Title: Cubic Elasticity
Subtitle: Rotation of tensor of elastic constants
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1 Introduction

This post discusses the relationship between stresses $\boldsymbol{\sigma}$ and strains $\boldsymbol{\varepsilon}$ in crystals with cubic symmetry, specifically focusing on FCC and BCC crystal structures. Furthermore, the rotation of these tensors in three-dimensional space is illustrated.
The figure below shows a cubic crystal, which includes simple cubic (left), body-centered cubic (middle), and face-centered cubic (right) structures. Two coordinate systems are presented: the crystal coordinate system (x_c, y_c, z_c), aligned with the $\langle 100 \rangle$ directions, and the global coordinate system (x, y, z), which is rotated relative to the crystal coordinate system about a vector $\boldsymbol{o}$ by an angle θ.

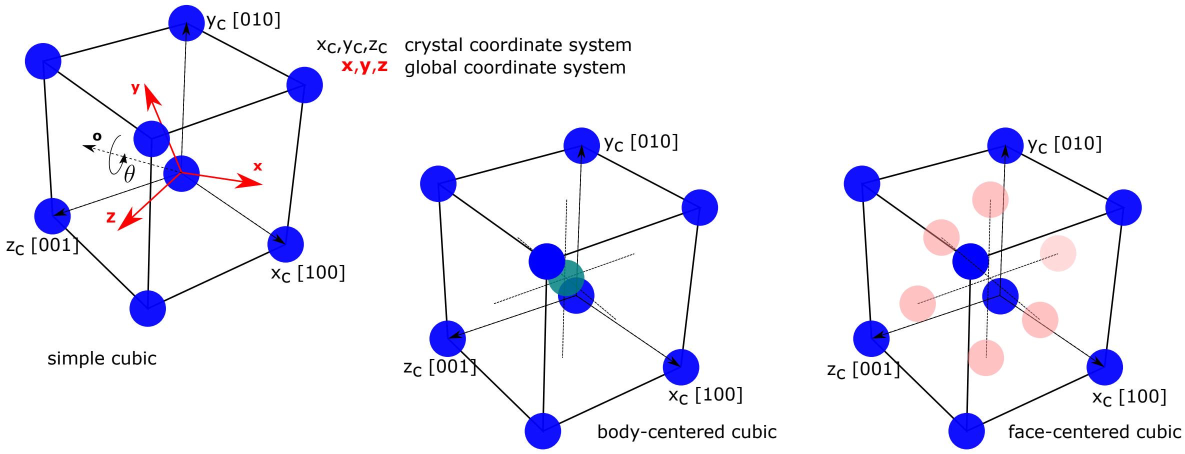

Figure 1: Example of a single crystal structure. Two coordinate systems are illustrated: crystal ($\boldsymbol{x}'$,$\boldsymbol{y}'$,$\boldsymbol{z}'$) and global ($\boldsymbol{x}$,$\boldsymbol{y}$,$\boldsymbol{z}$) coordinate system.

The simplest constitutive model describing the relationship between stress ($\boldsymbol{\sigma}$) and strain ($\boldsymbol{\varepsilon}$) in these crystal structures is linear, commonly referred to as Hooke's law. According to this law, stress is directly proportional to strain, therefore, we can write:

$$\begin{aligned} \sigma_{ij} &= \mathcal{D}_{ijkl}\varepsilon_{kl} \\ \boldsymbol{\sigma} &= \boldsymbol{D}\boldsymbol{\varepsilon} \end{aligned}, \tag{1}$$

where $\boldsymbol{\sigma}$ is a second-rank stress tensor, $\boldsymbol{\varepsilon}$ is a second-rank strain tensor, and $\boldsymbol{D}$ is a fourth-rank tensor of elastic constants. This relationship can be written in the crystal coordinate system using the Voigt notation as follows:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} D_{11} & D_{12} & D_{12} & 0 & 0 & 0 \\ D_{12} & D_{11} & D_{12} & 0 & 0 & 0 \\ D_{12} & D_{12} & D_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & D_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & D_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & D_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{bmatrix}, \tag{2}$$

which in 2D simplifies into

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & D_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{bmatrix}. \tag{3}$$

It is important to note that the constitutive law is formulated using engineering strain. The shear strain components of the engineering strain, denoted as γ_{ij}, are twice as large as the shear strain components of the tensorial strain, which can be expressed as $\gamma_{ij} = 2\varepsilon_{ij}$ for $i \neq j$. Assuming small deformations, the tensorial strain can be calculated as $\varepsilon_{ij} = 1/2\,(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$. Here, $\vec{u}$ is the displacement field.
Depending on this assumption, if we consider plane strain conditions where $\varepsilon_{zz} = 0$, the constants of the strain tensor in two dimensions remain the same: $C_{11} = D_{11}$, and $C_{12} = D_{12}$. On the other hand, if we assume plane stress conditions, ($\sigma_{zz} = 0$), $C_{11} = \frac{D_{11}^2 - D_{12}^2}{D_{11}}$, and $C_{12} = \frac{D_{11}D_{12} - D_{12}^2}{D_{11}}$.
A useful parameter for describing cubic anisotropy is the Zener ratio, which is a dimensionless number calculated as follows: D_{44}/D' where $D' = \frac{D_{11} - D_{12}}{2}$.
The elastic constants of selected materials, along with their corresponding Zener ratios, are summarized in the following table:

Table 1: Elastic constants of some FCC metals

Metal	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_{44}/C'
Pb[a]	55.6	45.4	19.4	3.8
Ag[a]	131.5	97.3	51.1	2.99
Au[a]	201	170	46	2.97
Cu[b]	225	153	115	3.19
Ni[a]	261	151	132	2.4
Al[a]	114	62	32	1.23
Pd[a]	232	176	71.2	2.45
Pt[a]	358	253	77.5	1.47

[a] = [1], [b] = [2]

2 Tensor rotation (rotation of elastic properties)

For interested readers, a more detailed analysis can be found in [3].
This section begins by defining the rotation matrix We denote rotated tensors by a prime symbol ($'$). A fourth-rank tensor is rotated as $\boldsymbol{D}' = \boldsymbol{T} \cdot \boldsymbol{D} \cdot \boldsymbol{T}^T$, while a second-rank tensor, such as stress, is rotated as $\boldsymbol{\sigma}' = \boldsymbol{R} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{R}^T$, where $\boldsymbol{R}$ is the rotation matrix.
Rotation ($\boldsymbol{R}$) and coordinate transformation ($\boldsymbol{Q}$) are distinct, with their relationship expressed as $\boldsymbol{R} = \boldsymbol{Q}^T$. To begin, we consider the general form of a rotation matrix:

$$\boldsymbol{R} = \begin{bmatrix} \cos(\boldsymbol{x}', \boldsymbol{x}) & \cos(\boldsymbol{y}', \boldsymbol{x}) & \cos(\boldsymbol{z}', \boldsymbol{x}) \\ \cos(\boldsymbol{x}', \boldsymbol{y}) & \cos(\boldsymbol{y}', \boldsymbol{y}) & \cos(\boldsymbol{z}', \boldsymbol{y}) \\ \cos(\boldsymbol{x}', \boldsymbol{z}) & \cos(\boldsymbol{y}', \boldsymbol{z}) & \cos(\boldsymbol{z}', \boldsymbol{z}) \end{bmatrix}. \tag{4}$$

The $\boldsymbol{T}$ matrix may then be assembled as

$$\boldsymbol{T} = \begin{bmatrix} \boldsymbol{T}^{(1)} & 2\boldsymbol{T}^{(2)} \\ \boldsymbol{T}^{(3)} & \boldsymbol{T}^{(4)} \end{bmatrix}, \tag{5}$$

where

$$\begin{aligned} T_{ij}^{(1)} &= R_{ij}^2 \\ T_{ij}^{(2)} &= R_{i\mathrm{mod}(j+1,3)} R_{i\mathrm{mod}(j+2,3)} \\ T_{ij}^{(3)} &= R_{\mathrm{mod}(i+1,3)j} R_{\mathrm{mod}(i+2,3)j} \\ T_{ij}^{(4)} &= R_{\mathrm{mod}(i+1,3)\mathrm{mod}(j+1,3)} R_{\mathrm{mod}(i+2,3)\mathrm{mod}(j+2,3)} + R_{\mathrm{mod}(i+1,3)\mathrm{mod}(j+2,3)} R_{\mathrm{mod}(i+2,3)\mathrm{mod}(j+1,3)} \end{aligned}, \tag{6}$$

where the modulo function is defined as

$$\mathrm{mod(i,3)} = \begin{cases} i & i \leq 3 \\ i - 3 & i > 3 \end{cases}. \tag{7}$$

2.1 Rotation about an axis $\boldsymbol{o} = (o_1, o_2, o_3)$, $|\boldsymbol{o}| = 1$

When rotation occurs about an arbitrary axis $\boldsymbol{o}$, the rotation matrix $\boldsymbol{R}$ simplifies to:

$$\boldsymbol{R} = \begin{bmatrix} o_1^2 + (1 - o1^2)\cos\theta & o_1o_2(1-\cos\theta) - o_3\sin\theta & o_1o_3(1-\cos\theta) + o_2\sin\theta \\ o_1o_2(1-\cos\theta) + o_3\sin\theta & o_2^2 + (1-o_2^2)\cos\theta & o_2o_3(1-\cos\theta) - o_1\sin\theta \\ o_1o_3(1-\cos\theta) - o_2\sin\theta & o_2o_3(1-\cos\theta) + o_1\sin\theta & o_3^2 + (1-o_3^2)\cos\theta \end{bmatrix} \tag{8}$$

2.2 Rotation of the Tensor of Elastic Constants $\boldsymbol{C}$

The constitutive law defines the tensor of elastic constants as a proportionality tensor relating stresses to **engineering strains**. The engineering strain shear terms γ_{ij} are twice as large as the tensorial strain shear terms ε_{ij}. Considering this, the tensor of elastic constants is rotated using the following equation:

$$\boldsymbol{C}' = \boldsymbol{TCAT}^{-1}\boldsymbol{A}^{-1} \tag{9}$$

where the matrix $\boldsymbol{A}$ (also known as the Reuter's matrix) is used to convert between the tensorial $\boldsymbol{\varepsilon}$ and engineering $\boldsymbol{\gamma}$ strains.

$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \tag{10}$$

The following Matlab script demonstrates how to rotate the tensor of elastic constants about an arbitrary vector $\boldsymbol{o}$. This script uses the background image of this post, in which the elastic constants D_{11}, D_{12}, and D_{44} are given in the crystal coordinate system, and the tensor of elastic constants is rotated into the global coordinate system (x, y, z).

Listing 1: Matlab example

```
% (c) 2018 Jakub Mikula
% PURPOSE:
% Example of tensor rotation about a general axis
% Rotating tensor of elastic constants about an arbitrary vector o
%
% INPUT:
%       > elastic constants D_11, D_12, D_44
%       > rotation axis o1, o2, o3
%       > rotation angle theta
% OUTPUT:
%       > rotated tensor of elastic constants in matrix form D_rot

% -----------------------------------------------------------

% Material : [GPa]
        D_11 = 190
        D_12 = 161
%D_44 = (D_11-D_12)/2 % uncomment for isotropic elasticity
        D_44 = 42.3

% Axis to rotate about
% Make sure that |o|=1
        o1 = 0
        o2 = 0
        o3 = 1

% Specify the angle [RAD]
        theta = -pi/4

% -----------------------------------------------------------

```

```
% Tensor of elastic constants (cubic elasticity) in the matrix form
% Voigth notation
D = [D_11 D_12 D_12 0 0 0
     D_12 D_11 D_12 0 0 0
         D_12 D_12 D_11 0 0 0
         0 0 0 D_44 0 0
         0 0 0 0 D_44 0
         0 0 0 0 0 D_44];

% Matrix due to the conversion from engineering to tensorial strain
R(:,:) = 0.0d0;
R(1,1) = 1.0d0;
R(2,2) = 1.0d0;
R(3,3) = 1.0d0;
R(4,4) = 2.0d0;
R(5,5) = 2.0d0;
R(6,6) = 2.0d0;

invR(:,:) = R(:,:);
invR(4,4) = .5d0;
invR(5,5) = .5d0;
invR(6,6) = .5d0;


% Rotating about an arbitrary axis (between crystal and global coordinate
    system)
R_cg=[o1^2+(1-o1^2)*cos(theta) o1*o2*(1-cos(theta))-o3*sin(theta) o1*o3*(1-cos(
    theta))+o2*sin(theta)
   o1*o2*(1-cos(theta))+o3*sin(theta) o2^2+(1-o2^2)*cos(theta) o2*o3*(1-cos(
       theta))-o1*sin(theta)
   o1*o3*(1-cos(theta))-o2*sin(theta) o2*o3*(1-cos(theta))+o1*sin(theta) o3
       ^2+(1-o3^2)*cos(theta)];


for i=1:3
for j=1:3

mmod = [1 1 1 1 1
                -1 2 2 2 2
                0 0 3 3 3
                1 1 1 4 4
                2 2 2 2 5];

 K1(i,j) = R_cg(i,j)^2;
 K2(i,j) = R_cg(i,mmod(j+1,3))*R_cg(i,mmod(j+2,3));
 K3(i,j) = R_cg(mmod(i+1,3),j)*R_cg(mmod(i+2,3),j);
 K4(i,j) = R_cg(mmod(i+1,3),mmod(j+1,3))*R_cg(mmod(i+2,3),mmod(j+2,3)) + ...
           R_cg(mmod(i+1,3),mmod(j+2,3))*R_cg(mmod(i+2,3),mmod(j+1,3));
end
end

T_cg(1:3,1:3) = K1;
T_cg(1:3,4:6) = 2.0d0*K2;
T_cg(4:6,1:3) = K3;
T_cg(4:6,4:6) = K4;

invT_cg(1:3,1:3) = K1';
invT_cg(1:3,4:6) = 2.0d0*K3';
invT_cg(4:6,1:3) = K2';
invT_cg(4:6,4:6) = K4';

% Rotated tensor of elastic constants
D_rot = T_cg*D*R*invT_cg*invR
```

2.3 Rotation of C About $\langle 001 \rangle$ in 2D

The rotation of the elastic constants can be derived using the following rotation matrices:

$$\boldsymbol{R}^{x_c} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \boldsymbol{R}^{y_c} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, \boldsymbol{R}^{z_C} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{11}$$

If we rotate the coordinate system about z_c ([001]) by an angle θ, we can express the equations above in the following form:

$$\begin{aligned} C'_{11} &= C_{11}\left(\cos^4\theta + \sin^4\theta\right) + 2C_{12}\sin^2\theta\cos^2\theta + C_{33}\sin^2 2\theta \\ C'_{12} &= C_{12}\left(\cos^4\theta + \sin^4\theta\right) + 2C_{11}\sin^2\theta\cos^2\theta - C_{33}\sin^2 2\theta \\ C'_{13} &= \tfrac{1}{2}C_{11}\sin 2\theta\cos 2\theta - \tfrac{1}{2}C_{12}\sin 2\theta\cos 2\theta - \tfrac{1}{2}C_{33}\sin 4\theta \\ C'_{21} &= C'_{12} \\ C'_{22} &= C'_{11} \\ C'_{23} &= -C'_{13} \\ C'_{31} &= C'_{13} \\ C'_{32} &= -C'_{13} \\ C'_{33} &= \tfrac{1}{2}C_{11}\sin^2 2\theta - \tfrac{1}{2}C_{12}\sin^2 2\theta + C_{33}\cos^2 2\theta \end{aligned}. \tag{12}$$

The following Matlab code is provided:

Listing 2: Matlab example

```
% Purpose:  rotate tensor of elastic constants C into C_rot by angle theta
% Define:   theta [1]
%           C [3x3]
% Output:   C_rot [3x3]

C_rot(1,1) = C(1,1)*(cos(theta)^4+sin(theta)^4) + 2*C(1,2)*sin(theta)^2*cos(theta)^2 + C(3,3)*sin(2*theta)^2;
C_rot(1,2) = C(1,2)*(cos(theta)^4+sin(theta)^4) + 2*C(1,1)*sin(theta)^2*cos(theta)^2 - C(3,3)*sin(2*theta)^2;
C_rot(1,3) = 0.5*C(1,1)*sin(2*theta)*cos(2*theta) - 0.5*C(1,2)*sin(2*theta)*cos(2*theta) - 0.5*C(3,3)*sin(4*theta);
C_rot(2,1) = C_rot(1,2);
C_rot(2,2) = C_rot(1,1);
C_rot(2,3) = -C_rot(1,3);
C_rot(3,1) = C_rot(1,3);
C_rot(3,2) = -C_rot(1,3);
C_rot(3,3) = 0.5*C(1,1)*sin(2*theta)^2 - 0.5*C(1,2)*sin(2*theta)^2 + C(3,3)*cos(2*theta)^2;
```

The derivatives of these with respect to the orientation θ are,

$$\begin{aligned} \frac{\partial C'_{11}}{\partial\theta} &= -4\sin\theta\cos\theta\left(2\cos^2\theta(C_{11} - C_{12}) - 4\cos^2\theta C_{33} - C_{11} + C_{12} + 2C_{33}\right) \\ \frac{\partial C'_{12}}{\partial\theta} &= 4\sin\theta\cos\theta\left(2\cos^2\theta(C_{11} - C_{12}) - 4\cos^2\theta C_{33} - C_{11} + C_{12} + 2C_{33}\right) \\ \frac{\partial C'_{13}}{\partial\theta} &= \cos^2 2\theta(2C_{11} - 2C_{12}) - 4C_{33}\cos^2 2\theta - C_{11} + C_{12} + 2C_{33} \\ \frac{\partial C'_{33}}{\partial\theta} &= \sin 4\theta(C_{11} - C_{12} - 2C_{33}) \end{aligned}. \tag{13}$$

The derivatives evaluated from the tensor of elastic constants vanish for isotropic materials, where C_{33} is related to C_{11} and C_{12} through the equation $C_{33} = \frac{C_{11} - C_{12}}{2}$. This property has interesting implications for nanocrystalline materials [4], where they are proportional to the bulk driving force contributing to grain boundary motion.
A Matlab code of the derivatives is provided below:

Listing 3: Matlab example

```
% Purpose:  rotate tensor of elastic constants C and calculate the derivative with respect to orientation theta into dC_rot
% Define:   theta [1]
%           C [3x3]
% Output:   dC_rot [3x3]
```

```

dC_rot(1,1) = -4*sin(theta)*cos(theta)*(2*cos(theta)^2*(C(1,1)-C(1,2)) - 4*cos(theta)^2*dC(3,3) - C(1,1) + C(1,2) + 2*C(3,3));
dC_rot(1,2) = 4*sin(theta)*cos(theta)*(2*cos(theta)^2*(C(1,1)-C(1,2)) - 4*cos(theta)^2*C(3,3) - C(1,1) + C(1,2) + 2*C(3,3));
dC_rot(1,3) = cos(2*theta)^2*(2*C(1,1)-2*C(1,2)) - 4*C(3,3)*cos(2*theta)^2 - C(1,1) + C(1,2) + 2*C(3,3);
dC_rot(2,1) = dC_rot(1,2);
dC_rot(2,2) = dC_rot(1,1);
dC_rot(2,3) = -dC_rot(1,3);
dC_rot(3,1) = dC_rot(1,3);
dC_rot(3,2) = -dC_rot(1,3);
dC_rot(3,3) = sin(4*theta)*(C(1,1) - C(1,2) - 2*C(3,3));
```

References

[1] Gene Simmons and Herbert F. Wang. Single crystal elastic constants and calculated aggregate properties. a handbook. 1971.

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[3] Minhang Bao. Chapter 6 - piezoresistive sensing. In Minhang Bao, editor, *Analysis and Design Principles of MEMS Devices*, pages 247–304. Elsevier Science, Amsterdam, 2005.

[4] Jakub Mikula, Shailendra P. Joshi, Tong-Earn Tay, Rajeev Ahluwalia, and Siu Sin Quek. A phase field model of grain boundary migration and grain rotation under elasto–plastic anisotropies. *International Journal of Solids and Structures*, 178-179:1–18, 2019.