

Details on Stress and Strain.

This handout is aimed at clearing up confusions about the second rank stress and strain tensors, and the fourth rank tensor connecting them, and the standard engineering "contraction" into 6-vectors and a 6x6 elastic constant matrix. It also addresses aspects of net forces and strain energy in terms of the two approaches.

Strain Definition

In a strained crystal a vector **R** becomes a vector **R'** as follows:

$$\mathbf{x}' = (1 + \frac{u_x}{x})\mathbf{x} + \frac{u_y}{y}\mathbf{y} + \frac{u_z}{z}\mathbf{z}$$

$$\mathbf{y}' = \frac{u_x}{x}\mathbf{x} + (1 + \frac{u_y}{y})\mathbf{y} + \frac{u_z}{z}\mathbf{z}$$

$$\mathbf{z}' = \frac{u_x}{x}\mathbf{x} + \frac{u_y}{y}\mathbf{y} + (1 + \frac{u_z}{z})\mathbf{z}$$

The deformation matrix e_{ij} is defined as:[‡]

$$e_{ij} = \frac{u_i}{x_j}$$

In terms of this matrix: $\mathbf{x}' = (1 + e_{11})\mathbf{x} + e_{12}\mathbf{y} + e_{13}\mathbf{z}$ (xyz cyclic). The deformation may be decomposed into a symmetric part (called strain) and an antisymmetric part (rotation).

$$\text{strain: } e_{ij} = \frac{1}{2} (e_{ij} + e_{ji}) \quad \text{rotation: } -e_{ij} = \frac{1}{2} (e_{ij} - e_{ji})$$

The strain part involves stretching or compressing bonds within the crystal, and results in a change in potential energy of the crystal (strain energy). The rotation part simply rotates the entire crystal. This does not change the internal strain energy of the solid. The symmetric 3x3 strain matrix has only 6 independent elements. It is convenient to define:

$$\vec{e} = (e_1, e_2, e_3, e_4, e_5, e_6) = (e_{11}, e_{22}, e_{33}, e_{23} + e_{32}, e_{31} + e_{13}, e_{12} + e_{21}),$$

$$\text{or } \vec{e} = \begin{pmatrix} \frac{u_x}{x} & \frac{1}{2} \frac{u_x}{y} + \frac{u_y}{x} & \frac{1}{2} \frac{u_z}{x} + \frac{u_x}{z} & e_1 & \frac{e_6}{2} & \frac{e_5}{2} \\ \frac{1}{2} \frac{u_x}{y} + \frac{u_y}{x} & \frac{u_y}{y} & \frac{1}{2} \frac{u_z}{y} + \frac{u_y}{z} & \frac{e_6}{2} & e_2 & \frac{e_4}{2} \\ \frac{1}{2} \frac{u_z}{x} + \frac{u_x}{z} & \frac{1}{2} \frac{u_z}{y} + \frac{u_y}{z} & \frac{u_z}{z} & \frac{e_5}{2} & \frac{e_4}{2} & e_3 \end{pmatrix}$$

[‡] The use of e for general deformation and e for symmetric strain is the one in the 7th edition of Kittel's *Introduction to Solid State Physics*, EXCEPT he uses $e_{xy} = e_6 = e_{xy} + e_{yx}$. The classic text by J.F. Nye, *Physical Properties of Crystals*, however, uses e for general deformation and e for symmetric strain.

In terms of the 6-vector description, $\mathbf{x} = (1 + e_1)\mathbf{x} + \frac{e_6}{2}\mathbf{y} + \frac{e_5}{2}\mathbf{z}$. The extra, inelegant factor of two in this equation results from a desire to have the energy equation (see last section) NOT contain extra factors of two.

Physical Meaning of various elements:

The vectors \mathbf{x} , \mathbf{y} and \mathbf{z} are orthogonal, but the primed coordinates are not. Both the overall volume (from diagonal strain elements) and the angles (from off-diagonal elements) will change.

Volume

A box of initial volume $v = xyz$ will (to first order in the small changes) change by a fractional amount :

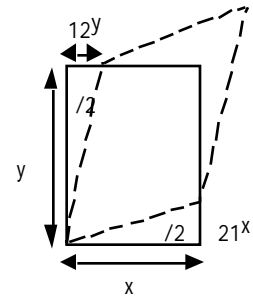
$$\begin{aligned} \frac{\Delta v}{v} &= \frac{(\Delta x)yz + (x)\Delta yz + (xy)\Delta z}{xyz} = \frac{\Delta x}{x} + \frac{\Delta y}{y} + \frac{\Delta z}{z} \\ &= Tr = e_1 + e_2 + e_3 \end{aligned}$$

Angles

The box is distorted by the off-diagonal strain elements. For example, consider an initial square in the xy plane. The deviation from right angles between the axes is given by[‡]:

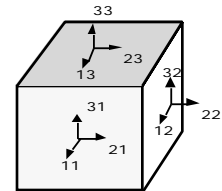
$$\Delta \theta = \theta' - \theta = e_6$$

Thus the components e_μ , $\mu = 1,2,3$ refer to the fractional change in length along the major axes, while the components e_μ , $\mu = 4,5,6$ refer to the change in angle between the major axes.



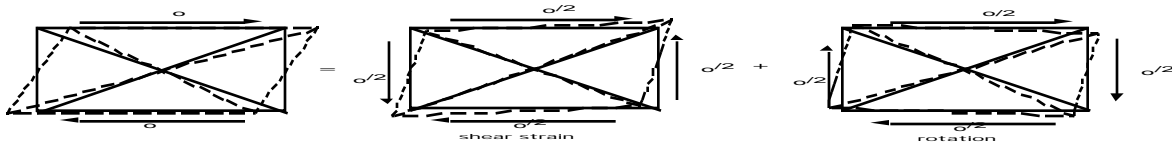
Stress Tensor

The stress tensor reflects the force per unit area on an oriented area of the solid. The first subscript gives the direction of the force, while the second gives the face of the cube on which it is acting. The sketch at the right shows the force per unit area on a cube with the x -face facing out, y to the right and z up. The units of stress are the same as those of pressure. Stress is applied like string tension: there are equal and opposite forces on the other (hidden) three faces of the cube.



Shear Stress and Rotation

The stress matrix that leads to strain in the crystal is symmetric, as may be seen from the following.



[‡]Besides the figure, this can also be seen from the dot product $\mathbf{x} \cdot \mathbf{y} = \frac{u_x}{y} + \frac{u_y}{x} = e_6$ for unit vectors, which is $\cos \theta = \sin(\frac{\theta}{2}) \sim \theta$ (defined in top figure, θ = angle between \mathbf{x} and \mathbf{y}).

Consider a case where the only non-zero stress component is $\tau_{21} = \tau_{12} = \tau_0$. It applies no net force, but the couple yields a net torque as well as a shear strain. It can be decomposed into a shear stress ($\tau_{21} = \tau_{12} = \tau_0/2$) and a rotation ($\tau_{21} = -\tau_{12} = \tau_0/2$) (see figure, which is a view down the $z(x_3)$ axis of a square in the xy plane). The rotation does not cause relative displacements of the atoms, and doesn't cost strain energy. Any work here leads to kinetic energy of rotation and not stored potential energy. The situation with $\tau_{xy} = \tau_{yx} = \tau_0/2$, on the other hand doesn't cause rotation around or displacement of the center of mass. Rather, it stores potential energy in the shear strain of the material.

Summary: If the cube is in equilibrium, with no torque, then $\tau_{ij} = \tau_{ji}$.

The symmetry again means there are only 6 independent components. For the stress, however, there is no extra factor of two in the definitions:

$$\tau = \begin{pmatrix} 1 & 6 & 5 \\ 6 & 2 & 4 \\ 5 & 4 & 3 \end{pmatrix}$$

Inhomogeneous Stress and Net Force

If the stress is homogeneous, there is no net force on the cube. However, if the stress is inhomogeneous, there is a net force, which arises from the difference between forces on opposing sides.

The force on a cube face is the product of the stress with the face area. The force in the i direction on the two i faces is then:

$$F_{ii} = \tau_{ii}^0 + \frac{\tau_{ij}}{x_i} \frac{x_j}{2} x_j x_k + - \tau_{ii}^0 - \frac{\tau_{ij}}{x_i} \frac{-x_j}{2} x_j x_k = \frac{\tau_{ij}}{x_i} x_j x_k,$$

where τ_{ii}^0 is the value of the stress tensor at the center of the cube and x_j denotes the length of the cube in the j direction. Summing over all six faces for a net force in the i direction we have:

$$F_i = \frac{\tau_{ii}}{x_i} x_i x_j x_k + \frac{\tau_{ij}}{x_j} x_j x_k x_i + \frac{\tau_{ik}}{x_k} x_k x_i x_j.$$

Each term contains the volume of the cube. The force on a unit volume of the solid may thus be rewritten in terms of a "divergence" of the stress matrix:

$$f_i = \frac{1}{v} F_i = \sum_j \tau_{ij}$$

which is compactly written as:

$$\vec{f} = \nabla \cdot \tau.$$

Note this requires the 3x3 description of stress. Converting to forces from the 6-vector requires going back to the 3x3 form.

Elastic Constants

The stress and strain second rank tensors are related by the fourth rank tensors compliance (\vec{s}) and stiffness (\vec{c}):

$$\epsilon_{ij} = c_{ijkl} e_{kl} \quad e_{ij} = s_{ijkl} \epsilon_{kl}$$

Note the inverse notation: the symbol c is referred to as stiffness (also called elastic constant) and the symbol s is referred to as compliance (also called modulus). Don't ask me why.

If we are interested in the storage of energy and not the translation or rotation of the crystal, the stress and strain tensors are symmetric. This means $c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk}$, and the 81 independent components reduce to 36. This is good, since we want to set up a 6x6 matrix connecting the 6-vector forms of the stress and strain.

The 36 stiffness components are related as $c_{ijkl} = C_{mn}$, with the compression:

ij	m
11	1
22	2
33	3
23	4
31	5
12	6

The 36 compliance components, on the other hand, have extra factors of 2 and 4 resulting from the different initial compression of the 3x3 to 1x6 forms in stress and strain:

$$\begin{aligned} s_{ijkl} &= S_{mn} && \text{both } m, n = 1, 2, 3 \\ 2s_{ijkl} &= S_{mn} && \text{either } m \text{ or } n = 4, 5, 6 \\ 4s_{ijkl} &= S_{mn} && \text{both } m, n = 4, 5, 6 \end{aligned}$$

The 36 components of the 6x6 elastic constants reduce to 21 independent components since $S_{mn} = S_{nm}$ and $C_{mn} = C_{nm}$. Only *triclinic* crystals, however, have 21 independent elastic constants. In an *isotropic* medium, symmetry reduces the number all the way to 2 independent constants, although they are talked about in 3 ways: Young's modulus (Y or E) is $1/s_{11}$, Poisson's ratio $\nu = -s_{12}/s_{11}$, and the Rigidity Modulus, $G = 1/s_{44} = 1/[2(s_{11}-s_{12})]$. In terms of the stiffness, they are usually written in terms of λ and μ (μ = shear modulus), $c_{11}=2\mu+\lambda$, $c_{12} = \lambda$, $c_{44} = \mu$. The Poisson ratio tells you the ratio of the compression in one dimension when you pull in the other -- typically around 0.25. In a *cubic* crystal there are 3 independent components, s_{11}, s_{12} and s_{44} , as you saw in your homework. In a *hexagonal* crystal (wurtzite, quartz, sapphire), there are 6: $s_{11}=s_{22}$, s_{33} , s_{12} , $s_{23}=s_{13}$, $s_{44}=s_{55}$, and s_{66} (the different axis is 3).

Aside on transforming crystal axes:

If you are growing a lattice-mismatched crystal in the [100] direction, then the distortions of the lattice are straightforward to determine from the standard xyz orientation of the stress-strain tensors. The elastic constants in their 6x6 form may be directly applied. However, if you are growing in a different direction, the ratio of expansion in the growth direction to compression in the surface plane is no longer given directly by the Poisson ratio. The best approach is to determine your initial

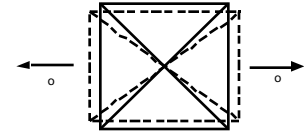
stress field in the growth coordinate system; rotate that into the xyz coordinate system; apply the elastic constants to determine the xyz strain components, and then rotate back to your growth coordinate system. See, for example, the application of (111) stress in the fourth HW set.

Energy Considerations

The discussion so far has centered on displacements -- strain -- and forces -- stress. A force acting through a displacement exerts work, and that work is stored as energy in the crystal. This relation between energy and elastic constants enables their calculation from band-structure and phonon calculations.

The discussion below is split between uniaxial stress, which is applied along one of the principal axes, and shear stress, which mixes axes.

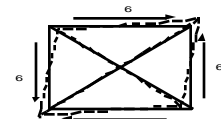
Uniaxial Stress



Consider a uniaxial stress, $\sigma_{11} = \sigma_1 = \sigma$. The unit cube increases in length along the x direction by $e_{11} = e_1 = S_{11} \sigma$, and decreases along the y (and z) directions by $e_{22} = e_2 = S_{12} \sigma$ (S_{12} is usually negative). Only the displacements in the direction of the force give non-zero work, storing potential energy. To determine work, compare to a spring, with a displacement $u_x = \frac{u_x}{x} x = e_1 x$, where $x =$ unit of length in the x direction, and a force $F = \sigma A = C_{11} e_1 A = C_{11} u_x (xA)$, where $A = yz =$ unit of area perpendicular to the x -direction.[‡] The differential work/unit volume is $dw = \sigma de_1$, which integrates to the stored potential energy density $u = \frac{1}{2} \sigma e_1 = \frac{1}{2} C_{11} e_1^2$. Uniaxial components in the y and z directions act in a similar manner.

If there are two uniaxial components simultaneously, then the net displacements must be used to calculate the work. For example imagine a stress σ_1, σ_2 , and all other components zero. The displacement in the x direction of a unit cube is now $e_{11} = e_1 = S_{11} \sigma_1 + S_{12} \sigma_2$. The force due to σ_2 , however, still does no work on the x displacement of the x -face (a y displacement of the x face is connected to shear, discussed below). In the absence of shear (pure combinations of uniaxial stress applied along the x, y and z axes), we have $u = \frac{1}{2} (\sigma_1 e_1 + \sigma_2 e_2 + \sigma_3 e_3)$, or equivalently $u = \frac{1}{2} (\sigma_{11} e_{11} + \sigma_{22} e_{22} + \sigma_{33} e_{33})$, but now the e 's (or the σ 's, depending on which is the dependent or independent variable) depend on all the other σ 's (or e 's).

Shear Stress



Shear stresses also enter the energy as a product of stress and displacement with the same subscript, which may be seen as follows. Consider a stress field of pure $\sigma_6 = \sigma_{xy} = \sigma_{yx}$ acting on a cube. The x relative displacement of the top and bottom faces (parallel to the σ_{xy} force) is $e_{xy} = \frac{e_6}{2}$, for a differential work element $dw_{tb} = \sigma_{xy} de_{xy} = \frac{1}{2} \sigma_6 de_6$. The vertical relative displacement of the left and right faces (parallel to the σ_{yx} force) is $e_{yx} = \frac{e_6}{2}$, for a differential work element of $dw_{rl} = \sigma_{yx} de_{yx} = \frac{1}{2} \sigma_6 de_6$. The potential energy change of the entire cube due to a pure σ_6 shear is then found from:

$$dw = dw_{tb} + dw_{rl} = \sigma_{xy} de_{xy} + \sigma_{yx} de_{yx} = \sigma_6 de_6$$

[‡] The force constant of a spring depends on the length of the spring, and whether you have a fat or skinny piece of the same material. Internally, however, the atoms can't know how big the spring really is. The relations we develop here connect a local property (elastic constants) with a macroscopic measurement (force constant).

$$u_6 = \frac{1}{2} \left(\tau_{xy} e_{xy} + \tau_{yx} e_{yx} \right) = \frac{1}{2} \tau_{66} e_6 = \frac{1}{2} C_{66} e_6^2$$

Note that by including the factors of two differently in the contraction of the stress and strain matrices, we are left *without* extra factors of 2 in the above equation.

Net Result

The differential work per unit volume done in deforming a solid is:

$$dw = \sum_{i,j=1}^3 \tau_{ij} de_{ij} = \sum_{m=1}^6 \tau_m de_m$$

Integrating the work, we find the potential energy density:

$$u_{strain} = \frac{1}{2} \sum_{m=1}^6 \tau_m e_m = \frac{1}{2} \sum_{m,n=1}^6 C_{mn} e_n e_m$$

We expect a force to be the derivative of the energy with respect to distance. The equivalent here is:

$$\frac{\partial u}{\partial e_m} = \sum_{n=1}^6 C_{mn} e_n = \tau_m$$

The force constants may be found similarly as:

$$\frac{\partial^2 u}{\partial e_m \partial e_n} = C_{mn} = C_{nm}$$