Stress and strain:

Euler angle과 좌표변환법

강의명: 소성가공 (MSA0026)

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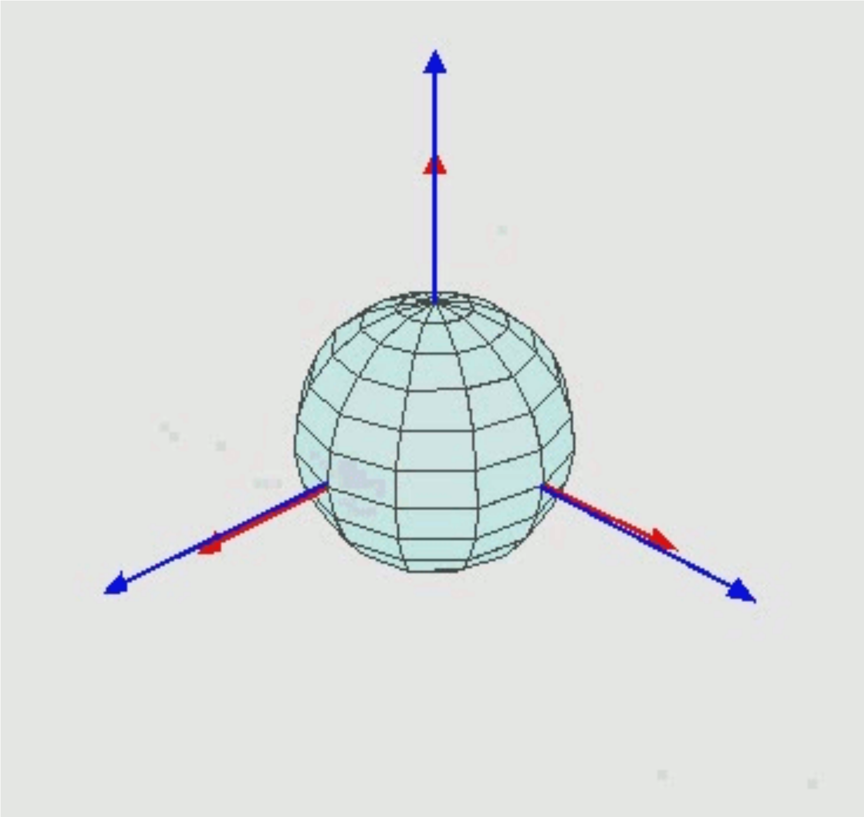
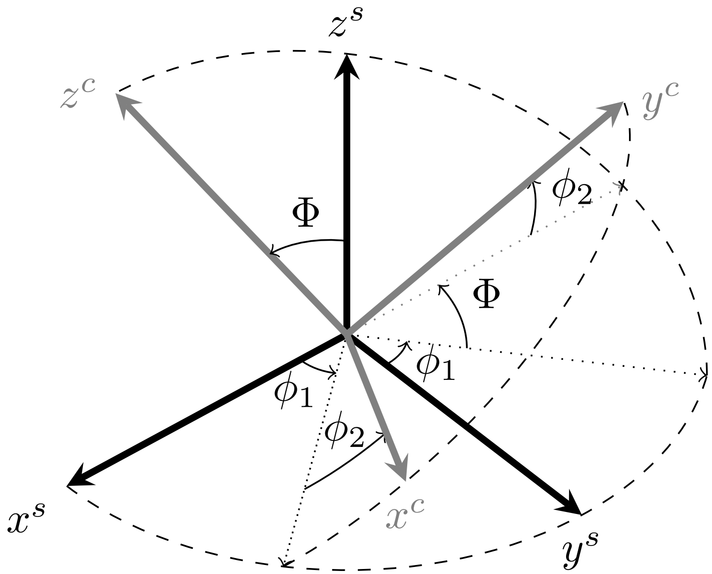
Euler angles





References:
https://en.wikipedia.org/wiki/Euler_angles
https://youngung.github.io/euler/

Euler angle을 이용한 3차원 좌표 변환

- Euler angle을 활용하여 두 삼차원 좌표계간의 관계를 표현할 수 있다.
- Euler angle를 사용하는 좌표변환법이 MSE에서 자주 쓰인다.
  1. 한 3차원 좌표에 $\mathbf{e}_3$축 (z-axis)을 바라보며 시계 반대방향으로 ϕ_1 만큼 회전
  2. 다음으로 1.로 인해 회전된 좌표계의 $\mathbf{e}_1$축을 바라보며 시계 반대방향으로 Φ 만큼 회전
  3. 다음으로 1-2.로 인해 회전된 좌표계를 다시 $\mathbf{e}_3$ 축을 바라보며 시계 반대방향으로 $\boldsymbol{\phi}_2$ 만큼 회전

$$\mathbf{R}^{\phi_1} = \begin{bmatrix} \cos\phi_1 & \sin\phi_1 & 0 \\ -\sin\phi_1 & \cos\phi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{R}^{\Phi} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & \sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{bmatrix}$$

$$\mathbf{R}^{\phi_2} = \begin{bmatrix} \cos\phi_2 & \sin\phi_2 & 0 \\ -\sin\phi_2 & \cos\phi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

위의 일련의 세 회전을 설명하는 '하나의' 좌표 변환 matrix를 다음을 통해 만들 수 있다.

$$\mathrm{R_{ij}} = \mathrm{R^c_{ik} R^b_{kl} R^a_{lj}}$$

$$\mathbf{R} = \mathbf{R}^{c} \cdot \mathbf{R}^{b} \cdot \mathbf{R}^{a}$$

$$\mathbf{R} \cdot \mathbf{v} = [\mathbf{R}^{c} \cdot \{\mathbf{R}^{b} \cdot (\mathbf{R}^{a} \cdot \mathbf{v})\}]$$

Recap: Einstein summation convention

Let’s practice #1

- Follow this link
- http://youngung.github.io/euler2ndtensor/
- You’ll find two links – one to open Google sheet another to download the sheet.

input	output												
			This excell sheet proves a means of coordinate system transformation										
				angle	radian								
			phi1	45	0.785								
	Three Euler angles		Phi	0	0.000								
			phi2	0	0.000								
							transformation matrix R				(transformation matrix)^t= R^t=R^-1		
	삼각 함수 값들												
	cos(phi1)	0.707	sin(phi1)	0.707			0.707	0.707	0.000		0.707	-0.707	0.000
	cos(Phi)	1.000	sin(Phi)	0.000			-0.707	0.707	0.000		0.707	0.707	0.000
	cos(phi2)	1.000	sin(phi2)	0.000			0.000	0.000	1.000		0.000	0.000	1.000
	2nd rank tensor in matrix form						R.T				R^t.R.T	**2nd rank tensor after coordinate transformation**	
	1	0	0				0.707	0.000	0.000		0.500	-0.500	0.000
	0	0	0				-0.707	0.000	0.000		-0.500	0.500	0.000
	0	0	0				0.000	0.000	0.000		0.000	0.000	0.000
	1st rank tensor (i.e., vector) in array form						R.v 1st rank tensor (vector) after coordinate transformation						
	1						0.70710678	-0.7071068	0				
	0												
	0												

Let’s practice #2

- At the bottom of the spread sheet you’ll find three separate matrices, which denote the three sequential rotation matrices.

$$\mathbf{R}^a = \begin{bmatrix} \cos\phi_1 & \sin\phi_1 & 0 \\ -\sin\phi_1 & \cos\phi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{R}^b = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & \sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{bmatrix} \quad \mathbf{R}^c = \begin{bmatrix} \cos\phi_2 & \sin\phi_2 & 0 \\ -\sin\phi_2 & \cos\phi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Below is to obtain the transformation matrix by multipliying the three sequential simpler rotation matrices.

g1				g2				g3			
	0.707	0.707	0.000		1.000	0.000	0.000		1.000	0.000	0.000
	-0.707	0.707	0.000		0.000	1.000	0.000		0.000	1.000	0.000
	0.000	0.000	1.000		0.000	0.000	1.000		0.000	0.000	1.000
g3 g2				g3g2g1							
	1.000	0.000	0.000		0.707	0.707	0.000				
	0.000	1.000	0.000		-0.707	0.707	0.000				
	0.000	0.000	1.000		0.000	0.000	1.000				

- Of course, these are functions of phi1, Phi, phi2 values available at the top.

input	output					
			This excell sheet proves a means of coordinate system transformation			
				angle	radian	
			phi1	45	0.785	
	Three Euler angles		Phi	0	0.000	
			phi2	0	0.000	
						transformation matı

Let's practice #3

- Follow this link:
- http://youngung.github.io/tensors/

$$a'_i = R_{ij} a_j$$
$$\sigma'_{ij} = R_{ik} \sigma_{kl} R_{jl}$$
$$\mathbb{M}'_{ijkl} = R_{im} R_{jn} \mathbb{M}_{mnop} R_{ko} R_{lp}$$

- Tensor transformation rule is implemented into a Fortran code

Let's practice #3 (Fortran)

```
program transform_vector
implicit none

dimension r(3,3), velocity_old(3), stress(3,3), velocity_new(3)
real*8 r, velocity_old, stress, th, velocity_new
integer i,j,k

!! the transformation matrix:
write(*,*)'Type: Rotation angle [in degree]:'
read(*,*) th
th = th* 3.141592 / 180. !! convert the degree to radian

r(:,:)=0.
r(1,1)=cos(th)
r(1,2)=sin(th)
r(2,1)=-sin(th)
r(2,2)=cos(th)
r(3,3)=1.

!! velocity
velocity_old(1)=30.
velocity_old(2)=0.
velocity_old(3)=0.

!! let's transform the velocity v`_i = r_ij v_j
do i=1,3
        velocity_new(i)=0.
do j=1,3
        velocity_new(i)=velocity_new(i)+r(i,j)*velocity_old(j)
enddo
enddo

!! print out the new velocity
write(*,*) 'old velocity'
write(*,'(3f5.1)') (velocity_old(i),i=1,3)
write(*,*) 'new velocity'
write(*,'(3f5.1)') (velocity_new(i),i=1,3)

end program transform_vector
```

변수 선언.
- E.g., R(3,3) is 'real' 실수, 그리고 (3,3) shape – 3x3 array

입력
- 'th' 라는 변수에 user가 각도를 입력하면 radian 값으로 변환한다.

Transformation matrix

'th' 라는 변수를 사용하여 3축을 잡고 ccw 회전시키는 transformation matrix를 만들어 변수 r에 저장

Velocity_old 변수 설정

Old coordinate system에 참조된 알고 있는 1차 텐서 velocity_old 변수를 설정 [30,0,0] array로 저장; ***1차 텐서는 벡터다**.

위 tensor를 변환하여 새로운 array에 저장

아래의 formula를 실행하여 1차 랭크 텐서 변환

$$v_i' = R_{ij} v_j$$

v 와 v`을 화면에 출력

Let's take a close look at the loop

```
do i=1,3
        velocity_new(i)=0.
do j=1,3
        velocity_new(i)=velocity_new(i)+r(i,j)*velocity_old(j)
enddo
enddo
```

1. In the above, each do-enddo pair
DO
ENDDO
allows you to form a loop: where integer i increases from 1 to 3, for each of which j increases from 1 to 3.

2. For instance, while i=1, you repeat
DO j=1,3
ENDDO

That means you perform

$$v_1^{new} = \sum_j^3 R_{1j} v_j^{old}$$

3. If you repeat Step 2 for i=2 and i=3 as well, you actually perform:

$$v_i^{new} = \sum_i^3 \sum_j^3 R_{ij} v_j^{old}$$

Remember that the above summation can be written short:

$$v_i^{new} = R_{ij} v_j^{old}$$

If you extend that idea for 2nd order tensor?

- Let's take an inverse approach for the 2nd order tensor transformation.
- We learned that the 2nd rank tensor transformation is done following the below rule:

$$\sigma'_{ij} = R_{ik}\sigma_{kl}R_{jl}$$

- The above can be implemented to a FORTRAN code such that

```
do i=1,3
do j=1,3
        s_new(i,j)=0.
do k=1,3
do l=1,3
        s_new(i,j)=s_new(i,j) + r(i,k)*s_old(k,l)*r(j,l)
enddo
enddo
enddo
enddo
```

- You might be able to find certain rules that are applicable when you implement the tensor transformation. Also, you might have found the Einstein convention is very useful particularly when the formula is translated into FORTRAN code.
- FORTRAN actually means 'FORMULA TRANSLATION'

Q. Extend that idea for 4th rank tensor

- Within elastic region, metal follows Hooke's law which writes as below:
  - $\sigma_{ij} = \mathbb{E}_{ijkl}\varepsilon_{kl}$
- (For advanced students) Can you write a short FORTRAN DO-ENDDO loop for the above operations?

Let’s practice #3 (Python)

```
import numpy as np
velocity_old=np.zeros(3)
velocity_new=np.zeros(3)
r=np.zeros((3,3))
velocity_old[0]=30.

th=raw_input('Type angle [in degree]: ')
th=np.pi*float(th)/180.

r[0,0]=np.cos(th)
r[0,1]=np.sin(th)
r[1,0]=-np.sin(th)
r[1,1]=np.cos(th)
r[2,2]=1.


## Apply v`_i = r_ij v_j
for i in xrange(3):
        for j in xrange(3):
                velocity_new[i]=velocity_new[i]+ \
        r[i,j]*velocity_old[j]

print 'old velocity'
print velocity_old
print 'new velocity'
print velocity_new
```

변수 선언.

- E.g., velocity_old와 velocity_new는 사이즈 3x1의 array
- R: 3x3 array;
- velocity_old 변수의 첫번째(0) element에 30 입력

입력

- ’th’ 각도 입력한후 Radian값으로 변환

Transformation matrix

- ’th’ 라는 변수를 사용하여 3축을 잡고 ccw 회전시키는 transformation matrix를 만들어 변수 r에 저장

위 tensor를 변환하여 새로운 array에 저장

- 아래의 formula를 실행하여 1차 랭크 텐서 변환
- $v_i' = R_{ij} v_j$

v 와 v`을 화면에 출력

Tensor and coordinate transformation

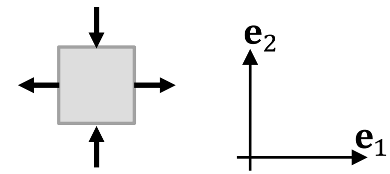
- Tensor is a method to represent physical quantities (and also some material properties).
- Physical quantities should remain the same even if you transform them to another coordinate system; The physical quantities should not be affected by the chosen coordinate system.
- But when you change the coordinate system, the values pertaining to individual components of the tensor may change.
- The values of components that are changing w.r.t. coordinate system are used when you need quantification of associated physical quantity (or material property). That's one of the reasons why you should learn how to apply the coordinate transformation to tensors.

Example: pure shear

- Pure shear is a term referring to a stress (or strain) state where only shear components are non-zero.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

I found the left is a simple shear state. Anything wrong with me?

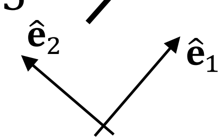


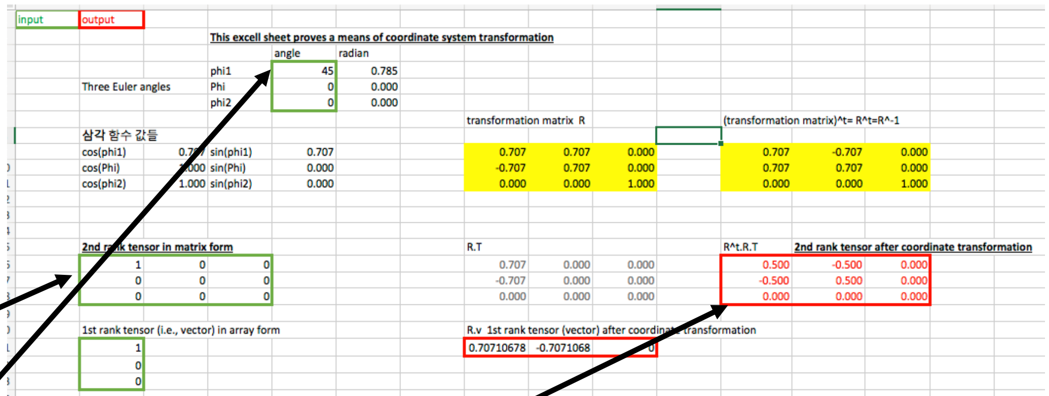
Let's check by using the spread sheet.

1. Put the given stress state value

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

2. Put $\phi_1 = 45\,°$
To obtain





input | output

This excell sheet proves a means of coordinate system transformation

Three Euler angles		angle	radian
	phi1	45	0.785
	Phi	0	0.000
	phi2	0	0.000

삼각 함수 값들

cos(phi1)	0.707	sin(phi1)	0.707
cos(Phi)	1.000	sin(Phi)	0.000
cos(phi2)	1.000	sin(phi2)	0.000

transformation matrix R

0.707	0.707	0.000
-0.707	0.707	0.000
0.000	0.000	1.000

(transformation matrix)^t= R^t=R^-1

0.707	-0.707	0.000
0.707	0.707	0.000
0.000	0.000	1.000

2nd rank tensor in matrix form

1	0	0
0	0	0
0	0	0

R.T

0.707	0.000	0.000
-0.707	0.000	0.000
0.000	0.000	0.000

R^t.R.T **2nd rank tensor after coordinate transformation**

0.500	-0.500	0.000
-0.500	0.500	0.000
0.000	0.000	0.000

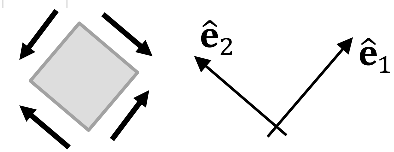
1st rank tensor (i.e., vector) in array form

1
0
0

R.v 1st rank tensor (vector) after coordinate transformation

0.70710678	-0.7071068	0

3. Check the new tensor component values referred to the new coordinate system



4. 새로운 좌표계에서는 pure shear state로 표현됨을 알 수 있다.

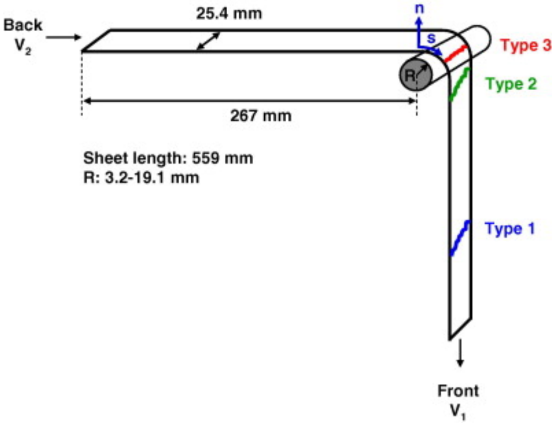
Q. 응력이 바뀐 것인가?

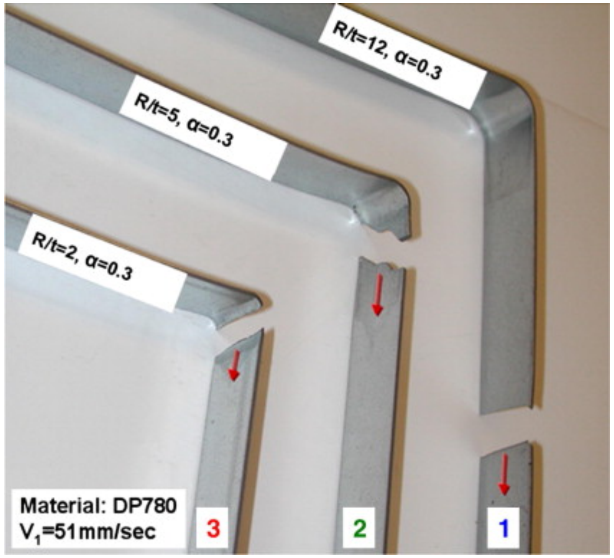
Advanced Example (기출)

- Elastic modulus ($\mathbb{E}$) is a 4th rank tensor and correlates the stress ($\boldsymbol{\sigma}$) and strain ($\boldsymbol{\varepsilon}$) in the elastic regime through
  - $\boldsymbol{\sigma} = \mathbb{E}\!:\boldsymbol{\varepsilon}$
- Note that the colon symbol in the above denotes the double inner dot operation such that
  - $\sigma_{\mathrm{ij}} = \mathbb{E}_{\mathrm{ijkl}}\varepsilon_{\mathrm{kl}}$
- Q1. Express σ_{23} in the function of $\mathbb{E}$ and $\boldsymbol{\varepsilon}$ by explicitly denoting the indices of the associated tensors; Do not contract the expression by using Einstein's summation convention; Do not use the summation symbol.
- Q2. How many separate equations are hidden?

Where coordinate system transformation is required?

- Stretch bending test
- The failure criterion is usually written in terms of strain (or stress) state referred to the coordinate that is attached to the plane of the sheet metal.
- Here, as you can see, the region of specimen that eventually fractures, flows over the roller, during which it bends and ’rotates’.
- Therefore, you would want to ‘transform’ the stress state that was once referred to the global coordinate to the local coordinate system that ‘rotates’ together with the material.



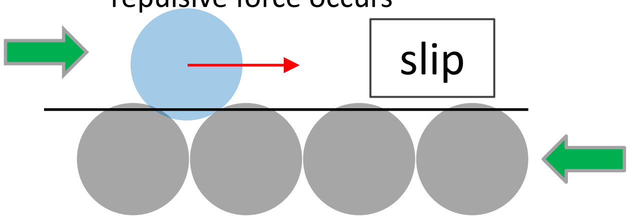


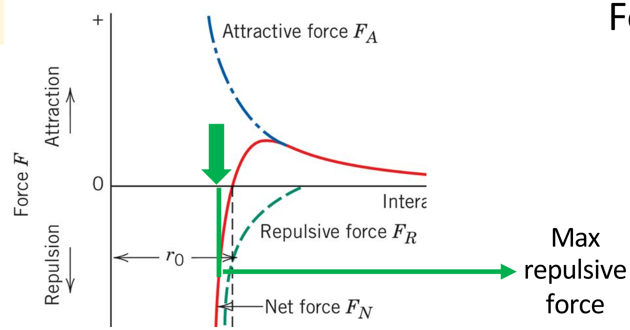
JH Kim et al, IJP 27, 2011

Where coordinate system transformation is required?

Critical Resolved Shear Stress

Atom position when maximum repulsive force occurs

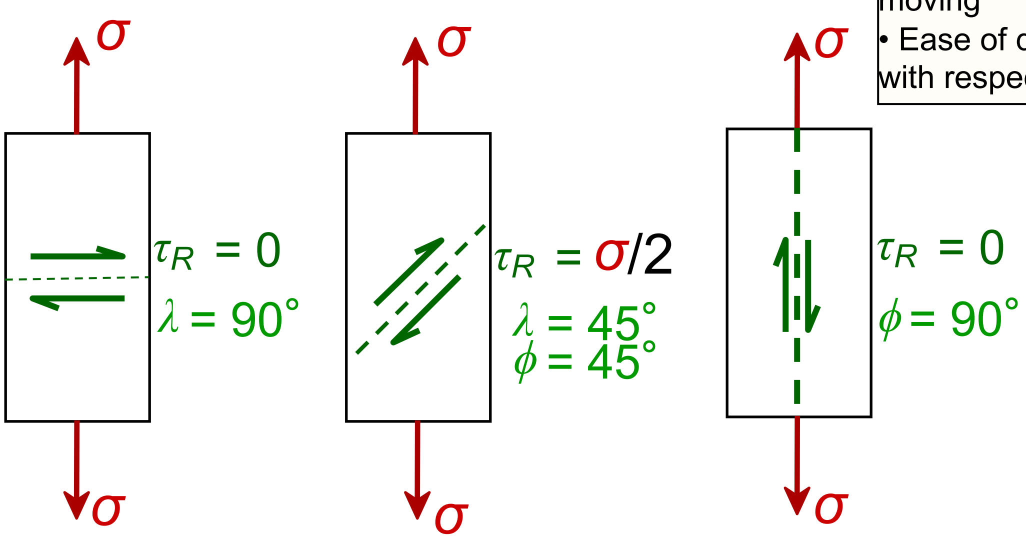




For dislocation to slip, this max. force should be overcome.

Max. repulsive force is closely related with the CRSS

- Condition for dislocation motion (= condition for plastic yielding):
  If RSS reaches a certain (critical) value, the dislocation will start moving
- Ease of dislocation motion depends on crystallographic orientation with respect to the external loading direction



$$\tau_{RSS} = \sigma \cos\lambda \cos\phi$$

$\cos\lambda \cos\phi$: Schmid's (orientation) factor

Dislocation slip condition (≈ atomic yield condition)

$$\tau_{RSS} \geq \tau_{CRSS}$$

Example: yield of single crystal

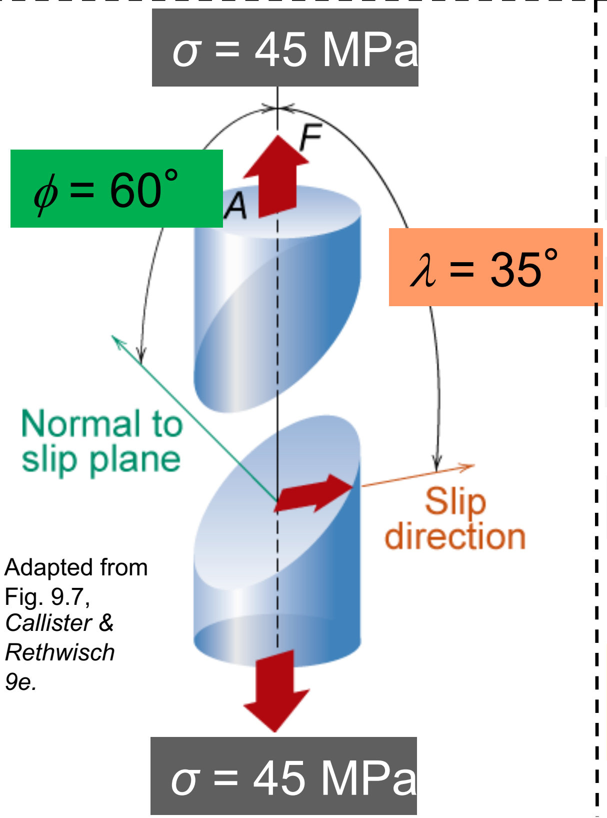
a) Will the single crystal yield?
b) If not, what stress is needed?

$\tau_{RSS} = \sigma \cos\lambda \cos\phi$

We learned this equation that correlates the external loading (σ) and the orientation of slip system (λ, ϕ).

Condition 1. External load of 45 MPa

Condition 2. Slip system characterized by $\lambda = 35°, \phi = 60°$



Adapted from Fig. 9.7, *Callister & Rethwisch 9e.*

Condition for dislocation to slip? → $\tau_{RSS} \geq \tau_{CRSS}$

Condition 1. $\tau_{CRSS} = 20.7$ MPa

Condition 2. $\tau_{RSS} = \sigma \cos\lambda \cos\phi$

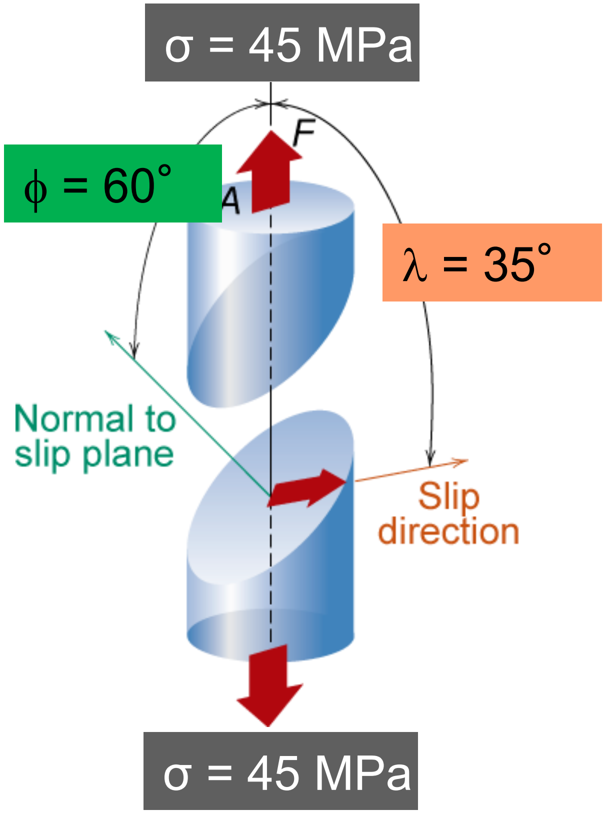
$= 45 \cos 35° \cos 60°$ [MPa]

$\approx 45 \times 0.819 \times 0.5 \approx 18.4$ [MPa]

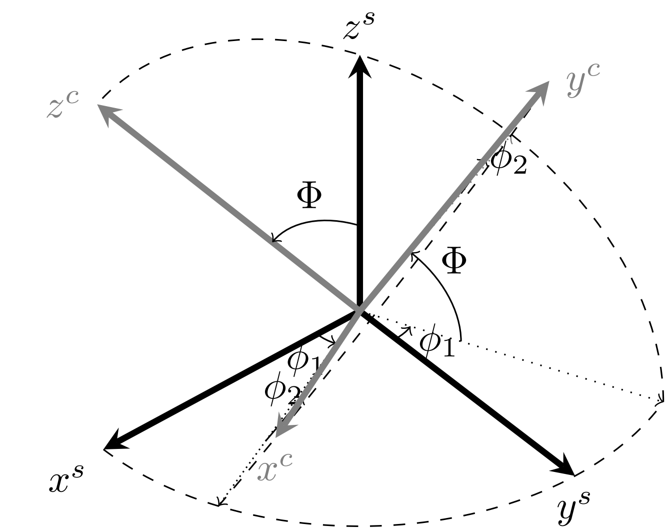
Check $\tau_{RSS} \ngeq \tau_{CRSS}$

45 MPa is not sufficient enough to cause this slip system ($\lambda = 35°, \phi = 60°$) to slip (yield)

Transformation for CRSS



$\phi_1 = 25°, \Phi = 60°, \phi_2 = 19°$



Transformation matrix that connects the loading axes to slip system axes.

This gives the transformation matrix like:

0.788	0.547	0.282
-0.495	0.291	0.819
0.366	-0.785	0.500

If you transform

0	0	0
0	0	0
0	0	45

You'll get

3.577	10.389	6.344
10.389	30.173	18.424
6.344	18.424	11.250

예제

- 다음의 2차 응력 텐서를 주어진 좌표변환 matrix를 사용하여 변환된 후의 값을 매트릭스 형태로 표현하여라.

- 현재 좌표계에서의 응력 텐서는 다음과 같은 형태로 보임:

100	0	0
0	100	0
0	0	100

- 좌표 변환 matrix는

0.788	0.547	0.282
-0.495	0.291	0.819
0.366	-0.785	0.500

예제 – 좌표 변환을 사용한 예제.

- 한 알루미늄 시편의 응력상태가 한 좌표계에서 응력 텐서를 사용하여 [[1,2,3],[2,5,6],[3,6,9]]로 주어져 있다.
- 알루미늄 시편의 (111) 결정면과 [1-10] 방향으로 RSS가 궁금하다.
- 만약 단결정의 결정좌표계(crystal coordinate system)와 응력텐서가 참조된 실험실좌표계(lab coordinate system)의 관계가 다음과 같은 transformation matrix로 주어진다면, RSS값은 얼마인가? Transformation matrix는 결정좌표계를 실험실 좌표계로 옮겨주는 것에 유의하라.

- 0.996 -0.087 0.006
- 0.086 0.981 -0.174
- 0.009 0.173 0.985

연습 문제

- ** http://youngung.github.io/euler2ndtensor/ 에 업로드된 spreadsheet를 활용하여 다음에 답하시오.
- Q1. 좌표계 A에 따른 응력 상태를 다음과 같이 행렬로 표현하였다. 해당 응력 상태를 좌표계 B로 변환하여 행렬로 표현하여라. 단, 좌표계 A에서 B로 변환은 다음의 Euler angle를 활용하여라: $\phi_1 = 45°, \Phi = 0°, \phi_2 = 0°$

100	0	0
0	0	0
0	0	0

- Q2. 위의 응력 상태를 다음의 Euler angle을 활용하여 변환하여 행렬로 나타내시오.

$$\phi_1 = 90°, \Phi = 0°, \phi_2 = 0°$$

- Q3. 위의 응력 상태를 다음의 Euler angle을 활용하여 변환하여 행렬로 나타내시오.

$$\phi_1 = 90°, \Phi = 45°, \phi_2 = 0°$$

연습 문제

- ** http://youngung.github.io/euler2ndtensor/ 에 업로드된 spreadsheet를 활용하여 다음에 답하시오.

- Q1. 좌표계 A에 따른 응력 상태를 다음과 같이 행렬로 표현하였다. 해당 응력 상태를 좌표계 B로 변환하여 행렬로 표현하여라. 단, 좌표계 A에서 B로 변환은 다음의 Euler angle를 활용하여라: $\phi_1 = 45°, \Phi = 0°, \phi_2 = 0°$

100	0	0
0	100	0
0	0	100

- Q2. 위의 응력 상태를 다음의 Euler angle을 활용하여 변환하여 행렬로 나타내시오.

$$\phi_1 = 90°, \Phi = 0°, \phi_2 = 0°$$

- Q3. 위의 응력 상태를 다음의 Euler angle을 활용하여 변환하여 행렬로 나타내시오.

$$\phi_1 = 90°, \Phi = 45°, \phi_2 = 0°$$

연습 문제

- 아래 행렬로 표현된 응력 상태는 어떠한 좌표변환에도 불변하는 것을 알 수 있다.

100	0	0
0	100	0
0	0	100

- Q. 좌표 변환에도 변화없는 물리량을 표현하기에 적절한 표현 방법은 무엇인가?
  - 1) 2nd rank tensor를 사용한다.
  - 2) 1st rank tensor를 사용한다.
  - 3) 0th rank tensor를 사용한다.
  - 4) 위 보기들 중에 적절한 답 없음

Project 문제

- 강의 시간에 활용된 Excel 혹은 Google spreadsheet (http://youngung.github.io/euler2ndtensor/)를 스스로 만들어 보시오.

Project 문제

- 강의 시간에 활용된 Excel 혹은 Google spreadsheet (http://youngung.github.io/euler2ndtensor/)를 활용하여 다음을 수행할 수 있는 spreadsheet를 만들어 보시오.

Target1: 주어진 임의의 stress state가 결정립에 가해질 때, 결정립이 가진 임의의 (hkl)[uvw]의 slip system에 해당하는 resolved shear stress를 구할 수 있는 spread sheet를 작성하시오.

Target2: 결정립의 방위가 (ϕ_1, Φ, ϕ_2)의 Euler angle로 주어진 FCC 결정 구조의 금속의 12개의 slip system 각각이 가질 resolved shear stress를 모두 구할 수 있는 spread sheet를 작성하시오.

Project 문제

- 앞서 target2을 통해 얻어진 spreadsheet를 computer program으로 작성하시오.