), \quad (34)$$

which is, pretty surprisingly, an *isotropic tensor*. That is, to leading order the elastic response of triangular lattice is isotropic, although the lattice is clearly not invariant to rotations. Explicitly, we have

$$u(\mathbf{E}) = \frac{\sqrt{3}k}{8} E_{ij} E_{kl} \left(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{kj} \right) = \frac{\sqrt{3}k}{8} \left((\text{tr } \mathbf{E})^2 + 2 \text{tr}(\mathbf{E}^2) \right) \quad (35)$$

As Eran will explain at length tomorrow, the relation between the stress and the strain is $\boldsymbol{\sigma} = \frac{\partial u}{\partial \boldsymbol{\varepsilon}} = C_{ijkl} \varepsilon_{kl}$ (note that I switched from \mathbf{E} to $\boldsymbol{\varepsilon}$, which is OK because we're in the linear approximation within which the two are identical). Thus,

$$\sigma_{ij}(\boldsymbol{\varepsilon}) = \frac{\sqrt{3}k}{4} \varepsilon_{kl} \left(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{kj} \right) = \frac{\sqrt{3}k}{4} \left(\delta_{ij} \text{tr } \boldsymbol{\varepsilon} + 2\varepsilon_{ij} \right) \quad (36)$$

$$\boldsymbol{\sigma} = \frac{\sqrt{3}k}{2} (\text{tr } \boldsymbol{\varepsilon}) \mathbf{I} + \frac{\sqrt{3}k}{4} \boldsymbol{\varepsilon} \quad (37)$$

As you'll see tomorrow, the form $\boldsymbol{\sigma} = \lambda(\text{tr } \boldsymbol{\varepsilon}) \mathbf{I} + 2\mu \boldsymbol{\varepsilon}$ for two constants λ, μ is the most general constitutive relation for linear isotropic materials. λ and μ are called Lamé coefficients (μ is also called the shear modulus). Note that the microscopic lengthscale a does not appear explicitly in the theory, a common situation in continuum theories (but if we were to include also strain-gradient terms, we could not have avoided having a in our equations).