5.2 Elasticity Theory, Energy , and Forces

## 5.2.1 General Remarks and Basics of Elasticity Theory

General Remarks

The **theory of elasticity** is quite difficult just for simple homogeneous media (no crystal), and even more difficult for crystals with dislocations - because the dislocation core cannot be treated with the linear approximations always used when the math gets tough.

- Moreover, *relatively simple* analytical solutions for e.g. the elastic energy stored in the displacement field of a dislocation, are only obtained for an *infinite* crystal, but then often lead to infinities.
- As an example, the energy of *one* dislocation in an otherwise perfect infinite crystal comes out to be infinite!

This looks not very promising. However, for *practical* purposes, very simple relations can be obtained in good approximations.

- This is especially true for the *energy per unit length*, the **line energy** of a dislocation, and for the forces between dislocations, or between dislocations and other defects.

A very good introduction into the elasticity theory as applied to dislocation is given in the text book **Introduction to Dislocations** of **D. Hull** and **D. J. Bacon**. We will essentially follow the presentation in this book.

The atoms in a crystal containing a dislocation are displaced from their perfect lattice sites, and the resulting **distortion** produces a **displacement field** in the crystal around the dislocation.

- If there is a *displacement* field, we automatically have a **stress field** and a **strain field**, too. Try not to mix up displacement, *stress* and *strain*!

If we look at the picture of the edge dislocation, we see that the region above the inserted half-plane is in **compression** - the distance between the atoms is smaller then in equilibrium; the region below the half-plane is in **tension**.

- The dislocation is therefore a source of **internal stress** in the crystal. In all regions of the crystal except right at the dislocation core, the stress is small enough to be treated by conventional *linear* elasticity theory. Moreover, it is generally sufficient to use *isotropic* theory, simplifying things even more.
- If we know what is called the **elastic field**, i.e. the *relative* displacement of all atoms, we can calculate the force that a dislocation exerts on other dislocations, or, more generally, any interaction with elastic fields from other defects or from external forces. We also can then calculate the energy contained in the elastic field produced by a dislocation.

Basics of Elasticity Theory

The first element of elasticity theory is to define the **displacement field $\underline{u}(x,y,z)$**, where $\underline{u}$ is a vector that defines the displacement of atoms or, since we essentially consider a continuum, the displacement of any point **P** in a strained body from its original (unstrained) position to the position **P'** in the strained state.

Displacement of *P* to *P'*
by displacement vector $\underline{u}$
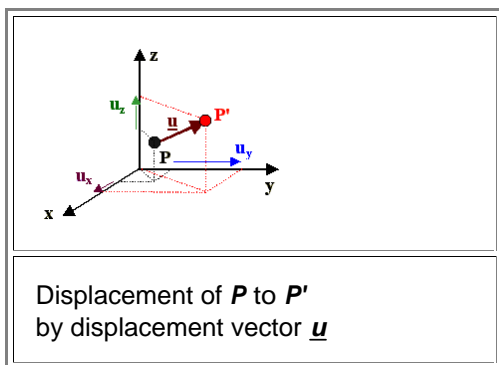
- The displacement vector $\underline{u}$**(x, y, z)** is then given by

$$\underline{u}(x, y, z) \ = \ \begin{matrix} u_X(x, y, z) \\ u_Y(x, y, z) \\ u_Z(x, y, z)] \end{matrix}$$

- The components u_x , u_y , u_z represent projections of $\underline{u}$ on the x, y, z axes, as shown above.

The vector field $\underline{u}$, however, contains not only uninteresting rigid body translations, but at some point (x,y,z) all the summed up displacements from the other parts of the body.

- If, for example, a long rod is just elongated along the x-axis, the resulting $\underline{u}$ field, if we neglect the contraction, would be

$$u_x = const \cdot x \qquad u_y = 0 \qquad u_z = 0$$

● But we are only interested in the *local* deformation, i.e. the deformation that acts on a volume element dV *after* it has been displaced some amount defined by the environment. In other words, we only are interested in the changes of the *shape* of a volume element that was a perfect cube in the undisplaced state. In the example above, *all* volume element cubes would deform into a rectangular block.

We thus resort to the local **strain** ϵ, defined by the nine components of the strain tensor acting on an elementary cube. That this is true for small strains you can prove for yourself in the next exercise.

● Applied to our case, the nine components of the **strain tensor** are directly given in terms of the first derivatives of the displacement components. If you are not sure about this, activate the link.

● We obtain the **normal strain** as the diagonal elements of the strain tensor.

$$\epsilon_{xx} = \frac{du_x}{dx} \qquad \epsilon_{yy} = \frac{du_y}{dy} \qquad \epsilon_{zz} = \frac{du_z}{dz}$$

● The **shear strains** are contained in the rest of the tensor:

$$\epsilon_{yz} = \epsilon_{zy} = \tfrac{1}{2} \cdot \left(\frac{du_y}{dz} + \frac{du_z}{dy} \right)$$

$$\epsilon_{zx} = \epsilon_{xz} = \tfrac{1}{2} \cdot \left(\frac{du_z}{dx} + \frac{du_x}{dz} \right)$$

$$\epsilon_{xy} = \epsilon_{yx} = \tfrac{1}{2} \cdot \left(\frac{du_x}{dy} + \frac{du_y}{dx} \right)$$

Within our basic assumption of linear theory, the magnitude of these components is **<< 1**. The normal strains simply represent the fractional change in length of elements parallel to the *x*, *y*, and *z* axes respectively. The physical meaning of the shear strains is shown in the following illustration
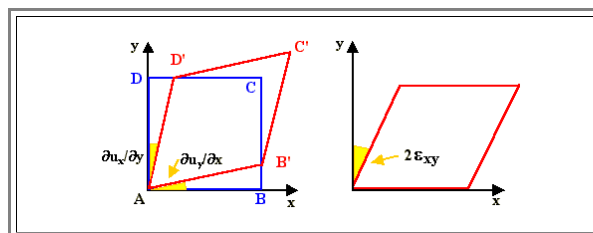
● A small area element **ABCD** in the *xy* plane has been strained to the shape **A B' C' D'** without change of area. The angle between the sides **AB** and **AD**, initially parallel to *x* and *y*, respectively, has decreased by $2\epsilon_{xy}$. By rotating, but not deforming, the element as shown on the right-hand side, it is seen that the element has undergone a simple shear. The simple shear strain often used in engineering practice is $2\epsilon_{xy}$, as indicated.

● The volume **V** of a small volume element is changed by strain to

$$V + \Delta V = V \cdot (1 + \epsilon_{xx}) \cdot (1 + \epsilon_{yy}) \cdot (1 + \epsilon_{zz})$$

● The fractional change in volume Δ, known as the *dilatation*, is therefore

$$\Delta = \frac{\Delta V}{V} = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$$

● Note that Δ is independent of the orientation of the axes *x, y, z*

Simple elasticity theory links the strain experienced in a volume element to the forces acting on this element. (*Difficult* elasticity theory links the strain experienced in any volume element to the forces acting on the macroscopic body!). The forces act on the surface of the element and are expressed as **stress**, i.e. as force per area. Stress is propagated in a solid because each volume element acts on its neighbors.

- A complete description of the stresses acting therefore requires not only specification of the magnitude and direction of the force but also of the orientation of the surface, for as the orientation changes so, in general, does the force.

- Consequently, nine components must be defined to specify the state of stress. This is shown in the illustration below.
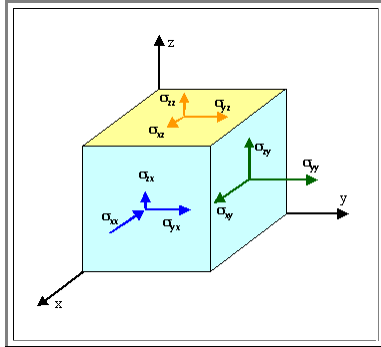
- We have a volume element, here a little cube, with the components of the stress shown as vectors

- Since on any surface an arbitrary force vector can be applied, we decompose it into **3** vectors at right angles to each other. Since we want to keep the volume element at rest (no translation and no rotation), the sum of all forces and moments must be zero, which leaves us with **6** independent components.

- The stress vectors on the other **3** sides are exactly the opposites of the vectors shown

- A picture of the components of the strain tensor would look exactly like this, too, of course.

- The component σ_{ij}, where **i** and **j** can be **x**, **y**, or **z**, is defined as the force per unit area exerted in the **+ i** direction on a face with outward normal in the **+ j** direction by the material *outside* upon the material *inside*. For a face with outward normal in the **– j** direction, i.e. the bottom and back faces in the figure above, σ_{ij} is the force per unit area exerted in the **– i** direction. For example, σ_{yz} acts in the positive **y** direction on the top face and the negative **y** direction on the bottom face.

- The six components with **i** unequal to **j** are the *shear* stresses. It is customary to abbreviate shear stresses with τ. In dislocation studies τ without an index then often represents the shear stress acting on the *slip plane* in the *slip direction* of a crystal.

- As mentioned above, by considering moments of forces taken about **x**, **y**, and **z** axes placed through the centre of the cube, it can be shown that rotational equilibrium of the element, i.e. net momentum **= 0**, requires

$$\tau_{zy} \ = \ \tau_{zy} \qquad \tau_{zx} \ = \ \tau_{xz} \qquad \tau_{xy} \ = \ \tau_{yx}$$

- It therefore does not matter in which order the subscripts are written.

- The three remaining components σ_{xx}, σ_{yy}, σ_{zz} are the *normal* components of the stress. From the definition given above, a *positive* normal stress results in *tension*, and a *negative* one in *compression*. We can define an **effective pressure** acting on a volume element by

$$p \ = \ - \ \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$$

For some problems, it is more convenient to use **cylindrical polar coordinates** (*r*, θ, *z*).

- This is shown below; the proper volume element of cylindrical polar coordinates, is essentially a "*piece of cake*".
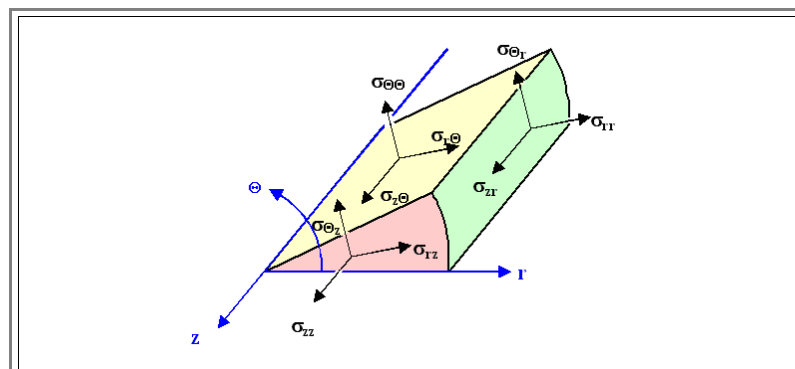
Is it a piece of cake indeed? Well - *no*!

- The picture above is straight form the really good book of **Introduction to Dislocations** of **D. Hull** and **D. J. Bacon**, but it is a little bit wrong. But since it was only used a basic illustration, it did not produce faulty reasoning or equations.
- The picture below shows it right - think about it a bit yourself. (Hint: Imagine a situation, where you apply an uniaxial stress and try to keep your volume element in place)
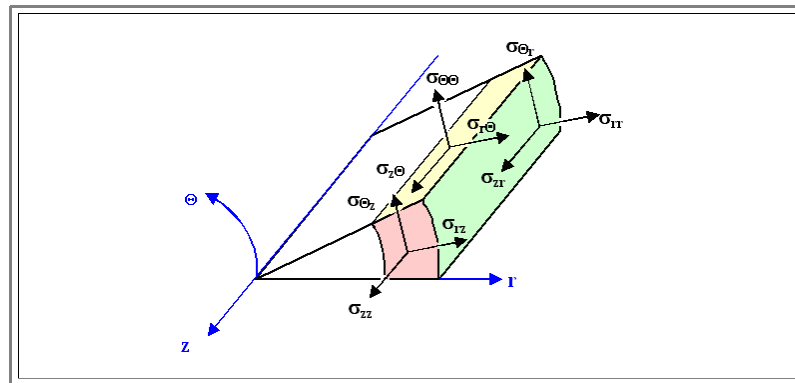
- The stresses are defined as shown above; the stress $\sigma_{z, \theta}$, e.g., is the stress in **z**-direction on the θ plane. The second subscript **j** thus denotes the plane or face of the "slice of cake" volume element that is perpendicular to the axis denote by the sunscript - as in the cartesian coordinate system <u>above</u>. The yellow plane or face thus is the θ plane, green corresponds to the **r** plane and pink denotes the **z** plane

Material Laws Relating Stress and Strain

In the simplest approximation (which is almost always good enough) *the relation between stress and strain is taken to be linear*, as in most "material laws" (take, e.g. "**Ohm's** law", or the relation between electrical field and polarization expressed by the dielectric constant); it is called "**Hooke's law**".

- Each strain component is linearly proportional to each stress component; in full generality for *anisotropic* media we have, e.g.

$$\epsilon_{11} = a_{11}\sigma_{11} + a_{22}\sigma_{22} + a_{33}\sigma_{33} + a_{12}\sigma_{12} + a_{13}\sigma_{13} + a_{23}\sigma_{23}$$

- For symmetry reasons, not all a_{ij} are independent; but even in the worst case (i.e. triclinic lattice) only **21** independent components remain.
- For *isotropic* solids, however, only *two* independent a_{ij} remain and Hooke's law can be written as

$$\sigma_{xx} = 2G \cdot \epsilon_{xx} + \lambda \cdot (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$$

$$\sigma_{yy} = 2G \cdot \epsilon_{yy} + \lambda \cdot (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$$

$$\sigma_{zz} = 2G \cdot \epsilon_{zz} + \lambda \cdot (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$$

$$\sigma_{xy} = 2G \cdot \epsilon_{xy}$$

$$\sigma_{yz} = 2G \cdot \epsilon_{xy}$$

$$\sigma_{zx} = 2G \cdot \epsilon_{zx}$$

- The two remaining material parameters λ and **G** are known as **Lamé constants**, but **G** is more commonly known as the **shear modulus**.

It is customary to use different elastic moduli, too. But for isotropic cubic crystals there are always only *two* independent constants; if you have more, some may expressed by the other ones.

- <u>Most frequently used</u>, and most useful are **Young's modulus**, **Y**, **Poisson's ratio**, ν, and the **bulk modulus**, **K**. These moduli refer to simple deformation experiments:
- Under uniaxial, normal loading in the longitudinal direction, **Young's modulus Y** equals the ratio of longitudinal stress to longitudinal strain, and **Poisson's ratio** ν equals the negative ratio of lateral strain to longitudinal strain. The **bulk modulus K** is defined to be $- p/\Delta V$ (**p** = pressure, ΔV = volume change). Since only two material parameters are required in Hooke's law, these constants are interrelated by the following equations

$$Y = 2G \cdot (1 + \nu)$$

$$\nu = \frac{\lambda}{2 \cdot (\lambda + G)}$$

$$K = \frac{Y}{3 \cdot (1 - 2\nu)}$$

Typical values of Y and ν for metallic and ceramic solids are in the ranges $Y = (40\text{-}600)\ \text{GNm}^{-2}$ and $\nu = (0.2 - 0.45)$, respectively.

Elastic Energy

A material under strain contains elastic energy - it is just the sum of the energy it takes to move atoms off their equilibrium position at the bottom of the potential well from the binding potential. Since energy is the sum over all displacements time the force needed for the displacement, we have:

- **Elastic strain energy E_{el}** per unit volume = one-half the product of stress times strain for each component. The factor **1/2** comes from counting twice by taking each component. Thus, for an element of volume **dV**, the elastic strain energy is

$$dE_{el} = \tfrac{1}{2} \cdot \sum_{i = x,y,z} \sum_{j = x,y,z} \sigma_{ij} \cdot \epsilon_{ij} \cdot dV$$

- For polar or cylindrical coordinates we would get a similar formula.

We do not actually have to calculate the energy with this formula (be grateful), but you must remember: If we have the stress field, we can calculate the strain field. If have both, we can calculate the energy.

- And if we have the energy we have (almost) everything! Minimizing the energy gives the equilibrium configuration; gradients of the energy with respect to coordinates give forces, and so on.