Tensor Properties of Materials

Lecture Notes

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1 Linear properties of materials

1.1 Linear response in materials

In physics we often use linear equations to quantitatively describe that some external cause results in a proportional response of the system. These relationships can be written formally as a linear equation of the form

$$\text{effect} = \text{proportionality factor} \times \text{cause}.$$

Here the cause is an external 'force' that we apply to our system (or material), while the proportionality factor is a constant property of our material. Given knowledge of these two quantities we can predict exactly how much is the resulting 'effect'. To be more concrete, let us consider now a few examples. First, recall that an electrical conductor has the property that if we apply an electric field E to it then a current density J will flow through it whose magnitude is proportional to E. The proportionality factor is the conductivity as

$$\underbrace{J}_{\text{current density}} = \underbrace{\sigma}_{\text{conductivity}} \times \underbrace{E}_{\text{electric field}} .$$

We could of course similarly write inverse relations, such as $E = \rho J$ which uses the resistivity $\rho = 1/\sigma$ as the (inverse) proportionality factor. Another example could be the electric susceptibility χ of a material which describes the proportionality between the electric field E and the electric polarisation P as

$$P = \epsilon_0 \chi E.$$

Yet another example is the thermal expansion coefficient α which expresses the proportionality between the extension of a material ϵ and the temperature difference ΔT we apply to the material as

$$\epsilon = \alpha \Delta T.$$

Recall that the extension is actually a strain ϵ and Hook's law relates it to the stress σ via the proportionality factor C that quantifies the stiffness of the material resulting in yet another linear relationship as

$$\sigma = C\epsilon. \tag{1}$$

The above equation is also often expressed in an inverse form as $\epsilon = s\sigma$ where $s = 1/C$ is the elastic compliance.

These equations are, however, only idealisations as in reality the response of a material is never perfectly linear. A response curve of a material is illustrated in Fig. 1(left): When the strain in the material is small then we see a perfectly linear strain-stress relationship as expected from Hook's law in Eq. (1). Depending on the properties of the material large

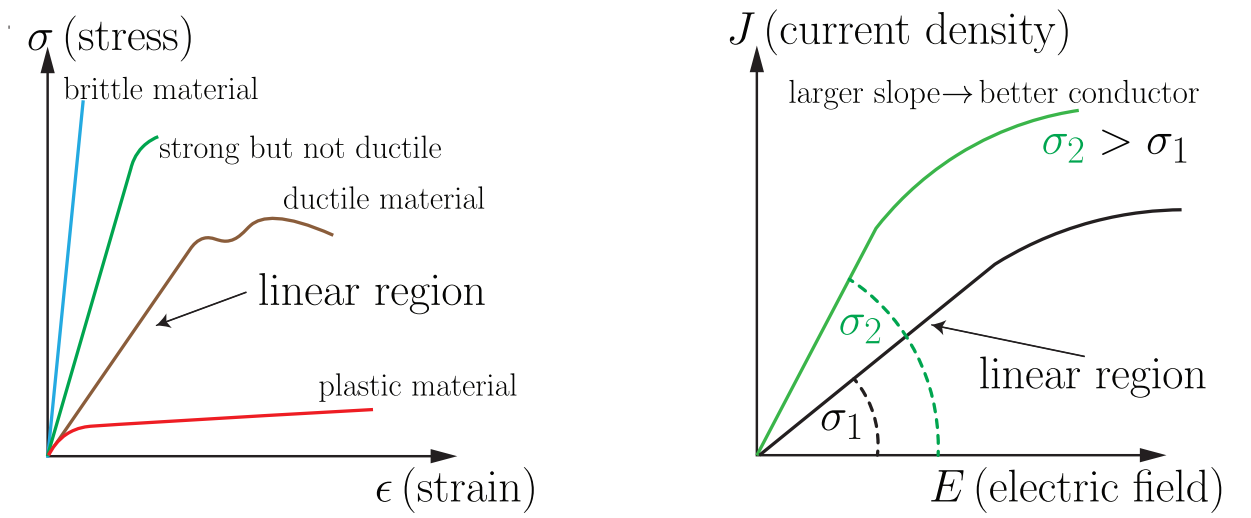


Figure 1: The cause and effect relationship is linear in the region where the material is only subject to a small cause. (left) Stress in different materials as a function of strain. The size of the linear region depends on properties of the material while the slope of the linear region is the stiffness of the material. (right) Current density as a function of the applied electric field. The proportionality factor is the electric conductivity σ and is the slope of the linear region. The material with the steeper slope σ_2 is the better conductor.

stresses may cause plastic deformations and we may see a deviation from Hook's law sooner or later. Similarly, we can imagine that if we induce a large enough current density in a conducting material then it might lead to a heating up. This heating up of the material then leads to a 'proportionality constant' that depends on the temperature ultimately leading to a non-linear response. If the current density is too large than heating may even lead to a complete breakdown.

We can mathematically formalise these observations using a Taylor expansion. In complete generality we can state that the effect $f(x)$ is a function of the cause x. For example, the current density is a function of the electric field as $f(x) = J(E)$. If we assume such a response function is smooth then we can express the dependence using a Taylor series as

$$f(x) = f(0) + f'(0)x + \tfrac{1}{2}f''(0)x^2 + \dots .$$

When the cause, here expressed as the variable x, is 'small' then the effect is almost perfectly linear as in the second third term the square x^2 of the small x can be negligibly small. Thus, the slope in the linear region in Fig. 1 is determined by the derivative $f'(x) = \sigma$ and this derivative is the proportionality in our cause-effect relations.

1.2 Isotropic and anisotropic properties

In Section 1.1 we considered several physical phenomena where a material is subject to an external cause which results in a linear response. However, both the cause and effect were expressed as a number and not as a vector. In a real, three-dimensional world a physical quantity may have both magnitude and direction and we need to use vectors to express them. It is often the case that the direction of the cause and effect are parallel, for example $\vec{J} = \sigma\vec{E}$, and the property of the material σ does not depend on the direction – resulting in the same cause-effect relationship from whichever direction we apply the electric field. For this reason, the proportionality factor, for example the conductivity σ, is a global property of the material and we can describe it just using a scalar. A material in which macroscopic properties are independent of the direction is called an isotropic material. Isotropic materials include the following.

- amorphous materials, for example glasses
- small-grained polycrystalline materials: even if the individual, small crystals are not isotropic, their properties average out on a macroscopic scale and polycrystalline materials are thus isotropic
- some crystals are isotropic due their high symmetry, for example linear response in cubic crystals is isotropic

On the other hand, if a material is anisotropic then both the magnitude and the direction of the effect depends on the directionality of the cause. In such a case we need to describe physical variables in terms of vectors and the proportionality factors in terms mathematical objects that can take into account directionality. We are interested in anisotropy because it is the key to so many technologies and applications, such as the following.

- Liquid crystals: appear in many applications, such as LCD screen, displays, digital watches
- fibre composites: many construction materials, such as wood, reinforced concrete
- single crystals: most crystal lattices
- Piezoelectricity: quartz oscillators are very commonly used, for example, for generating the clock frequency in computers. They are also used in gas lighters, stepper motors, high-precision positioning, sensors, but also in microphones
- many optical devices use anisotropy, such as polarisers, beam splitters

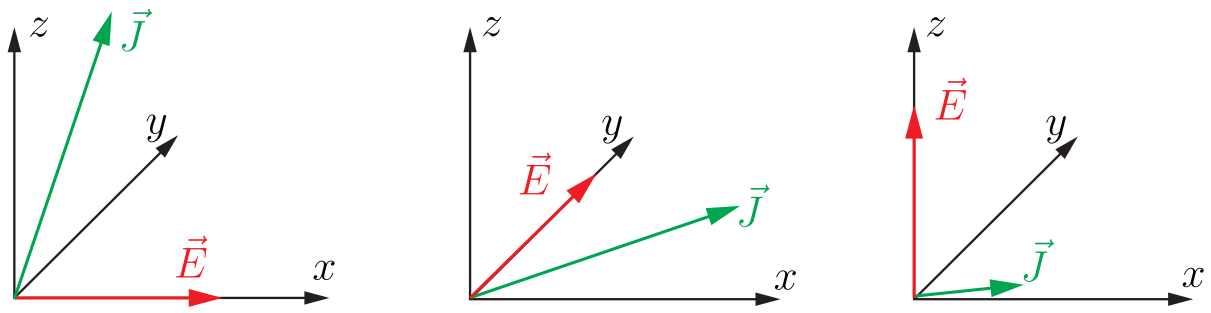


Figure 2: Thought experiment: We apply an electric field $\vec{E}$ to an anisotropic material from the three coordinate directions and measure the resulting components of the current density vector $\vec{J}$.

2 Tensors

2.1 Thought experiment in anisotropic materials

In the previous section we considered isotropic materials which have the property that a sufficiently small external cause, for example an external electric field $\vec{E}$, results in a proportional response that is independent of the direction of $\vec{E}$. We now consider an anisotropic material in which the response, in this example the current density, is not parallel with the electric field. We use vectors to describe both the effect $\vec{J} = (J_x, J_y, J_z)$ and the cause $\vec{E} = (E_x, E_y, E_z)$ and derive a higher mathematical object that correctly describes the anisotropy of the conductivity, which was previously just a proportionality factor σ.

Suppose we apply an electric field to a conductor such that $\vec{E}$ is parallel with the x direction of our coordinate system. We measure the resulting current density. We illustrate in Fig. 2(left) that the vector $\vec{J}$ that we measure has non-zero x, y and z vector entries and it is thus not parallel with $\vec{E}$. Assuming that the electric field is small enough such that the response of the material is linear, we can write down the following relation between cause and effect as

$$\vec{E} = (E_x, 0, 0) \quad \rightarrow \quad J_x = \sigma_{xx} E_x, \qquad J_y = \sigma_{yx} E_x, \qquad J_z = \sigma_{zx} E_x. \tag{2}$$

The proportionality factor between cause ($\vec{E}$) and effect ($\vec{J}$) is the conductivity of the material and we needed three such proportionality factors σ_{xx}, σ_{yx} and σ_{zx} for the following reasons. First, if we repeat the experiment and apply an electric field twice as large $E'_x = 2E_x$, we should measure a current density twice as large $|\vec{J}|' = 2|\vec{J}|$ due to linearity. Second, the two vectors in the two different experiments, $\vec{J}'$ and $\vec{J}$, should point to the same direction (since the electric field had the same direction in both experiments) and only their magnitude

should be different by a factor of 2. It is easy to verify that both properties are satisfied by Eq. (2). This is the reason why the proportionality factor must depend on two indexes, for example, σ_{yx} denotes the linear response in the y direction when an electric field is applied in the x direction.

We can repeat this thought experiment but now applying the electric field in the y direction as illustrated in Fig. 2(middle). We measure the following current densities as

$$\vec{E} = (0, E_y, 0) \quad \rightarrow \quad J_x = \sigma_{xy} E_y, \qquad J_y = \sigma_{yy} E_y, \qquad J_z = \sigma_{zy} E_y. \tag{3}$$

Here we had to introduce three more proportionality constants as the conductivities σ_{xy}, σ_{yy} and σ_{zy} to describe the material's response when the external electric field is applied only from the y direction. Finally we repeat the thought experiment for an electric field applied in the z direction as illustrated in Fig. 2(right). To describe the linear response of the material we need to introduce yet again three more conductivities as

$$\vec{E} = (0, 0, E_z) \quad \rightarrow \quad J_x = \sigma_{xz} E_z, \qquad J_y = \sigma_{yz} E_z, \qquad J_z = \sigma_{zz} E_z. \tag{4}$$

What happens when the electric field is applied from a direction that does not coincide with one of the axis vectors? For example, when the electric field vector is described by some arbitrary vector as $\vec{E} = (E_x, E_y, E_z)$? The answer is simple when the cause and effect are small enough so that the response of the material is linear. In this case all contributions in the x, y and z directions add up independently of each other. For example, we can sum all three contributions to the x component of the current density from the above three equations as $J_x = \sigma_{xx} E_x + \sigma_{xy} E_y + \sigma_{xz} E_z$. We can similarly do so for all components of the current density vector and find the complete response of the material is described by the linear system of equations as

$$\begin{aligned} J_x &= \sigma_{xx} E_x + \sigma_{xy} E_y + \sigma_{xz} E_z, \\ J_y &= \sigma_{yx} E_x + \sigma_{yy} E_y + \sigma_{yz} E_z, \\ J_z &= \sigma_{zx} E_x + \sigma_{zy} E_y + \sigma_{zz} E_z. \end{aligned} \tag{5}$$

2.2 Einstein summation convention

Eq. (5) describes a **linear** cause-effect relationship of an **anisotropic** material. In the following we want to write such equations more compactly and thus we need a way to distil the meaning of Eq. (5). We first introduce a more compact notation for axis vectors and corresponding vector entries.

Reminder 1. We denote the axis vectors of a right-handed Cartesian coordinate system as $\vec{x}_i$ where the free index i can take up any value between 1 and 3 as $\vec{x} = \vec{x}_1$, $\vec{y} = \vec{x}_2$ and $\vec{z} = \vec{x}_3$. We index the corresponding vector entries of vectors using numbers, for example $J_i = \vec{J} \cdot \vec{x}_i$, where again the index i can take up any values between 1 and 3 as $J_x = J_1$, $J_y = J_2$ and $J_z = J_3$.

This indexing scheme allows us to re-write Eq. (5) into the more compact form as

$$J_i = \sum_{j=1}^{3} \sigma_{ij} E_j. \tag{6}$$

We can even further simplify this equation by using the Einstein summation convention: We drop the summation sign and write Eq. (6) compactly as $J_i = \sigma_{ij} E_j$ because by convention we imply that the **repeated indexes are summed over**. For example, in the expression $\sigma_{ij} E_j$ the index j appears twice and thus we interpret this expression as

$$\sigma_{ij} E_j = \sum_{j=1}^{3} \sigma_{ij} E_j = \sigma_{i,1} E_1 + \sigma_{i,2} E_2 + \sigma_{i,3} E_3$$

Furthermore, the free index i can take up any value between 1 and 3 and thus both sides of the equation $J_i = \sigma_{ij} E_j$ refer to 3 entries of a vector, for example, the left-hand side is J_i refers to any of the three vector entries of $\vec{J}$.

Another way of compactly writing Eq. (5) is by recognising that the 9 numbers σ_{ij} can be arranged into a matrix of size 3×3. By convention the first index i indexes the columns of the matrix whereas the second index j indexes the rows. As such, the right-hand side of Eq. (5) expresses a matrix multiplying a column-vector as

$$\begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix},$$

which we can more compactly write as $\vec{J} = \boldsymbol{\sigma} \vec{E}$ where the matrix $\boldsymbol{\sigma}$ is denoted with bold symbols.

Summary 1. The conductivity in an anisotropic material (as illustrated in Fig. 2) can be compactly described using either a matrix-vector multiplication or an Einstein summation as

$$\text{matrix/vector:} \quad \vec{J} = \boldsymbol{\sigma} \vec{E}, \qquad\qquad \text{Einstein summation:} \quad J_i = \sigma_{ij} E_j.$$

We denote column vectors as $\vec{E}$ and refer to their vector entries as E_i while we denote matrices as $\boldsymbol{\sigma}$ and refer to their matrix entries as σ_{ij}.

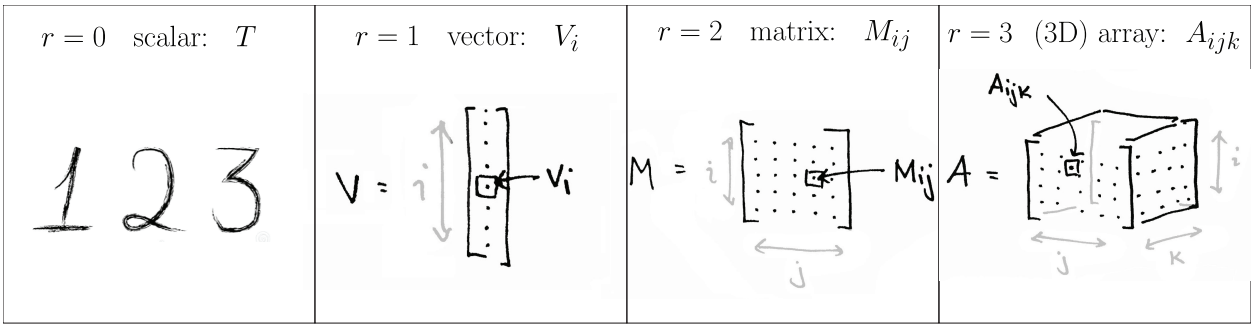


Figure 3: Tensors are rank-r arrays of numbers. For small ranks we can identify them with scalars ($r = 0$), vectors ($r = 1$) and matrices ($r = 2$). For ranks 3 and higher tensors become more complex to visualise.

2.3 What is a tensor?

We have introduced the Einstein summation convention in the previous section that allowed us compactly write equations where we sum over products of vector entries E_i and matrix entries σ_{ij}. While we can refer to the collection of matrix entries σ_{ij} as a matrix, it is important to note that matrices are not just a collection of numbers as they have some special properties. For example we can make sense of a matrix-matrix multiplication or the inverse of a matrix. If we forget about these special properties then σ_{ij} is nothing more than just a 3×3 array of numbers.

Simply put, a tensor, such as σ_{ij}, is an array of numbers and its rank refers to the number of free indexes it has which we illustrate in Fig. 3. For example, the collection of vector entries of a vector, such as T_i, is a rank-1 tensor. Similarly, the collection of matrix entries T_{ij} of a matrix is a rank-2 tensor. It is however important that matrices are not equivalent to rank-2 tensors as matrices have special properties (matrix multiplication, matrix inverse or matrix determinant) that tensors do not have. In another sense though tensors can be viewed as generalisations of vectors and matrices because we can define tensors with higher rank. For example, a three-dimensional array of numbers is a rank-3 tensor which then has 3 free indexes as T_{ijk}.

Why are we interested in using tensors? The reason is they can be a very useful set of tools in so many different applications. For example, we have already seen that we can express linear but anisotropic properties of materials using tensors of rank-2 (matrix) and rank-1 (vector). Furthermore, we will see that some properties of materials are described by higher rank tensors, for example in Section 5.8 we will use rank-4 tensors to describe the stiffness of materials.

As an aside, tensors are also very useful in applications not related to materials. For

explicit	Einstein conv.	matrix notation	type
$a = \sum_{i=1}^{3} v_i w_i$	$a = v_i w_i$	$a = \vec{v} \cdot \vec{w}$	vector/vector
$a_i = \sum_{j=1}^{3} T_{ij} v_j$	$a_i = T_{ij} v_j$	$\vec{a} = \mathbf{T} \cdot \vec{v}$	matrix/vector
$R_{ik} = \sum_{j=1}^{3} S_{ij} T_{jk}$	$R_{ik} = S_{ij} T_{jk}$	$\mathbf{R} = \mathbf{S} \cdot \mathbf{T}$	matrix/matrix
$R_{ij} = \sum_{k,l=1}^{3} S_{ijkl} T_{kl}$	$R_{ij} = S_{ijkl} T_{kl}$		

Table 1: Examples of equations involving tensors. We can explicitly write out a summation (left) that involves products of tensor entries. These can be simplified using the Einstein convention by dropping the summation signs – we assume all indexes are summed over that appear more than once. When the tensors involved are rank-1 or rank-2 then we can use convenient vector and matrix multiplications. When the rank of any of the tensors involved is higher than 2 then we need to resort to Einstein summations.

example, a widespread machine-learning software is called Tensor Flow. The reason is that weights in neural networks are modelled using tensors and Google even developed bespoke hardware for manipulating tensors (called tensor processing units) that have been used, for example, for text recognition in Street View. Tensors are also extremely useful in atomistic simulations of physical or chemical systems, for example, in approximating the wavefunction of a molecule. All these applications actually use tensors of rank much higher than 2.

In this lecture we are primarily motivated to go beyond matrices (rank-2) because certain properties of materials are described using higher-rank tensors. It was very convenient in Section 2.2 to use compact and intuitive matrix and vector multiplications, however, for ranks larger than 2 we must resort to tensors and Einstein summations. We will particularly focus on so-called Cartesian tensors. The reason is that in materials science and in physics we work in a three-dimensional, orthogonal, Cartesian coordinate system spanned by the axis vectors $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$ as introduced in Reminder 1. For example, the number E_1 refers to the electric field vector entry that we would measure along the $\vec{x}_1$ coordinate axis. Furthermore, we used the tensor entry σ_{13} to refer to the conductivity as the proportionality factor between the electric field that we applied in the direction $\vec{x}_3$ and the resulting current density that we would measure in the direction $\vec{x}_1$. In general, all indexes of a Cartesian tensor (for example i, j and k of T_{ijk}) refer to the corresponding coordinate axes of a Cartesian coordinate system [1]. We can use the Einstein summation to conveniently write various different matrix and vector operations as we summarise in Table 1.

[1] See the Wikipedia page for more information on Cartesian tensors.

Summary 2. A Cartesian tensor of rank r is an r-dimensional array of real numbers with r free indexes that each can take up values 1, 2 and 3 as they refer to the three axis vectors of a Cartesian coordinate system. When multiple tensors appear in an expression then we assume a summation over any index that appears more than once. For example, in the equation $R_{ij} = S_{abi}\, T_{abj}$ we sum over the repeated indexes a and b as

$$R_{ij} = S_{abi}\, T_{abj} = \sum_{a=1}^{3} \sum_{b=1}^{3} S_{abi}\, T_{abj}.$$

We have two free indexes, i and j, thus the result is a rank-2 tensor which we denoted as R_{ij}.

Question 1. As discussed, the expression $\sigma_{ij} E_j$ refers to a matrix multiplying a *column* vector. What does the analogous expression $\sigma_{ij} E_i$ refer to? Hint: we can use the transpose of the matrix (tensor) as $(\sigma^T)_{ij} = \sigma_{ji}$.

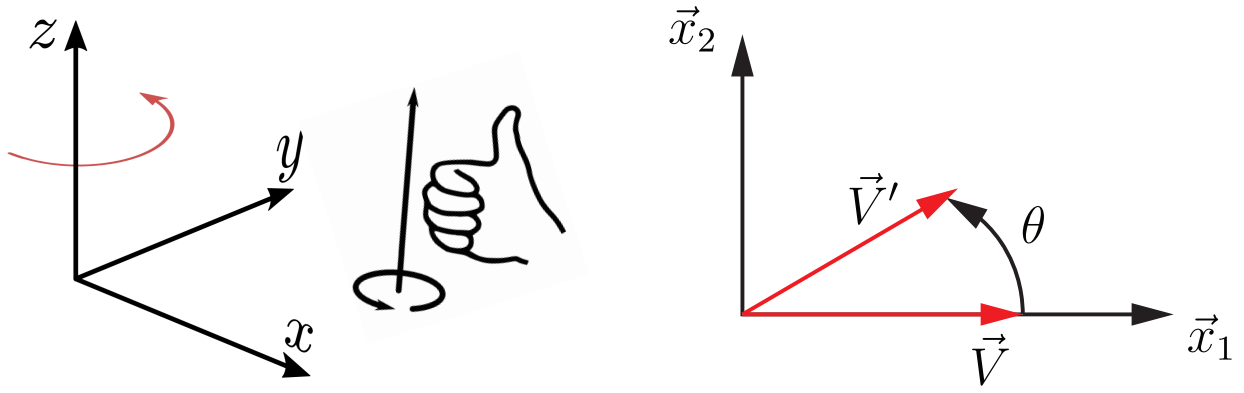


Figure 4: (left) A rotation around the z coordinate axis. By convention, rotations are right-handed. (right) the effect of a z rotation on a vector that is parallel with the x coordinate axis.

3 Coordinate system rotations

Properties of isotropic media do not change when we rotate the material or the external coordinate system. Anisotropic media, on the other hand, do depend on directionality. For example, when we apply an electric field $\vec{E}$ the resulting current density $\vec{J}$ is not necessarily parallel in an anisotropic material and thus we need to treat these quantities as vectors. However, as opposed to scalar quantities in isotropic materials, the vector entries of both $\vec{E}$ and $\vec{J}$ are always relative to a coordinate system. As such, even when the physical vectors are fixed, their vector entries do change as we change our coordinate system. We actually have complete freedom in choosing the coordinate system and our main motivation for doing so is that we can simplify the description of anisotropic materials when we view them in a special coordinate system. For this reason in this section we develop the necessary mathematical tools for compactly describing rotations using rotation matrices.

3.1 Basic rotations

Matrices are mathematical objects that we can view as a collection of rules how to take an 'input' vector and map it to an 'output' vector – more precisely, a matrix multiplies a vector $\vec{V}' = \mathbf{L}\vec{V}$ and transforms its vector entries so that we obtain the vector $\vec{V}'$. We now specifically focus on *rotations* of vectors and we will denote their transformation matrices as $\mathbf{L}$.

To illustrate, let us take a simple example of a rotation around the z coordinate axis. We

will use the right-hand rule as illustrated in Fig. 4(left) and a variable rotation angle that we denote with the symbol θ. We now want to analyse how the rotation matrix $\mathbf{L}$ transforms the entries of a vector via the matrix-vector multiplication $\mathbf{L}\vec{V}$.

Assume we are given a vector and for the sake of argument we assume this vector is parallel with the $\vec{x}_1$ axis vector as $V_1\vec{x}_1$ with length V_1. Fig. 4 illustrates the rotation of this vector around the z axis using the right-hand rule with a rotation angle θ. From Fig. 4(right) it is clear that the new vector after the rotation has the vector entries

$$\mathbf{L}\begin{bmatrix} V_1 \\ 0 \\ 0 \end{bmatrix} = V_1 \begin{bmatrix} \cos\theta \\ \sin\theta \\ 0 \end{bmatrix}. \tag{7}$$

This is of course a quite special case because our vector was chosen to be parallel with the $\vec{x}_1$ axis. For this reason we repeat the previous argument but now the vector we rotate is chosen such that is parallel with the $\vec{x}_2$ axis as $V_2\vec{x}_2$. We find the coordinates after rotation as

$$\mathbf{L}\begin{bmatrix} 0 \\ V_2 \\ 0 \end{bmatrix} = V_2 \begin{bmatrix} -\sin\theta \\ \cos\theta \\ 0 \end{bmatrix}. \tag{8}$$

We could also repeat the previous argument with a vector that is parallel with the $\vec{x}_3$ axis, however, it would be unchanged under our rotation around the z axis. For this reason we can write

$$\mathbf{L}\begin{bmatrix} 0 \\ 0 \\ V_3 \end{bmatrix} = V_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{9}$$

But how about the rotation of any vector? For example an arbitrary vector that we can write as $\vec{V} = (V_1, V_2, V_3)$? We actually already have all ingredients to answer this question and we just need to combine the above equations together. First, we denote the vector that we obtain after the rotation with a prime as $\vec{V}' = \mathbf{L}\vec{V}$. Second, we write our original vector $\vec{V}$ as a sum of its components as $\vec{V} = V_1\vec{x}_1 + V_2\vec{x}_2 + V_3\vec{x}_3$ and apply the rotation to the individual components

$$\vec{V}' = \mathbf{L}\vec{V} = \mathbf{L}\begin{bmatrix} V_1 \\ 0 \\ 0 \end{bmatrix} + \mathbf{L}\begin{bmatrix} 0 \\ V_2 \\ 0 \end{bmatrix} + \mathbf{L}\begin{bmatrix} 0 \\ 0 \\ V_3 \end{bmatrix}. \tag{10}$$

We have already evaluated the rotation of the first component in Eq. (7), the rotation of the second component in Eq. (8), and the rotation of the third component in Eq. (9). We just copy back the right-hand sides of those equations and find our desired matrix-vector equation as

$$\vec{V}' = V_1\begin{bmatrix} \cos\theta \\ \sin\theta \\ 0 \end{bmatrix} + V_2\begin{bmatrix} -\sin\theta \\ \cos\theta \\ 0 \end{bmatrix} + V_3\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{11}$$

One can show (we will discuss this in the next section) that due to Eq. (10), the column vectors in Eq. (11) must be the column vectors of the transformation matrix $\mathbf{L}$, and thus $\mathbf{L}$ must have the form

$$\mathbf{L} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \equiv R_z.$$

This is actually the elementary z rotation matrix which most textbooks use as a mathematical definition of the rotation around the z axis, see for example the Wikipedia page. While above we evaluated the matrix of rotations around the z axis, similarly we could repeat our analysis and rotate vectors around the x or y axes to find the other two basic rotation matrices.

Summary 3. The three basic rotation matrices rotate any column vector by an angle of θ around one of the three Cartesian coordinate axes as

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \qquad R_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, \qquad R_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{12}$$

We discuss in Appendix A that we can construct any rotation matrix, for example, a rotation around a tilted vector, by multiplying at most three basic rotations together.

Question 2. Verify the x and y basic rotation matrices by drawing their effect on vectors as in Fig. 4.

Question 3. Suppose the homogeneous electric field between two large parallel charged plates is described by the vector $\vec{E} = (0.1, 0.5, 0.9)$. We rotate the two plates by 120° around the $\vec{x}_3$ axis. What is the electric field vector $\vec{E}'$ after the rotation of the plates.

3.2 Orthogonal and rotation matrices

In the previous section we introduced basic rotations that rotate around one of the standard axes, for example, around the x axis. How about a rotation around an arbitrary axis? For example, a rotation around an axis that is halfway between the z and x axes? It turns out we can express any rotation in terms of a 3×3 rotation matrix $\mathbf{L}$. Conversely, any 3×3 matrix is a rotation matrix if it satisfies the two properties: First, its row and column vectors must be mutually orthogonal – such a matrix is called an orthogonal matrix. Second, a rotation

matrix $\mathbf{L}$ has determinant one. Both properties are important as we can use the rotation matrix to rotate a set of coordinate axes (basis vectors) as $\vec{x}'_1 = \mathbf{L}\vec{x}_1$, $\vec{x}'_2 = \mathbf{L}\vec{x}_2$, and $\vec{x}'_3 = \mathbf{L}\vec{x}_3$ into a new set of coordinate axes (we have denoted the new axes with a prime).

Note 1. The matrix entries L_{ij} of the transformation matrix are actually cosines of angles between the axes $\vec{x}_i$ and $\vec{x}'_j$. The reason is the following. The coordinate axis $\vec{x}'_j$ is the j^{th} column vector of $\mathbf{L}$ and the i^{th} vector entry of $\vec{x}'_j$ is given by the scalar product $\vec{x}_i \cdot \vec{x}'_j$. This scalar product is actually given by the cosine of the angles between the *old axes* $\vec{x}_i$ and *new axes* $\vec{x}'_j$ and thus $L_{ij} = \cos\theta_{ij}$. For example, θ_{12} is angle between the old axis $\vec{x}_1$ and the new axis $\vec{x}'_2$.

Property 1 (Determinant): The property that $\mathbf{L}$ must have determinant 1 ensures that a right-handed basis remains right handed (with determinant -1 it could be changed to a left-handed one).

Property 2 (Orthogonality): Without loss of generality, we can assume that $\vec{x}_i$ are just the standard coordinate axes in which case the new coordinate axes $\vec{x}'_i$ are column vectors of the rotation matrix. For example, $\vec{x}'_2$ is the second column vector as

$$\vec{x}'_2 = \mathbf{L}\vec{x}_2 = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} L_{12} \\ L_{22} \\ L_{32} \end{bmatrix}.$$

In some sense we have already verified this property: in the example in Eq. (7) we evaluated how the z rotation acts on the vector $V_1\vec{x}_1$ and we found it is rotated into V_1 times the first column vector of the rotation matrix. Similarly, in Eq. (8), and in Eq. (9) we obtained vectors proportional to the second and third column vectors of $\mathbf{L}$.

In general, the column vectors of $\mathbf{L}$ form a coordinate system and it is therefore necessary that they be mutually orthogonal. For example, we want that the scalar product between the first and second axes (column vectors) are zero as

$$L_{i1}L_{i2} = \vec{x}'_1 \cdot \vec{x}'_2 = 0,$$

while we also want the axes (column vectors) be normalised as

$$L_{i1}L_{i1} = \vec{x}'_1 \cdot \vec{x}'_1 = 1.$$

We can summarise all equation of this kind very compactly using our Einstein convention as $L_{ij}L_{ik} = \delta_{jk}$, where the Kronecker delta symbol is a rank-2 tensor that evaluates to 1 when $j = k$ and otherwise it evaluates zero. The equation $L_{ij}L_{ik}$ expresses the scalar product between the basis vector $\vec{x}'_j$ and $\vec{x}'_k$, which is indeed 1 if $j = k$ and zero otherwise. In fact, the Kronecker delta symbol is the identity matrix $\mathbb{1}$ in matrix notation and we can re-write the equation as a matrix-matrix product using that $L_{ij}L_{ik} = (L^T)_{ji}L_{ik}$ which allows us to finally state the defining property of orthogonal matrices.

Summary 4. Orthogonal matrices have mutually orthogonal column and row vectors and thus satisfy the property

$$\mathbf{L}^T\mathbf{L} = \mathbb{1}, \qquad L_{ij}L_{ik} = \delta_{jk},$$

using matrix notation and using tensor notation, respectively.

Most importantly, the above property immediately guarantees us that the transpose is the inverse operation $\mathbf{L}^T = \mathbf{L}^{-1}$. We will make use of this property, for example to undo the effect of a rotation on a vector as $\mathbf{L}^T V' = V$.

Whenever we rotate vectors with a rotation matrix as $\mathbf{L}\vec{V}$ we change its vector entries. This can be interpreted as an *active rotation* that turns $\vec{V}$ into another vector $\vec{V}'$. We now detail in the next section that, at the same time, the transformation of the vector entries by $\mathbf{L}\vec{V}$ can be interpreted such that $\vec{V}$ remains unchanged and only the coordinate axes are being transformed (via the inverse rotation $\mathbf{L}^T$) into a new set of coordinate axes as $\vec{x}'_i = \mathbf{L}^T\vec{x}_i$. This is a *passive rotation* and it changes the vector entries because the vector entries are always relative to a coordinate system.

3.3 Passive rotation of vectors

In Section 3.1 we interpreted the rotation matrix $\mathbf{L}$ such that it acts on a vector $\vec{V}$ and rotates it into another vector $\vec{V}'$ but we described the vector entries of both vectors using the same coordinate system. This is called an *active rotation*. At the same time, rotation matrices also express coordinate axis transformations. For example, if we take a vector that represents something physical, such as an electric field $\vec{E}$, then we would expect this vector is unchanged as a physical quantity should not change when we change our coordinate system. We can repeat the thought experiment in Section 3.1 but now rotating the coordinate system with a negative angle while keeping the vector unchanged $\vec{V}$ as illustrated in Fig. 5 (right) – surprisingly we find the process results in exactly the same transformation of vector entries. This is called a *passive rotation*.

We can show mathematically that the rotation of a vector and the (inverse) rotation of a coordinate system has the same effect on the vector entries as we always specify vector entries *relative to a coordinate system* [2]. First, a passive rotation rotates the coordinate vectors with an inverse rotation as, for example, $\vec{x}'_1 = \mathbf{L}^T\vec{x}_1$. We can calculate the entries of

[2]See also the discussion in Sec 4.2 in: Goldstein, H., C. Poole and J. Safko, Classical Mechanics, 3rd Edition, San Francisco: Addison Wesley, 2002

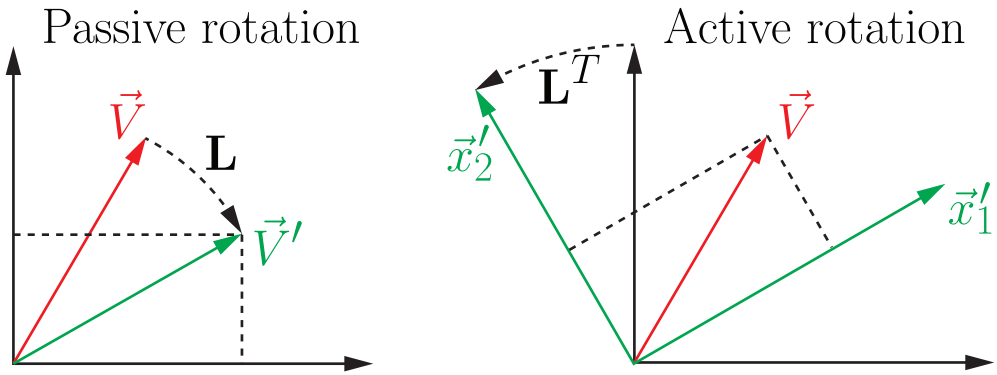


Figure 5: (left) an active rotation $\mathbf{L}$ keeps the coordinate system unchanged and rotates the vector $\vec{V}$ into another vector $\vec{V}' = \mathbf{L}\vec{V}$. (right) A passive rotation inversely rotates the coordinate axes as $\vec{x}_i' = \mathbf{L}^T\vec{x}_i$ but leaves the vector unchanged. Passive and active rotations have the same effect on the vector entries: The vector entries of the unchanged vector $\vec{V}$ in the new coordinate system are exactly those of $\vec{V}'$.

the unchanged vector $\vec{J}$ in the new coordinate system using the scalar product, for example

$$\text{passive rotation:} \qquad J_1' = \vec{J}\cdot\vec{x}_1' = \vec{J}\cdot\left(\mathbf{L}^T\vec{x}_1\right). \tag{13}$$

On the other hand, if we interpret the transformation as an active rotation as we did in Section 3.1 then our transformation matrix formally rotates the vector $\vec{J}$ into a new vector $\vec{J}' = \mathbf{L}\vec{J}$ whose vector entries can be calculated in the unchanged coordinate system as

$$\text{active rotation:} \qquad J_1' = \vec{J}'\cdot\vec{x}_1 = \left(\mathbf{L}\vec{J}\right)\cdot\vec{x}_1. \tag{14}$$

We can now immediately confirm that the vector entry J_1' is the same in case of both active and passive rotations: in a scalar product it does not matter whether a matrix multiplies the vector on the left or the transpose of the matrix multiplies the vector on the right as $(\mathbf{L}\vec{u})\cdot\vec{v} = \vec{u}\cdot\left(\mathbf{L}^T\vec{v}\right)$. This confirms that indeed the right-hand sides of Eq. (13) and Eq. (14) are equivalent.

Question 4. Show the equivalence of scalar products $(\mathbf{A}\vec{u})\cdot\vec{v} = \vec{u}\cdot\left(\mathbf{A}^T\vec{v}\right)$ for any matrix $\mathbf{A}$ and any vector $\vec{u}$ and $\vec{v}$. Hint: rewriting the equation in the Einstein convention helps.

Since in this lecture we are interested in how the entries of a vector or a tensor change under a transformation, rather than how the coordinate system is changed, we use the convention of active rotations. This is also a more natural interpretation of rotation matrices: a matrix acts on a vector and transforms it into another vector. We can of course interchangeably refer to the rotation matrix either as an active rotation or as an inverse a passive

rotation. However, by making one interpretation default any instruction, such as "apply a right-handed x rotation with an angle $\pi/2$", unambiguously identifies an active rotation of a vector or the passive rotation with an angle $-\pi/2$ and not the other way around.

The interpretation as an active transformation is indeed the more common one, especially in programming, scripting and mathematical software, see for example the Wikipedia article, or the relevant wolfram and mathematica and Matlab pages.

Summary 5. A rotation matrix $\mathbf{L}$ satisfies $\mathbf{L}^T = \mathbf{L}^{-1}$ and det$\mathbf{L} = 1$ and expresses a transformation of vector entries due to a change of basis: Changing the coordinate axes $\vec{x}_i' = \mathbf{L}^T\vec{x}_i$ transforms the vector entries of all vectors. This transformation has the same effect on the vector entries as an **active rotation** of the vector as

$$\vec{J}' = \mathbf{L}\vec{J}, \qquad\qquad J_i' = L_{ij}J_j. \tag{15}$$

By convention, $\mathbf{L}$ multiplies **column vectors** from the left.

Question 5. Calculate the matrix $\mathbf{L}$ of the rotation that actively rotates column vectors by an angle $\pi/2$ around the axis that is halfway between the $\vec{x}_2$ and $\vec{x}_3$ axes (the rotation axis is in the direction [011]). See solution in Appendix B.1.

3.4 Rotations of tensors

We are now equipped with all tools to derive how tensors transform under a change of basis. As in the case of vectors, we will be interested in how the entries of a tensor transform due to a change of coordinate system and we thus derive the active rotation of a tensor.

Suppose a tensor that expresses the relation between a cause and an effect, for example the relation between the current density $\vec{J}$ and electric field $\vec{E}$. Imagine we know all tensor entries σ_{ij} because we determined them in the experiment in Section 2.1 so we can write the linear relationship

$$\vec{J} = \boldsymbol{\sigma}\vec{E}. \tag{16}$$

When we determined these tensor entries in Section 2.1 we used a specific coordinate system – we can refer to it as our original coordinate system. However, imagine that for some reason we would like to re-write the above cause and effect in a different coordinate system, for example, because we hope this way Eq. (16) will simplify – indeed we sill see later that in certain coordinate systems the equation greatly simplifies. As we discussed in the previous section, when we rotate our coordinate system then the vector entries of all vectors change which we expressed using a rotation matrix that acts on the original vectors $\vec{J}' = \mathbf{L}\vec{J}$ and

$\vec{E}' = \mathbf{L}\vec{E}$, formally actively rotating them into new vectors. We can apply the inverse rotation to transform the new vectors back to the original ones as $\vec{J} = \mathbf{L}^T\vec{J}'$ and $\vec{E} = \mathbf{L}^T\vec{E}'$ and substitute back the expressions for the original vectors in Eq. (16) as

$$\mathbf{L}^T\vec{J}' = \boldsymbol{\sigma}\mathbf{L}^T\vec{E}'.$$

Let us now multiply both sides of the above equation with $\mathbf{L}$ from left to obtain

$$\mathbf{L}\mathbf{L}^T\vec{J}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T\vec{E}'$$

We can simplify the left-hand side of the equation by using the orthogonality of rotation matrices as $\mathbf{L}\mathbf{L}^T = \mathbb{1}$ to finally obtain the expression

$$\vec{J}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T\vec{E}'.$$

If here we denote the matrix $\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$ then it is immediately clear that the above equation expresses a cause and effect relation just like Eq. (16) but expressed in a new coordinate system as

$$\vec{J}' = \boldsymbol{\sigma}'\vec{E}'.$$

Summary 6. Changing coordinate axes transforms vector entries according to a transformation matrix $\mathbf{L}\vec{J}$ as detailed in Summary 5. Entries of a rank-2 tensor (matrix) are then transformed by rotating the tensor (matrix) using the same rotation matrix as

$$\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T, \qquad \sigma'_{ij} = L_{ik}\sigma_{kl}L_{jl}.$$

So far, we only made an informal statement that a tensor is an "array of numbers" but have not yet precisely stated what is a tensor. The generalisation of the above transformation rule is actually the main defining property of a general tensor.

Note 2. A Cartesian tensor is a rank-r array of real numbers $T_{i_1 i_2 \ldots i_r}$ with the following property. Given a transformation of the Cartesian coordinate system that transforms entries of vectors as $V'_i = \mathbf{L}_{ij}V_j$, a tensor must transform according to (see the Wikipedia page)

$$T'_{i_1 i_2 \ldots i_r} = L_{i_1 j_1}L_{i_2 j_2}\cdots L_{i_r j_r}\,T_{j_1 j_2 \ldots j_r}.$$

Question 6. Show that if we apply the general definition of a tensor in Note 2 to the special case of a rank-2 tensor, we obtain our formula in Summary 6 as expected. Hint: substitute $r = 2$ and substitute the indexes, for example $i_1 = i$, $i_2 = j$, etc.

3.5 Principal axis system

In the previous section we saw that rank-2 tensors transform according to the equation $\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$ when we change the coordinate system. Here a rotation $\mathbf{L}$ is always an orthogonal transformation and maps a rank-2 tensor $\boldsymbol{\sigma}$ onto another rank-2 tensor $\boldsymbol{\sigma}'$. We now want to find a special rotation that maps our tensor to a diagonal form. This will help us to better understand properties of the material because the rotated tensor reveals important information about, for example, symmetries of a crystal. But, let us first recollect a very important property of orthogonal matrices, namely, that they can be used to bring any symmetric matrix into a diagonal form.

Reminder 2. Recall that a symmetric matrix $\mathbf{M}$ has real entries and satisfies $\mathbf{M}^T = \mathbf{M}$. Such matrices have real eigenvalues λ_i and arranging eigenvectors of $\mathbf{M}$ into the orthogonal matrix $\mathbf{L}$ as columns allows us to write $\mathbf{M}$ as a "rotated" diagonal matrix

$$\mathbf{M} = \mathbf{L} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \mathbf{L}^T.$$

As a consequence of Reminder 2 we can diagonalise any rank-2 tensor that satisfies the symmetry $\sigma_{ij} = \sigma_{ji}$, or equivalently in matrix from $\boldsymbol{\sigma}^T = \boldsymbol{\sigma}$, by rotating the coordinate system. The rotation transforms our coordinate system into a special one, called the **principal axis system**, in which the tensor becomes diagonal as

$$\mathbf{L}^T\boldsymbol{\sigma}\mathbf{L} = \begin{bmatrix} \sigma_1^{pas} & 0 & 0 \\ 0 & \sigma_2^{pas} & 0 \\ 0 & 0 & \sigma_3^{pas} \end{bmatrix} \equiv \boldsymbol{\sigma}^{PAS}. \tag{17}$$

Here the column vectors of $\mathbf{L}$ are the eigenvectors $\vec{x}_i^{pas}$ which we refer to as the *principal axes*. The eigenvalues σ_i^{pas} are the *principal components*, for example, here σ_i^{pas} are principal conductivities. These principal axes are eigenvectors of $\boldsymbol{\sigma}$ in the sense that they satisfy the eigenvalue equation

$$\boldsymbol{\sigma}\vec{x}_i^{pas} = \sigma_i^{pas}\vec{x}_i^{pas}. \tag{18}$$

Interestingly, it is a direct consequence of this eigenvalue equation that along the principal directions we find a parallel **cause** and **effect**. To show this we first write our general cause and effect equation $\vec{J} = \boldsymbol{\sigma}\vec{E}$ assuming that the cause, the electric field, is parallel with one of the principal axes and thus substitute $\vec{E} = \vec{x}_i^{pas}$. We find the equation

$$\vec{J} = \boldsymbol{\sigma}\vec{x}_i^{pas},$$

which is exactly the left-hand side of the eigenvalue equation in Eq. (18). For this reason we substitute back the right-hand side of the eigenvalue equation in Eq. (18) as

$$\vec{J} = \sigma_i^{pas} \vec{x}_i^{pas}.$$

We now recollect that the electric field was parallel with the principal direction $\vec{x}_i^{pas} = \vec{E}$ and thus find

$$\vec{J} = \sigma_i^{pas} \vec{E}.$$

In the above equation the anisotropic tensor property appears to behave like an **isotropic** property (parallel cause and effect) – but note that this is only true along the principal directions, when $\vec{E}$ is parallel with one of the three principal axes, and we would see anisotropic behaviour for vectors of any other direction.

Question 7. Recall from Reminder 2 that we can write any symmetric matrix $\mathbf{M}$ as a rotated diagonal matrix as $\mathbf{M} = \mathbf{L}\mathbf{D}\mathbf{L}^T$. Although $\mathbf{L}$ must be an orthogonal matrix, it is not necessarily a proper rotation. A proper rotation satisfies $\det \mathbf{L} = 1$. Show that we can always choose $\mathbf{L}$ with $\det \mathbf{L} = 1$ and thus Reminder 2 can always be interpreted as a proper rotation of a diagonal matrix. Hint: Using the properties of the determinant as $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$ and $\det(\mathbf{A}^T) = \det(\mathbf{A})$ helps. See the solution in Appendix B.2.

4 Visualisation and Crystal Symmetries

4.1 Implicit equation

By now we have developed all necessary mathematical tools to work with tensors and to analyse their properties in the principal axis system. In this section we consider how properties of materials determine tensor properties, such as symmetries of crystals. We will first develop visualisation tools that are quite intuitive as they use simple geometric objects rather than abstract matrices or vectors. The primary advantage of using these visualisation surfaces is that they clearly reflect symmetry properties of tensors. We will see that single crystals can have high symmetry which then manifests in tensor properties that we can directly infer from their visualisations.

The geometric objects we will use are three-dimensional surfaces. Such surfaces can be specified using so-called *implicit* equations or implicit functions. But first, what are implicit functions? Usually we use *explicit* functions, such as $f(x, y) = ax + b + y$ for variables x and y. This equation tells us explicitly that the function value $f(x, y)$ is computed for any argument x and y just by multiplying x with a and adding b and y to the result. In contrast, in an implicit function we relate the variables x and y to each other via an implicit equation that sets constraints that the solution must satisfy. For example, a two-dimensional circle of unit radius is defined by a set of points that satisfy the constraint

$$\text{2D circle:} \qquad x^2 + y^2 = 1.$$

Indeed, this constraint is only satisfied by points that are of unit distance from the origin which is the defining property of a unit circle as illustrated in Fig. 6(b). Similarly, we could consider a circle whose radius is larger or smaller than 1 by rescaling both variables with the desired radius r as $x^2/r^2 + y^2/r^2 = 1$. Following a similar logic, we can write down an implicit equation for an ellipse: we similarly rescale the x and y variables but we use two different scaling factors a and b. The resulting implicit equation is

$$\text{2D ellipse:} \qquad x^2/a^2 + y^2/b^2 = 1,$$

and it defines a 2D ellipse of width $2a$ and height $2b$ as illustrated in Fig. 6(b). In order to specify surfaces in three dimensions we use three variables x, y and z. The generalisation of the unit circle is then the unit sphere which we can specify similarly using the implicit equation

$$\text{3D sphere:} \qquad x^2 + y^2 + z^2 = 1,$$

which is illustrated in Fig. 6(c). The ellipsoid is the generalisation of the ellipse in three dimensions and rescaling the variables x, y, and z, yields its implicit equation as

$$\text{3D ellipsoid:} \qquad x^2/a^2 + y^2/b^2 + z^2/c^2 = 1.$$

In the following we want to extract an implicit equation from a tensor.

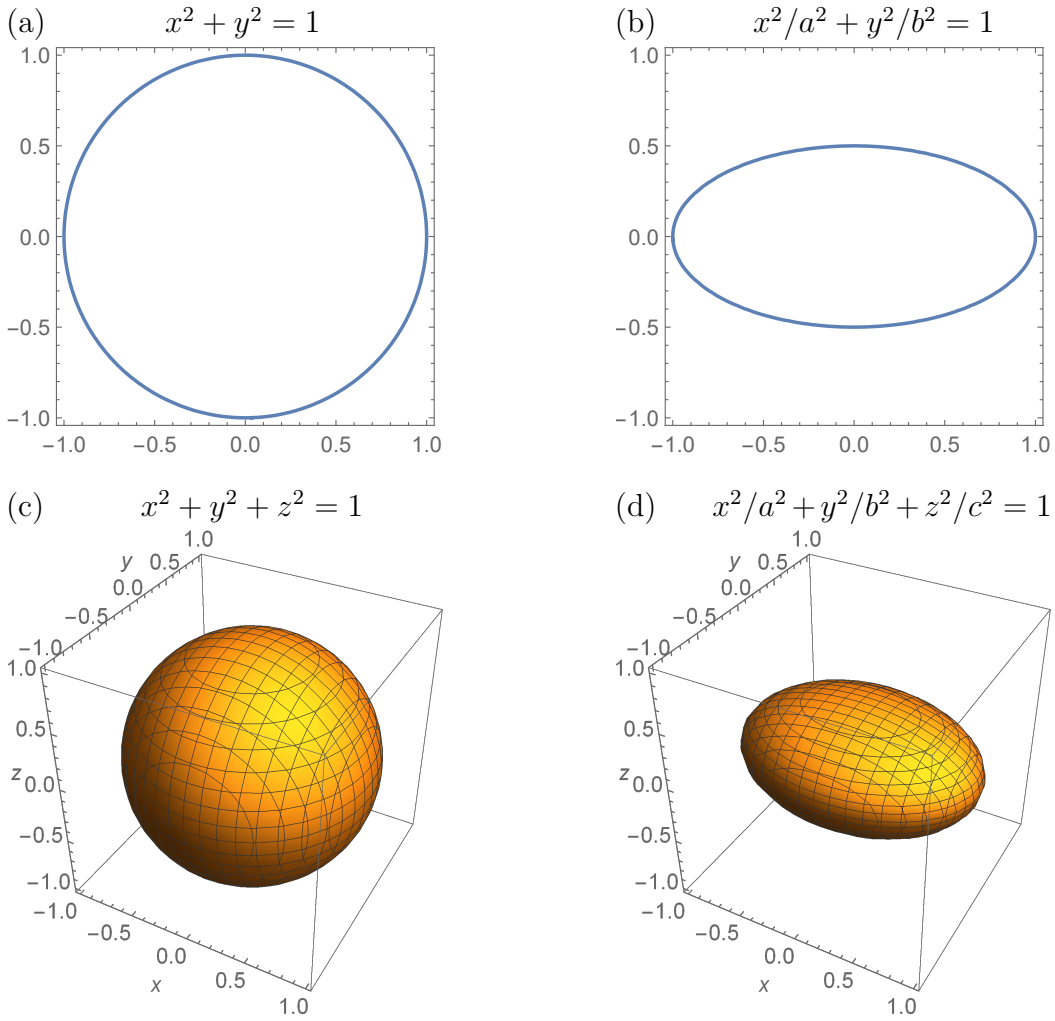


Figure 6: Examples of implicit equations and visualisation of their solutions. (a) 2D circle (b) 2D ellipse (c) 3D sphere (d) 3D ellipsoid.

4.2 Visualising tensors as surfaces

Assume we are given a fixed, rank-2 tensor as a symmetric matrix $\mathbf{T}$. We want to extract a 3D surface from $\mathbf{T}$ that is characteristic to the tensor. We specify this surface as an implicit equation that depends on the three variables x, y and z. First, we arrange the variables into the coordinate (column) vector $\vec{x} = (x, y, z)^T$. Second, we multiply this column vector with our tensor as $\vec{v} = \mathbf{T}\vec{x}$, similarly to how we described physical cause-effect relations. Finally, we define our implicit equation using the scalar product $\vec{x} \cdot \vec{v}$ between the original coordinate vector $\vec{x}$ and $\vec{v}$. This scalar product is actually the length of the parallel component between $\vec{v}$ and $\vec{x}$ as illustrated in Fig. 7. We can now express our implicit equation mathematically

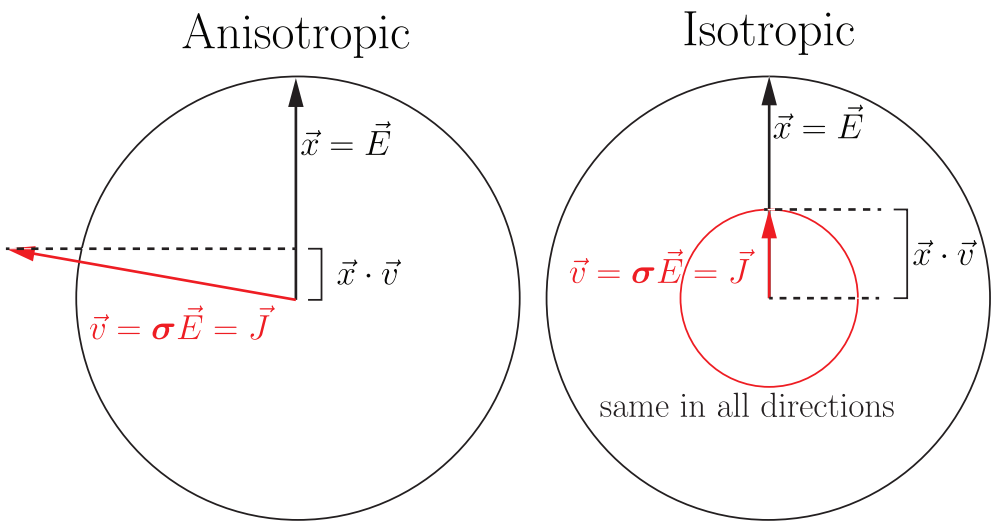


Figure 7: (left) The representation surface is the collection of points $\vec{x}$ that result in the parallel component $\vec{x} \cdot \vec{v} = 1$. Suppose a coordinate-dependent electric field $\vec{x} = \vec{E}$: the representation surface of the conductivity tensor $\boldsymbol{\sigma}$ can be though of as the parallel component $\vec{x} \cdot \vec{v} = \vec{J} \cdot \vec{E}$ between the current density and the electric field due to the cause-effect relation $\vec{v} = \vec{J} = \boldsymbol{\sigma}\vec{E}$. (right) In isotropic materials $\vec{J}$ is always proportional to the electric field with the constant proportionality as $\sigma\vec{E}$, hence the representation surface is a sphere.

as

$$\text{all } \vec{x} \text{ that satisfy:} \qquad \vec{x}^T \mathbf{T} \vec{x} = \vec{x} \cdot \underbrace{(\mathbf{T}\vec{x})}_{\vec{v}} = 1 \qquad \text{for fixed } \mathbf{T}.$$

This equation is only satisfied by points $\vec{x}$ that produce a parallel component $\vec{x} \cdot \vec{v}$ of unit length – and these form points on a surface in 3D that we will refer to as the representation surface of the tensor $\mathbf{T}$. The meaning of the scalar product $\vec{x} \cdot \vec{v}$ is illustrated in Fig. 7 using the example of a cause-effect relationship whereby the vector $\vec{x} = \vec{E}$ is an electric field and the tensor is a conductivity as $\mathbf{T} = \boldsymbol{\sigma}$. The vector $\vec{v}$ is then given by the current density $\vec{J} = \boldsymbol{\sigma}\vec{E}$ and the scalar product then refers to the length of the parallel component between the cause ($\vec{E}$) and effect ($\vec{J}$).

Summary 7. The representation surface of a symmetric, rank-2 tensor is the 3D surface that consist of points $\vec{x} = (x, y, z)^T$ that satisfy the implicit equation $\vec{x}^T \mathbf{T} \vec{x} = 1$.

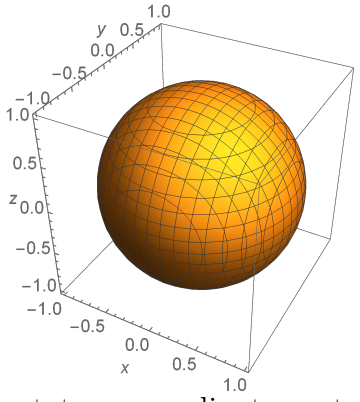
4.3 Examples of surfaces

Let us first consider the simplest case of an isotropic material. Recall that in an isotropic material a tensor $\mathbf{T}$ can be treated as a scalar (or equivalently as a scalar multiple of the identity matrix as $T\mathbb{1}$). In this case our representation surface can be simplified considerably as

$$1 = \vec{x} \cdot (\mathbf{T}\vec{x}) = T\vec{x} \cdot \vec{x}.$$

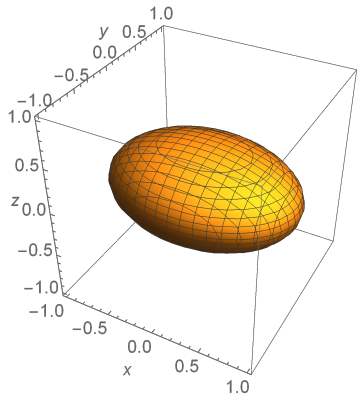
Here the scalar product of the vector with itself is actually the distance of the corresponding point from the origin as $\vec{x} \cdot \vec{x} = x^2 + y^2 + z^2$. We thus find the implicit equation of a sphere of radius $\sqrt{1/T}$ as

Isotropic material: $\quad 1/T = x^2 + y^2 + z^2$



Let us now consider a tensor that is given with respect to a coordinate system that is aligned perfectly with the Principal Axis System. In this case the tensor is diagonal with three non-zero entries as $\mathbf{T} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ and thus our vector can be simplified as $\vec{v} = \mathbf{T}\vec{x} = (\lambda_1 x, \lambda_2 y, \lambda_3 z)^T$. Let us further assume that the principal components are all positive resulting in the implicit equation

principal components > 0: $\quad 1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2$



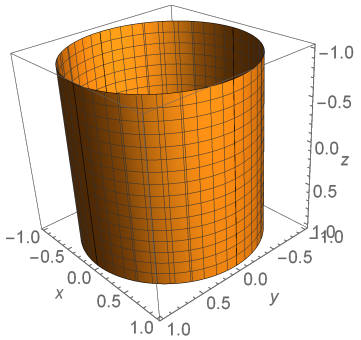
This is the equation for an ellipsoid whose parameters a, b and c are determined by the inverse square roots of the principal components $a = \lambda_1^{-1/2}$, $b = \lambda_2^{-1/2}$, $c = \lambda_3^{-1/2}$.

But what happens when the tensor has negative principal components (eigenvalues)? Although we do not expect a conductivity to be negative, we will consider several tensors later that can have negative principal components. We obtain surfaces that are more general than ellipsoids: Generally any equation of the form $1 = \vec{x}^T\mathbf{T}\vec{x}$ for any symmetric matrix $\mathbf{T}$

is called a quadric and when the coordinate system aligns with the principal axes then the quadric equation simplifies to $1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2$. The difference to an ellipsoid is that the principal components here can be either negative or zero and we can imagine implicit equations, such as $1 = \lambda_1 x^2 - \lambda_2 y^2$ via the eigenvalues $(\lambda_1, \lambda_2, \lambda_3) = (1, -1, 0)$.

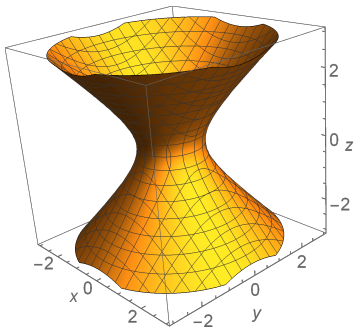
Let us consider the case when we have a zero eigenvalue via the following example: imagine that we have a series of tensors $\mathbf{T}_n$ which we index by n and imagine that each has principal components $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, 1/n)$ that depend on the index n. As all eigenvalues are positive, the corresponding representation surfaces are all ellipsoids. However, each successive ellipsoid in the series has a height $c = \lambda_3^{-1/2} = \sqrt{n}$ that is larger than the previous one. As we keep increasing the index n we find that the height of the ellipsoid grows to infinity. Indeed, we find that the limit corresponds to the eigenvalues $\lim_{n\to\infty}(1, 1, 1/n) = (1, 1, 0)$ whose representation surface is a cylinder as

one p. comp. zero $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, 0)$



Similarly, we could also consider the case when one of the eigenvalues is negative. While we can think about a cylinder (zero eigenvalue) as an infinite number of identical 2D circles stacked on top of each other, a negative eigenvalue $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, -1)$ corresponds to an infinite number of 2D circles stacked on top of each other but the radius of these circles grows as we increase the distance from the origin along the z coordinate. This surface is called a hyperboloid of one sheet as

one p. comp. negative $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, -1)$



Question 8. In the case when the tensor has two negative eigenvalues as, e.g., $(\lambda_1, \lambda_2, \lambda_3) = (1, -1, -1)$, we obtain a hyperboloid of two sheets. Draw this surface or use computer software to visualise it.

For three negative eigenvalues we do not have a real solution of the implicit equation but

in such an instance we could just take $-\mathbf{T}$ and visualise this tensor. In most usual physical phenomena we do not expect to come across negative principal components, in fact, some physical phenomena can only have positive proportionality constants, such as the electrical conductivity. However, in some instances we do have negative proportionality constants, such as in the case of the magnetic susceptibility of a diamagnetic material. Moreover, we will later use tensors to describe physical variables rather than proportionality constants, and those variables can indeed have either negative or zero principal components.

4.4 Rotational properties

How do these surfaces look when the coordinate axes don't exactly align with the principal axes? In other words, what happens when the tensor is not diagonal? In such an instance the equation $\vec{x}^T\mathbf{T}\vec{x} = 1$ becomes really complicated as it is a sum of many terms.

Question 9. When we expand the equation $\vec{x}^T\mathbf{T}\vec{x} = 1$ for a diagonal tensor $\mathbf{T} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ and a position vector $\vec{x} = (x, y, z)^T$ it is only a sum of three terms as $1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2$. Expand the equation $\vec{x}^T\mathbf{T}\vec{x} = 1$ assuming that $\mathbf{T}$ is a full matrix with matrix entries, $T_{1,1}$, $T_{1,2}$, $T_{1,3}$ etc. How many terms does the result have?

We can actually understand how these surfaces look without trying to handle these complicated equations. The reason is that we can diagonalise any symmetric matrix just by rotating the coordinate system due to the property summarised in Reminder 2. We thus take our representation quadric $1 = \vec{x}^T\mathbf{T}\vec{x}$ and substitute the tensor $\mathbf{T}$ with its diagonalised form as $\mathbf{T} = \mathbf{L}\mathbf{D}\mathbf{L}^T$. Here $\mathbf{D}$ is a diagonal matrix and $\mathbf{L}$ is a rotation. The resulting implicit equation is

$$1 = (\mathbf{L}^T\vec{x})^T\mathbf{D}(\mathbf{L}^T\vec{x}),$$

but it is not obvious the above is still a representation quadric. Here, we can interpret the expression $\mathbf{L}^T\vec{x}$ such that it is a rotation of the coordinate vector. We can thus introduce the notation $\mathbf{L}^T\vec{x} = \vec{x}'$ for a position vector $\vec{x}'$ in a rotated coordinate system. Indeed, the result is now clearly a representation quadric in a rotated coordinate system

$$1 = (\vec{x}')^T\mathbf{D}\vec{x}'.$$

Most importantly, this is the representation quadric of a diagonal tensor that we already know how to interpret as we discussed in Section 4.3. Fig. 8 illustrates that the representation quadric of any symmetric tensor $\mathbf{T}$ (Fig. 8(left)) is obtained as follows. First, we diagonalise $\mathbf{T}$, second, we visualise the diagonal matrix $\mathbf{D}$ and third, by rotating the coordinate system we obtain the representation quadric of the general matrix $\mathbf{T}$.

Importantly, the converse holds too: Just by looking at Fig. 8(left) we see that the representation quadric of $\mathbf{T}$ is a cylinder of radius 1 whose axis of symmetry is 45° off

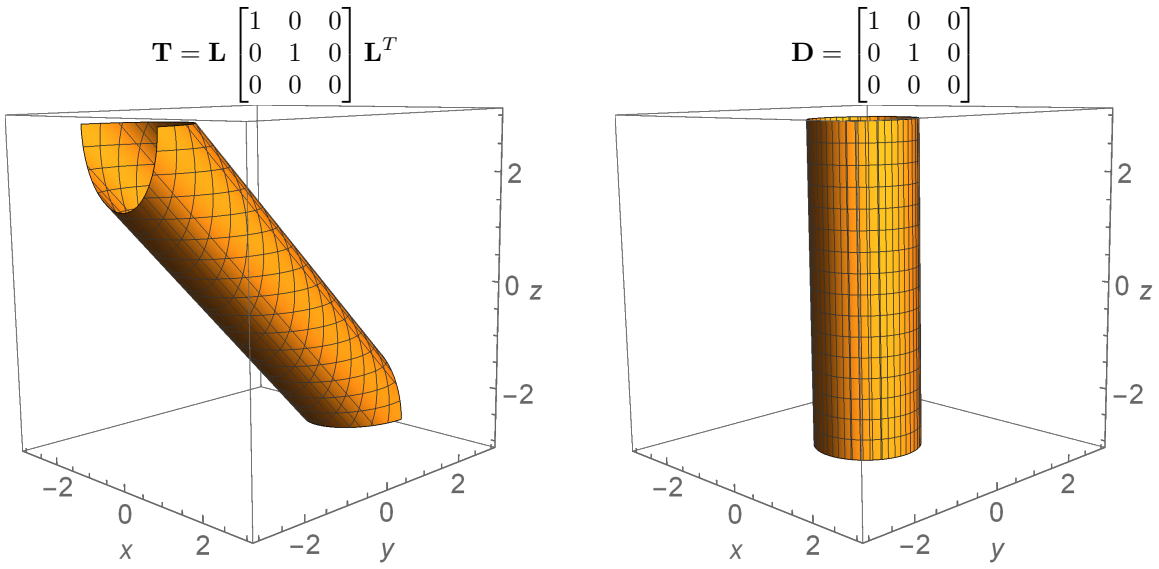


Figure 8: The representation quadric of any symmetric tensor $\mathbf{T}$ can be understood by transforming the tensor into a diagonal form via a rotation: Here $\mathbf{L}$ is a rotation of 45° around $\vec{x}_1$. (left) As we rotate the tensor into the Principal Axis System it becomes diagonal and we can immediately infer its representation quadric based on the eigenvalues (diagonal entries). For example, here they are $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, 0)$ and therefore the representation quadric of $\mathbf{D}$ is a cylinder of radius 1.

between the y and z axes. From this description we can immediately tell that $\mathbf{T}$ must have eigenvalues $(\lambda_1, \lambda_2, \lambda_3) = (1, 1, 0)$ since it is a cylinder of radius 1 and we can also tell that its eigenvectors (principal directions) must be 45° off from the coordinate axes.

Question 10. What is the representation quadric of the tensor $\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$? Hint: diagonalising the matrix first helps to determine the representation quadric.

4.5 Effect of crystal structure

Properties of a crystalline material depend on symmetries of the crystal. As such, if a property of a material is described by a tensor then the tensor, as well as its representation surface, must have the same symmetry properties as the crystal. This is summarised by Neumann's principle.

cryst. syst.	quadric orientation	params.	tensor
cubic	sphere	1	$\begin{bmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & T \end{bmatrix}$
tetragonal, hexagonal, trigonal	symm. around x_3	2	$\begin{bmatrix} T_1 & 0 & 0 \\ 0 & T_1 & 0 \\ 0 & 0 & T_3 \end{bmatrix}$
orthorhombic	x_1, x_2, x_3 parallel to diads	3	$\begin{bmatrix} T_1 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_3 \end{bmatrix}$
monoclinic	x_2 parallel to diad	4	$\begin{bmatrix} T_{11} & 0 & T_{13} \\ 0 & T_{22} & 0 \\ T_{13} & 0 & T_{33} \end{bmatrix}$
triclinic	-	6	$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{bmatrix}$

Table 2: Tensor properties of a crystalline material must contain symmetries of the crystal. Symmetry properties of the 7 crystal systems constrain what principal directions and principal components the corresponding tensors can have.

Neumann's principle: *Any physical property of a crystal must include the symmetry elements of the point group of the crystal.*

The symmetry of the tensor may actually be higher but must include at least the symmetry elements of the crystal. Furthermore, the crystal symmetry axes determine the principal axis system (the principal directions). Table 2 summarises symmetry properties of the 7 crystal systems and the possible eigenvalues (principal components) of the corresponding tensors.

- A cubic crystal has a high symmetry and it only has 1 degree of freedom. The corresponding tensors must be proportional to the identity matrix and the material must thus be isotropic.
- tetragonal, hexagonal and trigonal lattices have an axis of symmetry around the $\vec{x}_3$ axis and thus their tensors must have two identical eigenvalues. This also means that their representation surfaces must have a rotational symmetry around the $\vec{x}_3$ axis, such as a symmetric ellipsoid with axes $a = b$.

5 Applications of tensors

We are now equipped with all necessary mathematical tools to work with tensors. So far our motivation to using tensors was to describe the linear response in anisotropic materials. In these applications the tensors typically express properties of materials, for example, the electric conductivity is a proportionality factor in the equation $\vec{J} = \boldsymbol{\sigma}\vec{E}$. Here we consider some more advanced applications of tensors. In these applications the tensors don't always express properties of the materials but rather they are used to express a physical variable, such as mechanical stress and strain.

5.1 Stress tensor

As we apply forces to a solid body it becomes deformed. Stress is used to describe these forces in a way that the description is independent of the size or the shape of the body. Stress is defined as the force divided by the area it is acting on. For example, if we apply a tension force F to stretch a wire of radius r, the stress is defined as the tension relative to the cross-sectional area as

$$\sigma = \frac{F}{\pi r^2}. \tag{19}$$

Indeed, as we apply a multiple of the tension, for example $4F$ to a wire of radius $2r$, then the stress remains the same σ as the same forces pull the atoms in the wire apart.

In three dimensions, we model stress by taking a infinitesimally small cube of the material and analyse what forces act upon it – and we assume that the stress is homogeneous and all parts of the material experience the same forces. The three edges of the cube are parallel with our coordinate axes $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$ as illustrated in Fig. 9. Each of the six faces of the cube can be described by an axis vector $\vec{x}_1$, $-\vec{x}_1$, $\vec{x}_2$, $-\vec{x}_2$, and $\vec{x}_3$, $-\vec{x}_3$. We only need to take into account what forces act on the three faces of the cube that correspond to the three axis vectors $\vec{x}_1$, $\vec{x}_2$ and $\vec{x}_3$, while the forces acting on the opposite faces must be equal and opposite as the total force acting on the cube in equilibrium must be zero. Consider the force acting on the face that corresponds to the axis $\vec{x}_1$: this force has some component that is parallel with the axis σ_{11} but it can also have components in the other two directions which we denote as σ_{21} and σ_{31} as illustrated in Fig. 9(left). We similarly repeat this analysis for the other two faces and find the 9 tensor entries that describe the stress tensor as forces acting on the three faces of the cube

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}. \tag{20}$$

Since stress is described by a rank-2 tensor, it relates two vectors to each other. For this reason, we can define the traction vector $\vec{T}$ as a force per unit area that acts on the

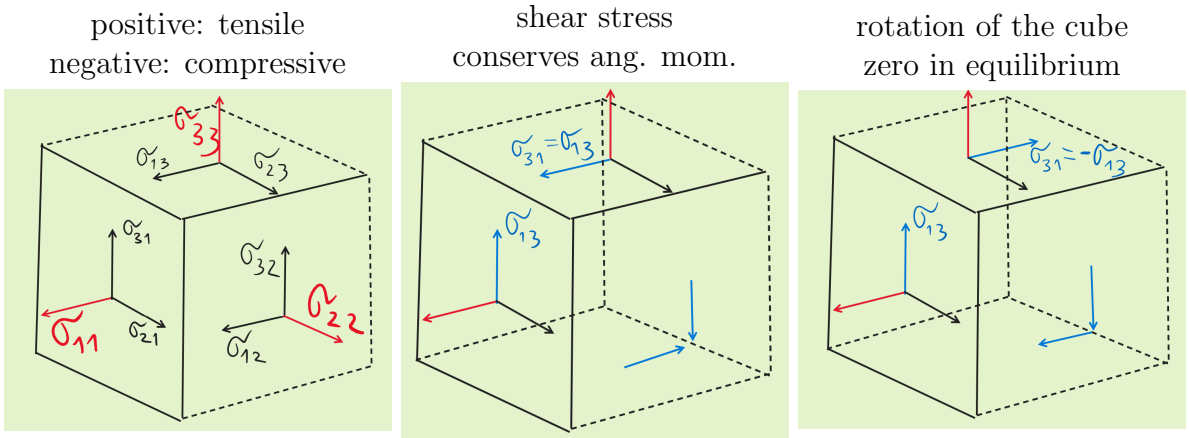


Figure 9: We analyse stress by taking a small cube of the material such that the edges of the cube are parallel with the coordinate axes. (left) Tensile and compressive stresses (red arrows) correspond to diagonal entries of the stress tensor. (middle) Shear stresses (blue arrows) correspond to off-diagonal entries of the symmetrised stress tensor as $\boldsymbol{\sigma}^s$. (right) Off diagonal entries of the antisymmetrised stress tensor $\boldsymbol{\sigma}^a$ try to rotate the cube (blue arrows). The stress tensor is thus symmetric due to the conservation of angular momentum (no rotation).

plane represented by an area vector $\vec{n}$. Here, an area vector is a vector whose direction is perpendicular to the plane and its length is identical to the area of the plane. The stress tensor relates these two vector quantities to each other as

$$\vec{T} = \boldsymbol{\sigma}\vec{n}, \qquad T_i = \sigma_{ij} n_j. \tag{21}$$

This equation expresses the relationship between two rank-1 tensors (vectors) using a rank-2 tensor, just like in the case of cause and effect relations. As such it also guarantees the rotational property $\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$ from Summary 6. The important conceptual difference here is that the stress tensor is not a property of the material, it is rather a physical variable.

Note 3. The expression in Eq. (21) is also commonly stated in terms of **row vectors** as $\vec{T}^T = \vec{n}^T \boldsymbol{\sigma}_{row}$, see for example the Wikipedia page[3]. The transpose of this tensor is equivalent to the one in Eq. (21) as $\boldsymbol{\sigma}_{row} = \boldsymbol{\sigma}^T$.

[3]The generalisation of row and column vectors are covariant and contravariant tensors – while one transforms according to $\mathbf{L}^T$ the other transforms according to $\mathbf{L}$. Here we only work in orthogonal, Cartesian coordinate systems and all tensor entries are real numbers – we referred to these as Cartesian tensors in Summary 2 and in Note 2. For Cartesian tensors there is no distinction between covariance and contravariance, see the Wikipedia page. For example, the tensors $\boldsymbol{\sigma}_{row}$ and $\boldsymbol{\sigma}$ obey the same rotational transformation rule

5.2 Stress tensor in equilibrium

The red arrows in Fig. 9 (left) visualise the tensor entries σ_{11}, σ_{22} and σ_{33} which correspond to forces that act perpendicular to the faces of the cube. Such a force can be either tensile (positive value) or compressive (negative value). For example, if a tensile force σ_{11} acts on a face $\vec{x}_1$ then a compressive force $-\sigma_{11}$ must act on the opposite face $-\vec{x}_1$ such that these forces cancel each other out in equilibrium.

The other tensor entries are forces that act parallel to the faces. For example, the tensor entry σ_{12} is the force that acts on the $\vec{x}_2$ face but in the $\vec{x}_1$ direction. It simplifies the following argument if we first decompose our tensor into symmetric and antisymmetric parts. Recall that a symmetric matrix is unchanged under a transposition $(\boldsymbol{\sigma}^s)^T = \boldsymbol{\sigma}^s$ while an antisymmetric matrix picks up a negative sign under a transposition $(\boldsymbol{\sigma}^a)^T = -\boldsymbol{\sigma}^a$. We can actually write any matrix as a sum of a symmetric and an antisymmetric matrix as $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$.

Question 11. We can define the symmetric part of a matrix as $2\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\sigma}^T$ and the antisymmetric part as $2\boldsymbol{\sigma}^a = \boldsymbol{\sigma} - \boldsymbol{\sigma}^T$. Verify that by transposing these matrices they only pick up a sign ± 1.

For these reasons, we can write the stress tensor as a sum of a diagonal matrix, a symmetric matrix with zeros in the diagonal and an antisymmetric matrix with zeros in the diagonal as

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \underbrace{\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}}_{\text{tensile}} + \underbrace{\begin{bmatrix} 0 & \sigma^s_{12} & \sigma^s_{13} \\ \sigma^s_{12} & 0 & \sigma^s_{23} \\ \sigma^s_{13} & \sigma^s_{23} & 0 \end{bmatrix}}_{\text{shear}} + \underbrace{\begin{bmatrix} 0 & \sigma^a_{12} & \sigma^a_{13} \\ -\sigma^a_{12} & 0 & \sigma^a_{23} \\ -\sigma^a_{13} & -\sigma^a_{23} & 0 \end{bmatrix}}_{\text{rotation}}. \tag{22}$$

The first part, the diagonal matrix corresponds to the aforementioned stresses that act perpendicular to the faces and they are illustrated as red arrows in Fig. 9(left). The second matrix in Eq. (22) is off-diagonal and symmetric and it corresponds to so-called shear stresses. These shear stresses are illustrated in Fig. 9(middle) as blue arrows. The third matrix in Eq. (22) is antisymmetric and off-diagonal and these terms correspond to a rotation of the cube. The blue arrows in Fig. 9(right) form a circle and correspond to forces that try to rotate the cube. In equilibrium, due to Cauchy's conservation of angular momentum, these terms must be zero and thus the stress tensor must be symmetric $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^s$.

5.3 Principal stresses

We saw that in equilibrium the stress tensor is symmetric as $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$ and from Reminder 2 we know that any such matrix can be diagonalised. After diagonalisation we obtain the

stress type	principal comps.	example	tensor
uniaxial	1 non-zero σ_k	pulling wire	$\mathrm{diag}(\sigma_1, 0, 0)$
biaxial	2 non-zero σ_k	force on thin plate	$\mathrm{diag}(\sigma_1, \sigma_2, 0)$
triaxial	3 non-zero σ_k	-	$\mathrm{diag}(\sigma_1, \sigma_2, \sigma_3)$
hydrostatic	3 identical $\sigma_k < 0$	pressure p in fluid	$\mathrm{diag}(-p, -p, -p)$
pure shear	special biaxial	rod torsion	$\mathrm{diag}(-\sigma, \sigma, 0)$

Table 3: Examples where the shape and quality of a material determine what principal components the stress tensor can have.

principal components and principal vectors. Note that $\boldsymbol{\sigma}$ is not a property of material but rather a physical variable and thus the principal components and principal axes are not related to symmetry properties of the crystal.

In Table 3 we summarise a few scenarios when the shape and quality of the object determine properties of the stress tensor.

- Imagine a wire that is being stretched. As we set up our coordinate system such that the wire is parallel with the $\vec{x}_1$ coordinate axis, the tensor becomes diagonal. This is called a uniaxial stress and it only has a single non-zero principal component as shown in Table 3.
- A biaxial stress can be, for example, due to a force that pulls a thin plate and the corresponding stress tensor then only has two non-zero principal components.
- Hydrostatic pressure in a liquid has a stress tensor that is proportional to the identity matrix as $-p\mathbb{1}$. The proportionality factor is $-p$ and its negative sign reflects the fact that the pressure is compressive.
- We can consider a pure shear stress as illustrated in Fig. 9(middle) with the blue arrows. As we will see later we can apply a 45° rotation to this tensor to obtain the diagonal form $\mathrm{diag}(-\sigma, \sigma, 0)$.

In general the stress tensor represents a physical variable, more concretely a force per unit area. But given a stress tensor, what is the 'magnitude' of this physical variable? For example, when a physical variable is described by a vector then we can conveniently use the norm of the vector to express the magnitude of the physical property. Unfortunately, there is no obvious metric of magnitude for matrices.

Note 4. We expect that the 'magnitude' of a physical property must not depend on what coordinate system we use. In order to quantify the norm of a tensor property, we need to use matrix invariants, such as the trace $\mathrm{Tr}(A)$, the determinant or so-called matrix norms, for example $\mathrm{Tr}(A^T A)$. These matrix invariants do not change when we rotate our matrix.

5.4 Strain in 1D

If we apply force or stress to a material, it becomes deformed. We refer to this deformation as strain and express it as the ratio of the extension of the body relative to the original distance. The extension of the body is measured as the change in distance between two points in the body. We first consider a 1-dimensional example, such as a wire that is being stretched. Suppose we select and analyse a small interval of this wire, for example, the interval $(x, x + \Delta x)$ which has a length Δx. This is illustrated in in the top part of Fig. 10(left). Imagine that after stretching the wire, the interval has been increased to $(x + u, x + \Delta x + u + \Delta u)$ which is illustrated in the bottom part of Fig. 10(left). We can define the extension per unit length as

$$\text{strain} = \frac{\text{increase in length}}{\text{original length}} = \Delta u / \Delta x.$$

This expression is, however, only valid if the extension of the material is homogeneous which is illustrated with the red linear curve in Fig. 10(right).

The black curve in Fig. 10(right) shows the profile of a material in which the strain is not homogeneous. In such an instance we need to consider small intervals Δx, in fact the limit when the interval becomes very small as

$$\text{strain} = \lim_{\Delta x \to 0} \frac{\Delta u}{\Delta x} = \frac{\mathrm{d}u}{\mathrm{d}x}. \tag{23}$$

The strain ϵ is thus the derivative of the displacement $u(x)$ with respect to the position x. Indeed, when the strain is homogeneous, such as in the red curve in Fig. 10(right), then then the extension $u(x)$ is a linear function of x whose derivative, the strain, is a constant. In such a case the Taylor expansion only contains the first two terms which lead to the equation $u(x) - u(0) = \epsilon x$.

5.5 Strain in 3D

In the previous example we only considered a material in 1 dimension where we could describe the coordinate with a number x. As we want to treat materials in three dimensions we need

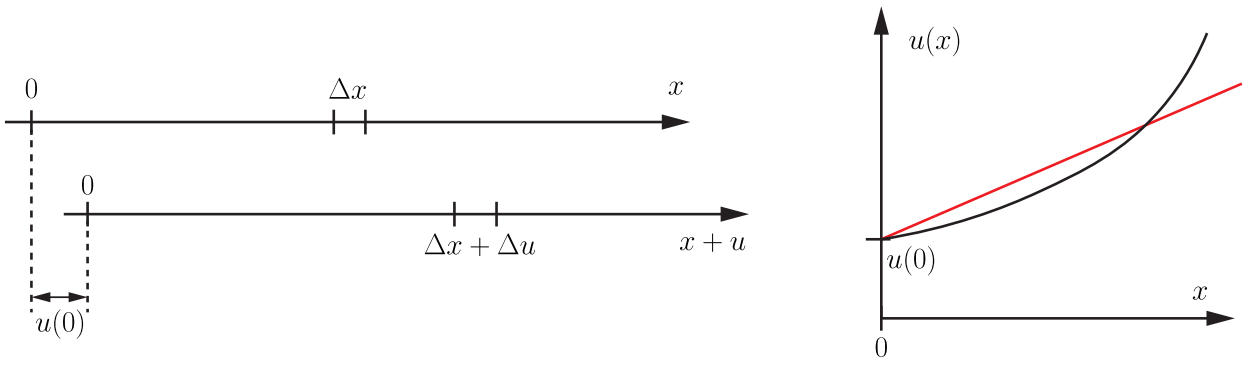


Figure 10: (left) A 1D wire before and after stretching. The interval of length Δx is extended to an interval of length $\Delta x + \Delta u$ due to stretching. Strain is the increase in length Δu relative to the original length Δx. (right) The extension $u(x)$ might be a non-linear function of the coordinate x and thus the strain is more generally the derivative $\frac{\mathrm{d}u}{\mathrm{d}x}$.

to describe the coordinate as a column vector $\vec{x} = (x_1, x_2, x_3)^T$ and similarly the extension as a column vector $\vec{u} = (u_1, u_2, u_3)^T$. The strain in 3D is then a direct generalisation of the 1-dimensional derivative in Eq. (23): in 3D we have to consider each of the three vector entries of $\vec{u}$ and compute *partial derivatives* with respect to each vector entry of $\vec{x}$ as

$$\tilde{\epsilon}_{ij} = \frac{\partial u_i}{\partial x_j}.$$

These partial derivatives form a tensor as $\tilde{\epsilon}_{ij}$. We have seen in Section 5.2 that the anti-symmetric part of the matrix as $(\tilde{\epsilon}_{ij} - \tilde{\epsilon}_{ji})/2$ tries to rotate the material. For this reason, we only consider the symmetric part of the above tensor and define the strain tensor as the rank-2, symmetric tensor

$$\epsilon_{ij} = (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})/2.$$

Similarly as in Section 5.2 we can decompose this symmetric strain tensor as a sum of a diagonal matrix and a purely off-diagonal matrix as

$$\boldsymbol{\epsilon} = \underbrace{\begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}}_{\text{uniaxial extension}} + \underbrace{\begin{bmatrix} 0 & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & 0 & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & 0 \end{bmatrix}}_{\text{shear}}.$$

The diagonal entries ϵ_{11}, ϵ_{22}, ϵ_{33} are the uniaxial extensions per unit length. The off-diagonal entries in the matrix are shear strains – these of course depend on the coordinate system and, for example, in the principal axis system all off-diagonal entries are zero. When the strain is homogeneous, then the extension vector $\vec{u}(x)$ is a linear function of the coordinate vector and we can thus write $\vec{u}(\vec{x}) - \vec{u}(0) = \boldsymbol{\epsilon}\vec{x}$.

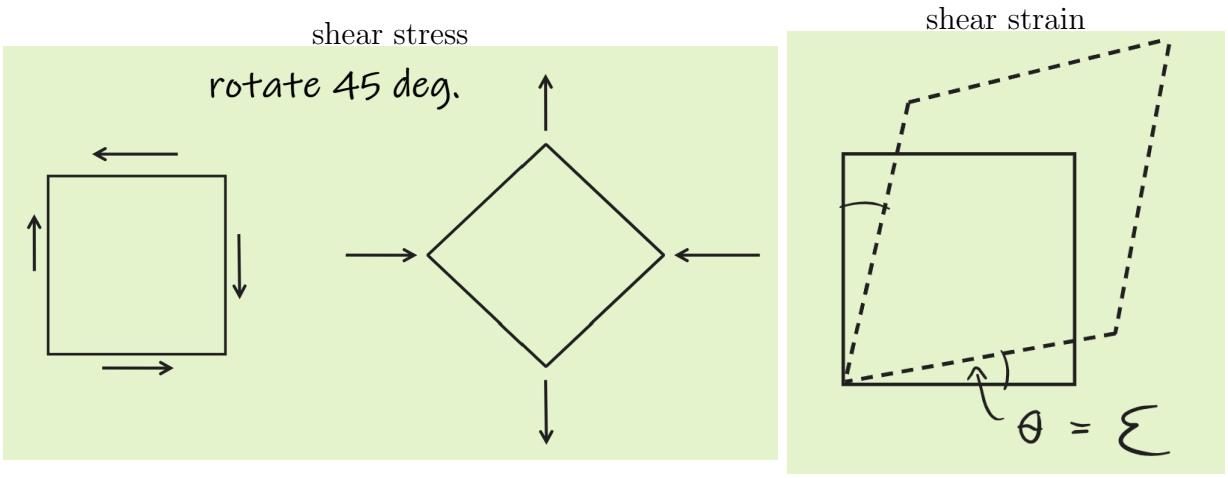


Figure 11: Pure shear stress (left) and strain (right) in a cube of material. (left) Shear tensors can be diagonalised by a 45° rotation. (right) The angle of deformation of the material is approximately the matrix entry ϵ when ϵ is small.

5.6 Pure shear stress and strain

Suppose we have a material undergoing pure shear stress or strain. Pure shear stress is illustrated in Fig. 11(left) while pure shear strain is illustrated in Fig. 11(right). The corresponding stress and strain matrices are

$$\boldsymbol{\sigma} = \begin{bmatrix} 0 & \sigma & 0 \\ \sigma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \boldsymbol{\epsilon} = \begin{bmatrix} 0 & \epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Above both matrices can be diagonalised by a 45° rotation of the coordinate system, which can also be thought of as an active rotation of the material as illustrated in Fig. 11(left). After diagonalization, both matrices have only two non-zero eigenvalues as $\pm\sigma$ and $\pm\epsilon$. Fig. 11(left) illustrates that after the diagonalising rotation the principal stresses act along the $\vec{x}_1$ and $\vec{x}_2$ coordinate axes with compressive and tensile stresses as $\pm\sigma$, respectively.

Shear strain deforms the cubic material in Fig. 11(right) into a rhombic material. Using the definition of the strain, we can derive the angle of deformation as

$$\epsilon = \epsilon_{12} = (\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1})/2 = \tan(\theta) \approx \theta. \tag{24}$$

In the third equation we used that the derivative $\frac{\partial u_1}{\partial x_2}$ expresses the tangent of the angle θ and in the last equation we used the Taylor expansion of the tangent function as $\tan(x) = x + \ldots$ for small x.

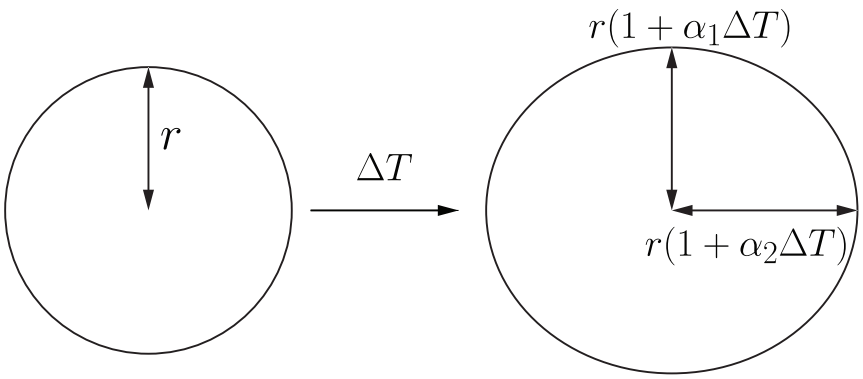


Figure 12: A sphere of material is heated up uniformly such that its temperature is raised by a small amount ΔT. The sphere is deformed into an ellipsoid.

5.7 Strain tensor via thermal expansion

Suppose a material is heated up uniformly by a small amount such that its temperature increases by a small ΔT – we assume that all parts of the material were initially of the same temperature and all parts are heated up by exactly the same change of temperature. Under these assumptions the extension of the material caused by the heating is proportional to the temperature and thus the components of the strain tensor (ϵ_{ij}) are proportional to the thermal expansion coefficients (α_{ij}) as

$$\boldsymbol{\epsilon} = \boldsymbol{\alpha}\Delta T, \qquad \epsilon_{ij} = \alpha_{ij}\Delta T.$$

Here ϵ_{ij} is a symmetric tensor and since ΔT is just a scalar multiplication factor, α_{ij} must also be a symmetric tensor too. Since the tensor α_{ij} is a property of the material, the principal components and principal directions (eigenvalues and eigenvectors) are determined by the crystal symmetry according to von Neuamnn's principle. For example, the principal components $\epsilon_i = \alpha_i\Delta T$ express the expansion along the crystal directions. These principal components α_i are typically positive, but in some instances they can be negative too. In the most typical case when α_i are positive, the corresponding representation surface of ϵ_{ij} and α_{ij} are ellipsoids as we discussed in Section 4.3.

As we heat up a ball of material, it gets deformed into an ellipsoid. The expansion along the principal directions can be described in terms of the principal components as $\epsilon_i = \alpha_i\Delta$. Fig. 12 illustrates that initially the sphere had a radius r and after heating up the material, the sphere is transformed into an ellipsoid with axes

$$a = r(1+\alpha_1\Delta T), \qquad b = r(1+\alpha_2\Delta T), \qquad c = r(1+\alpha_3\Delta T). \tag{25}$$

While the sphere had a volume $V = \frac{3}{4}\pi r^3$ the resulting ellipsoid has a volume $V' = \frac{3}{4}\pi abc$ that depends on the magnitude of the three axes. We can simplify the expression for the

new volume V' assuming that the change of temperature ΔT is small as

$$V' = V + (\alpha_1 + \alpha_2 + \alpha_3)V\Delta T + \ldots, \tag{26}$$

where we have neglected all terms that contain $(\Delta T)^2$ or $(\Delta T)^3$. Finally, the increase of volume can be calculated for small ΔT as

$$\Delta V \approx (\alpha_1 + \alpha_2 + \alpha_3)V\Delta T. \tag{27}$$

Notice that here the sum of principal components is actually the trace of the matrix $\alpha_1 + \alpha_2 + \alpha_3 = \mathrm{Tr}\boldsymbol{\alpha}$. The trace is actually a matrix invariant as noted in Note 4 and it can thus be used as a valid measure of the magnitude of the tensor $\boldsymbol{\alpha}$. In conclusion, the volume expansion of a material is approximately proportional to the trace of its thermal expansion tensor – and the trace is not dependent on the coordinate system used.

5.8 Hooke's law and linear elasticity

Recall Hooke's law that describes the force in a 1-dimensional spring as

$$F = kx.$$

The generalisation of Hooke's law relates stress and strain in an elastic material. As both the stress and strain are rank-2 tensors (they are physical variables), in order to relate them to each other we need to use rank-4 tensors. The stiffness tensor c_{ijkl} is the analogue of the spring constant k from the above equation and it relates stress and strain via the Einstein summation

$$\sigma_{ij} = c_{ijkl}\,\epsilon_{kl}.$$

So far, we have used convenient matrix and vector notations to describe how a rank-2 tensor relates two vectors to each other. In contrast, here we need to resort to Einstein summations as rank-4 tensors are more general than matrices as we discussed in Section 2.3.

Since every index in the tensor c_{ijkl} can take up 3 values, overall there are $3^4 = 81$ tensor entries in a rank-4 Cartesian tensor. While for rank-2 tensors (matrices) we only had 9 entries, we could even reduce them to 6 entries since the matrices we considered were symmetric. Similarly, we can exploit symmetry properties of the stiffness tensor: In general we only have 21 independent tensor entries in c_{ijkl} due to the following symmetries. The symmetry of the stress and strain tensors $\sigma_{ij} = \sigma_{ji}$ and $\epsilon_{kl} = \epsilon_{lk}$ implies the symmetry of the stiffness tensor as $c_{ijkl} = c_{jikl}$ and $c_{ijkl} = c_{ijlk}$, respectively. Furthermore, in crystals the strain tensor ϵ_{kl} inherits symmetry properties of the crystal which then further reduces the number of independent components in the stiffness tensor. For example, in orthorhombic crystals the stiffness tensor has 9 independent entries, in hexagonal crystals it has 5 independent entries, and in cubic crystals it only has 3 independent entries.

Appendix

A Constructing rotation matrices

Here we discuss how we can take a physically defined operation, such as a "rotation around an axis that is halfway between the x and z axes" and calculate its rotation matrix $\mathbf{L}$.

a if the physical operation is a rotation around one of the axis vectors than we can immediately use one of the three elementary rotation matrices from Eq. (12).

b if the physical operation is specified as a series of elementary rotations, e.g, "rotate first around the x axis, then around the y axis ..." then we can simply construct $\mathcal{L}$ as a matrix product of the elementary rotation matrices. In fact, this is the conventional way to construct any rotation from the composition of only 3 elementary rotations that rotate around only 2 axes. This is called the Euler angle convention and is detailed, for example, in the Wikipedia article.

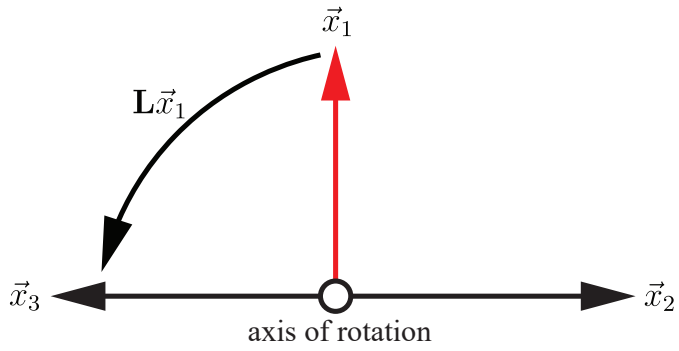
c We may need to find the rotation matrix that corresponds to a rotation around an angle that is not one of the standard axes and then we cannot use the above two techniques. In such a case the simplest way to evaluate the rotation matrix is by analysing how the standard basis vectors are rotated. This is explained in more detail in Appendix B.1.

B Solutions

B.1 Solution of Question 5

We can calculate the active rotation matrix by evaluating how it acts on the standard basis vectors as discussed in Section 3.1: For example, the vector $\vec{x}_1' = \mathbf{L}\vec{x}_1$ will be the first column vector of $\mathbf{L}$ etc.

By drawing how the three coordinate axes are rotated we can determine column vectors of $\mathbf{L}$. For example, the first column vector $\vec{x}_1' = \mathbf{L}\vec{x}_1$ is obtained by looking at the rotation axis from the top and performing the rotation that maps the $\vec{x}_1$ axis to a vector that is halfway between the $\vec{x}_2$ and $-\vec{x}_3$ axes as $\mathbf{L}\vec{x}_1 = (0, 1, -1)^T/\sqrt{2}$ as



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We could repeat this similarly and draw the rotations for the other two axes and find the vector entries as

$$\mathbf{L}\begin{bmatrix}1\\0\\0\end{bmatrix} = \begin{bmatrix}0\\\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}\end{bmatrix}, \qquad \mathbf{L}\begin{bmatrix}0\\1\\0\end{bmatrix} = \begin{bmatrix}-\frac{1}{\sqrt{2}}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}, \qquad \mathbf{L}\begin{bmatrix}0\\0\\1\end{bmatrix} = \begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}. \tag{28}$$

We finally arrange these vectors as column vectors into the transformation matrix $\mathbf{L}$ as

$$\begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

B.2 Solution of Question 7

We compute the determinant of both sides of the equation $\mathbf{M} = \mathbf{L}\mathbf{D}\mathbf{L}^T$ as

$$\det \mathbf{M} = \det(\mathbf{L}^T\mathbf{D}\mathbf{L}),$$

and use the property of determinants that $\det(\mathbf{A}\mathbf{B}) = \det(\mathbf{A})\det(\mathbf{B})$ as

$$\det(\mathbf{L}^T\boldsymbol{\sigma}\mathbf{L}) = \det(\mathbf{L}^T)\det(\mathbf{D})\det(\mathbf{L})$$

Since the determinant is the product of eigenvalues, and $\mathbf{M}$ has the same eigenvalues as $\mathbf{D}$, we know their determinants must be the same as $\det \mathbf{M} = \det \mathbf{D}$. This allows us to write that

$$1 = \det(\mathbf{L}^T)\det(\mathbf{L}).$$

Using the property of determinants that $\det(\mathbf{L}^T) = \det(\mathbf{L})$ we find that the determinant of the orthogonal matrix is allowed to be either plus or minus one as $\det(\mathbf{L}) = \pm 1$. We can thus always choose an orthogonal transformation $\mathbf{L}$ that is a proper rotation with determinant one.