Applications of Coordinate Transformation

강의명: 금속가공학특론 (AMB2004)

정영웅

창원대학교 신소재공학부

YJEONG@CHANGWON.AC.KR

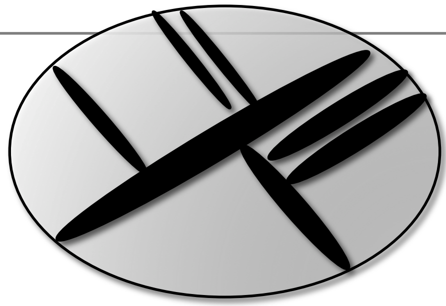
연구실: #52-212 전화: 055-213-3694

HOMEPAGE: HTTP://YOUNGUNG.GITHUB.IO

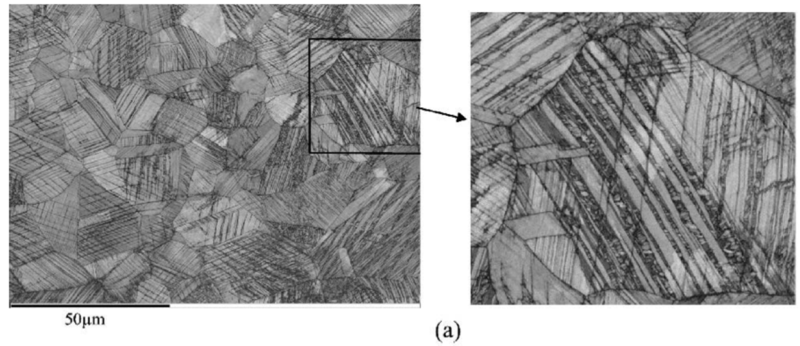
Coordinate transformation 예제

- Variant selection
- Schmid’s law와 비교

Variant selection

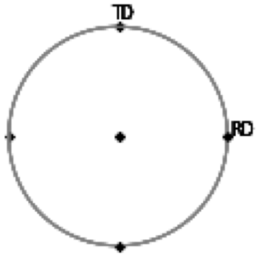


Schematic illustration of martensitic transformation

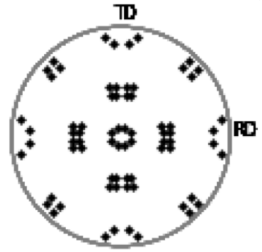


Gey, N.; Petit, B. & Humbert, M. Electron backscattered diffraction study of ε/α` martensitic variants induced by plastic deformation in 304 stainless steel Metallurgical and Materials Transactions A, Springer Boston, 2005, 36, 3291-3299

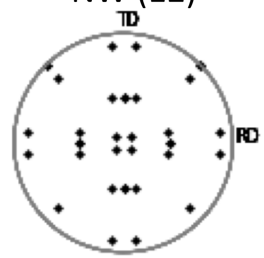
Mother austenite



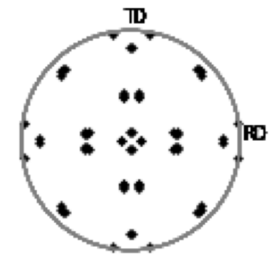
KS (24)



NW (12)



WLR-Bhadeshia (24)



Transformation matrix between axes of parent austenite and child? a_{ij}

$$a_{ij}^{\alpha' \text{ var.} \leftarrow \gamma} = \begin{bmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

How to obtain transformation matrix (a_{ij})?
We'll study it step-by-step in case you know
1). Habit plane and direction of parent (austenite)
2). Habit plane and direction of child (martensite)

Variant selection

Example of martensite variant selections

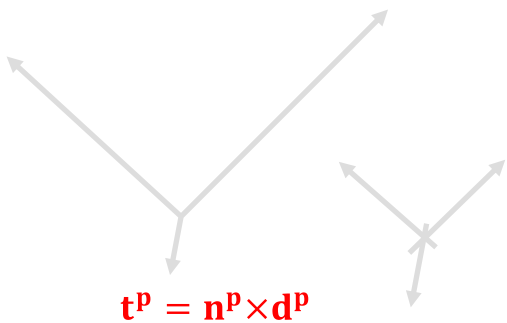
Superscript p(γ) and c(α) denote
- parent (i.e., γ austenite)
- child (i.e., a α martensite variant)

1). Habit plane and direction of parent (austenite)
2). Habit plane and direction of child (martensite)

$$(111)^{\gamma}[110]^{\gamma} \parallel (110)^{\alpha}[111]^{\alpha}$$

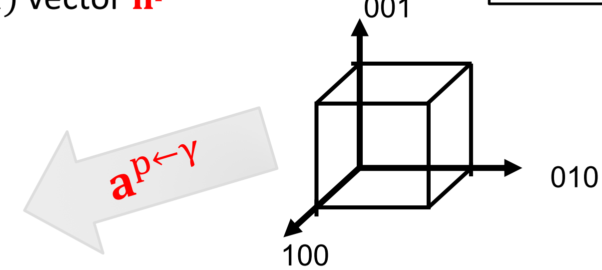
$$\begin{bmatrix}1\\0\\0\end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}$$

$\frac{1}{\sqrt{2}}(1,1,0)$ vector $\mathbf{d}^{\mathrm{p}}$ $\frac{1}{\sqrt{3}}(1,-1,1)$ vector $\mathbf{n}^{\mathrm{p}}$



$\mathbf{t}^{\mathrm{p}} = \mathbf{n}^{\mathrm{p}} \times \mathbf{d}^{\mathrm{p}}$

γ Austenite

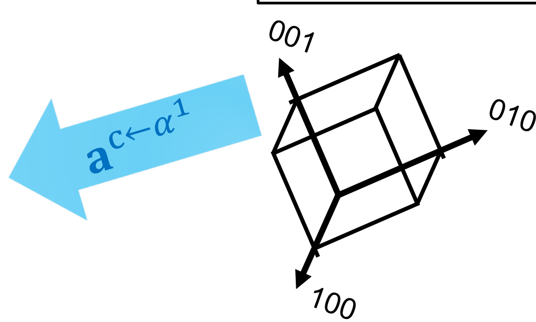


$$\boldsymbol{a}_{\mathrm{ij}}^{\mathrm{p}\leftarrow\gamma} = \begin{bmatrix} \mathrm{n}_1^{\mathrm{p}} & \mathrm{d}_1^{\mathrm{p}} & \mathrm{t}_1^{\mathrm{p}} \\ \mathrm{n}_2^{\mathrm{p}} & \mathrm{d}_2^{\mathrm{p}} & \mathrm{t}_2^{\mathrm{p}} \\ \mathrm{n}_3^{\mathrm{p}} & \mathrm{d}_3^{\mathrm{p}} & \mathrm{t}_3^{\mathrm{p}} \end{bmatrix}$$

$\frac{1}{\sqrt{2}}(1,1,1)$ vector $\mathbf{d}^{\mathrm{c}}$ $\frac{1}{\sqrt{3}}(1,-1,0)$ vector $\mathbf{n}^{\mathrm{c}}$

$\mathbf{t}^{\mathrm{c}} = \mathbf{n}^{\mathrm{c}} \times \mathbf{d}^{\mathrm{c}}$

α^1 Martensite

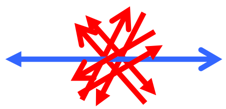


$$\boldsymbol{a}_{\mathrm{ij}}^{\mathrm{c}\leftarrow\alpha^1} = \begin{bmatrix} \mathrm{n}_1^{\mathrm{c}} & \mathrm{d}_1^{\mathrm{c}} & \mathrm{t}_1^{\mathrm{c}} \\ \mathrm{n}_2^{\mathrm{c}} & \mathrm{d}_2^{\mathrm{c}} & \mathrm{t}_2^{\mathrm{c}} \\ \mathrm{n}_3^{\mathrm{c}} & \mathrm{d}_3^{\mathrm{c}} & \mathrm{t}_3^{\mathrm{c}} \end{bmatrix}$$

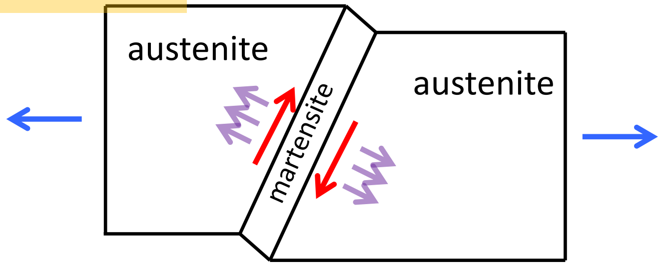
Note that P axes and C axes are physically equivalent

Variant selection

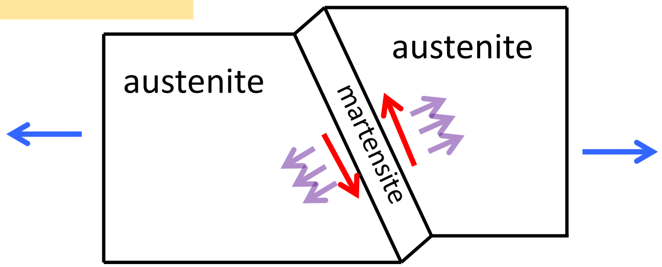
$$\boxed{\mathbf{a}_{ij}^{\alpha^1\leftarrow\gamma}} = \mathbf{a}^{\alpha^1\leftarrow c} \cdot \mathbf{a}^{p\leftarrow\gamma} = \left(\mathbf{a}^{c\leftarrow\alpha^1}\right)^{T} \cdot \mathbf{a}^{p\leftarrow\gamma} = a_{ki}^{c\leftarrow\alpha^1} a_{kj}^{p\leftarrow\gamma} = \sum_{k}^{3} a_{ki}^{c\leftarrow\alpha^1} a_{kj}^{p\leftarrow\gamma}$$



Variant 1



Variant 2



$U^{i} = \boldsymbol{\sigma}{:}\,\boldsymbol{\varepsilon}_{i}^{tr}$. with index i to denote i-th variant

⋮

Principal of maximum energy:

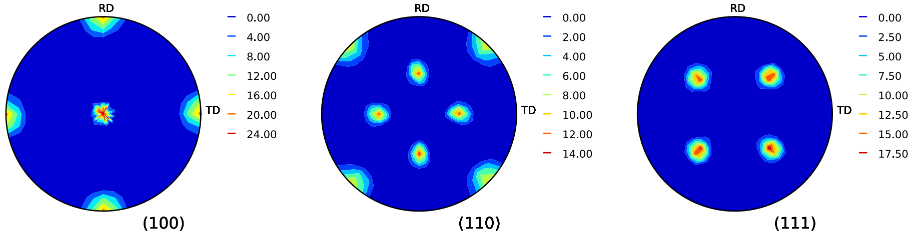
$U^{1} = \boldsymbol{\sigma}{:}\,\boldsymbol{\varepsilon}_{1}^{tr} \ldots U^{2} = \boldsymbol{\sigma}{:}\,\boldsymbol{\varepsilon}_{2}^{tr} \quad \ldots. \quad U^{24} = \boldsymbol{\sigma}{:}\,\boldsymbol{\varepsilon}_{24}^{tr}$

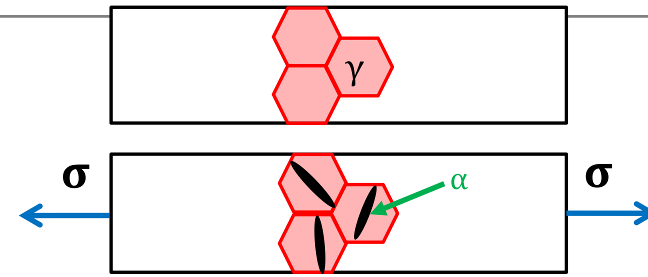
Variant 24

Transformation characteristic strain $\boldsymbol{\varepsilon}^{tr}$ is a tensor. Over the calculation of U, stress and strain tensors should be written in the same axes; thus need correct transformation matrices (orientation)

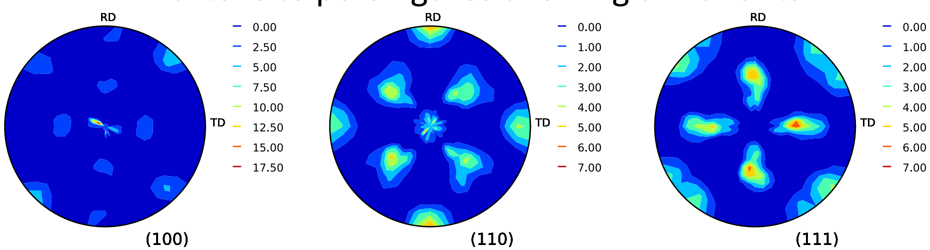
Variant selection (Benchmark test)

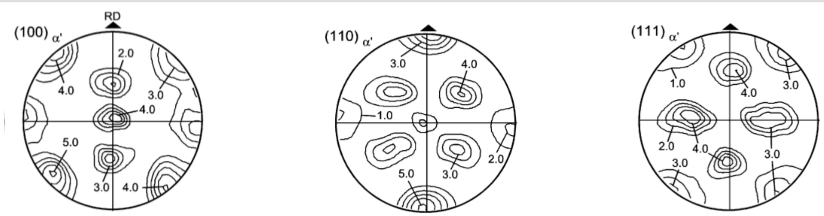
Cube textured 100% austenitic polycrystal



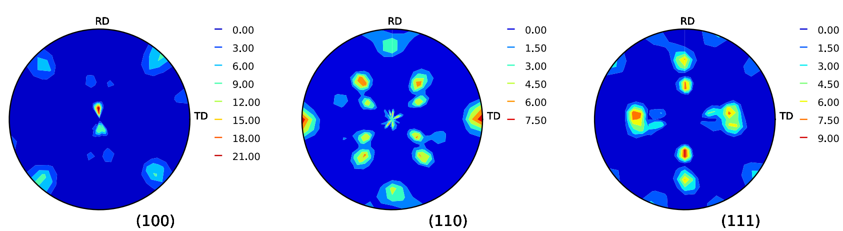


Martensite pole figures allowing all variants





Humbert MSEA (2007)

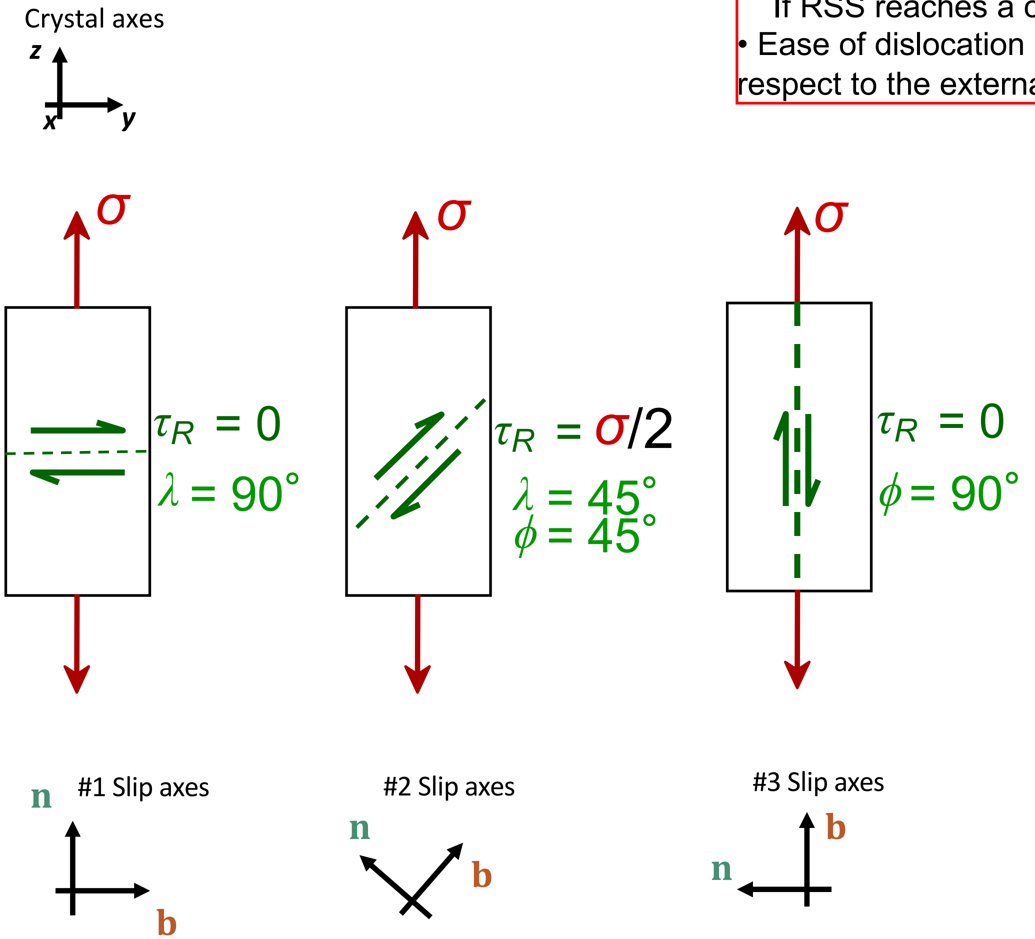


WLR:
$\gamma \rightarrow \alpha$

- Humbert, M.; Petit, B.; Bolle, B. & Gey, N. *Materials Science and Engineering: A,* **2007**
- Kundu, S. & Bhadeshia, H. *Scripta Materialia,* **2006**

Coordinate transformation and Schmid law, Schmid factor

- 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



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

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

Dislocation slip condition
(≈ atomic yield condition)

$$\tau_{\mathrm{RSS}} = \tau_{\mathrm{CRSS}}$$

Example: yield of single crystal

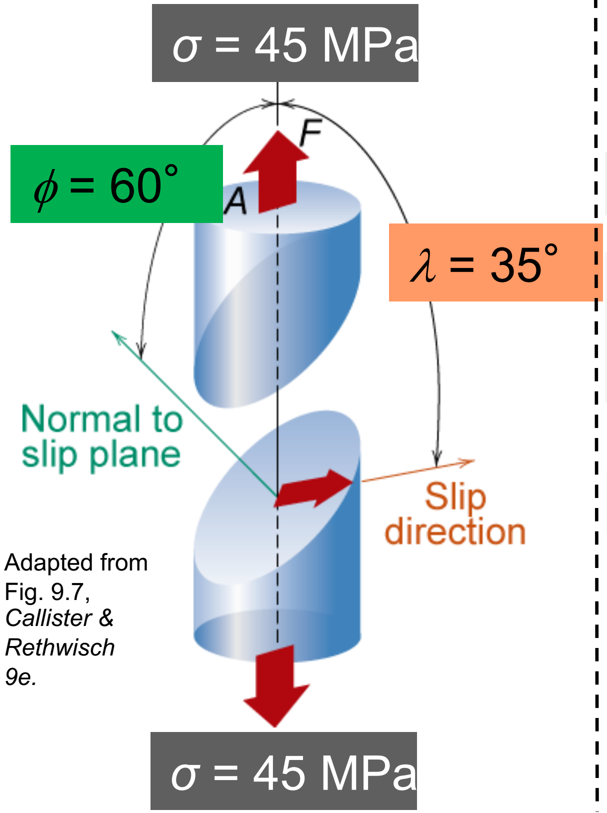
a) Will the single crystal yield?
b) If not, what stress is needed?

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

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. $\tau_{CRSS} = \boxed{20.7}$ MPa

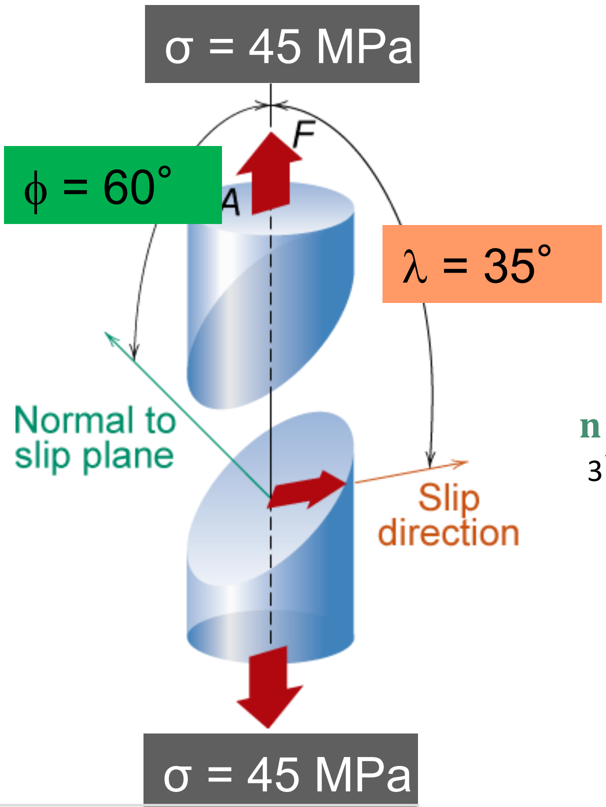
Condition 2. $\tau_{RSS} = \sigma \cos\lambda \cos\phi$
$= 45 \cos 35° \cos 60°$ [MPa]
$\approx 45 \times 0.819 \times 0.5 \approx \boxed{18.4}$ [MPa]

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

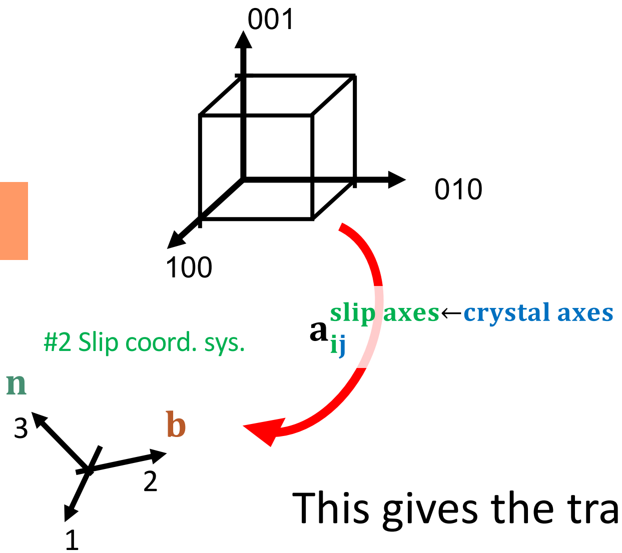
Remember this value

45 MPa is not sufficient enough to cause this slip system ($\lambda = 35°, \phi = 60°$, with $\tau_{CRSS} = 20.7$ MPa) to slip (yield)

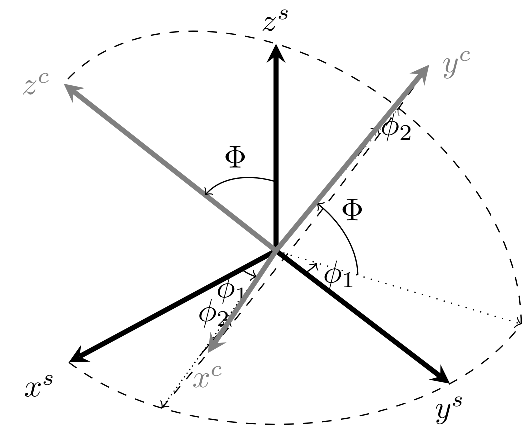
Transformation: stress in CA to that in Slip. Axes.



Single crystal axes



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



This gives the transformation matrix like:

$a_{ij}^{\text{slip axes}\leftarrow\text{crystal axes}}$ =

0.788	0.547	0.282
-0.495	0.291	0.819
0.366	-0.785	0.500

Matrix form of the stress tensor $\boldsymbol{\sigma}$ in crystal axes

0	0	0
0	0	0
0	0	45

$$\sigma_{ij}^{SA} = \sum_{k}^{3}\sum_{l}^{3} a_{ik}a_{jl}\sigma_{kl}^{CA} = a_{ik}a_{jl}\sigma_{kl}^{CA} = \mathbf{a}\cdot\boldsymbol{\sigma}^{CA}\cdot\mathbf{a}^{T}$$

Matrix form of the stress tensor in slip system axes

3.577	10.389	6.344
10.389	30.173	18.424
6.344	18.424	11.250

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]

Finding resolved shear stress = Stress tensor transformation

- 가령, 단결정 결정립이 응력 텐서 $\boldsymbol{\sigma}$ 를 받는 상태를 생각해보자.
- 여러분이 관심있는 slip system은, 결정면 방향 (denoted by vector **n**)과 슬립 방향 (denoted by **b**) 으로 표현되며, 다음과 같은 resolved shear stress 를 가진다:

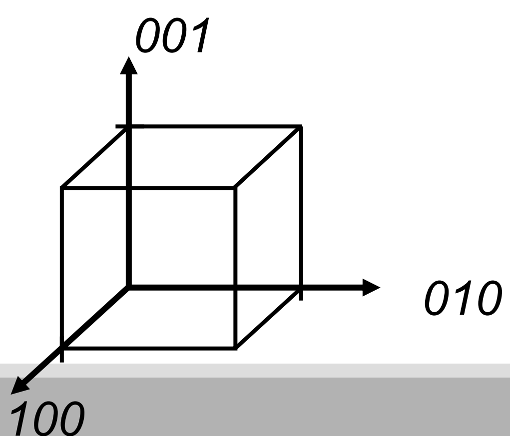
$$\boxed{\tau_{\mathrm{RSS}} = \boldsymbol{\sigma} \cdot \mathbf{n} \cdot \mathbf{b} = \sigma_{ij} n_i b_j}$$

- 더욱더 일반화 시켜, 임의의 slip system s를 대상으로 표현하자면…

$$\boxed{\tau^{s}_{\mathrm{RSS}} = \boldsymbol{\sigma} \cdot \mathbf{n}^{s} \cdot \mathbf{b}^{s}}$$

- 실례를 들자.

Cubic unit cell에 의한 crystal axes



예를 들어, $\mathbf{n}^{s}$와 $\mathbf{b}^{s}$ 는 각각 [1,1,1]/sqrt(3). [1,1,0]/sqrt(2)

$$\tau^{s}_{\mathrm{RSS}} = (\boldsymbol{\sigma} \cdot \mathbf{n}^{s} \cdot \mathbf{b}^{s}) = \sigma_{ij} n^{s}_{i} b^{s}_{j} = \sum_{i}^{3} \sum_{j}^{3} \sigma_{ij} n^{s}_{i} b^{s}_{j}$$

$n^{s}_{i} b^{s}_{j} \rightarrow \mathbb{m}^{s}_{ij}$ (Schmid tensor; will see more precise definition later)

Schmid factor is a special case of Schmid tensor when the crystal is imposed to a uniaxial stress state

Stress transformation in Schmid law

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

$$\boxed{\tau^{s}_{RSS} = \boldsymbol{\sigma}\cdot\mathbf{n}^{s}\cdot\mathbf{b}^{s}} = \sigma_{ij} n^{s}_{i} b^{s}_{j} = \sum_{i}^{3}\sum_{j}^{3} \sigma_{ij} n^{s}_{i} b^{s}_{j}$$

$$\boldsymbol{\sigma}^{\text{Crystal Axes}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix} \mathbf{e}^{CA}_{i} \otimes \mathbf{e}^{CA}_{j}$$

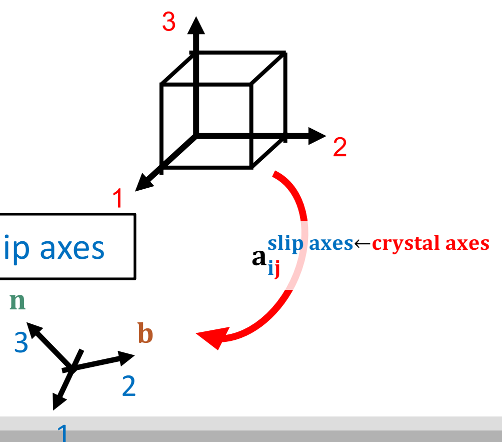
Schmid law is merely a special case of stress tensor transformation (= Finding a resolved shear stress component to a particular slip system under uniaxial stress state).

Recall

$$\begin{array}{cc} & \text{Old co. sys.} \\ & \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \end{bmatrix} \\ \text{New co. sys.} \begin{bmatrix} \acute{\mathbf{e}}_1 \\ \acute{\mathbf{e}}_2 \\ \acute{\mathbf{e}}_3 \end{bmatrix} & \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \end{array}$$

$$\boxed{\tau^{s}_{RSS} = \sigma^{(Xtal)}_{33} n^{s,(Xtal)}_{3} b^{s,(Xtal)}_{3}} \boxed{= \sigma^{(Xtal)}_{33}\left(\mathbf{a}^{Xtal\leftarrow(Slip)}\cdot\mathbf{n}^{(Slip)}\right)_{3}\left(\mathbf{a}^{Xtal\leftarrow(Slip)}\cdot\mathbf{b}^{(Slip)}\right)_{3}}$$

Single crystal axes



Slip axes

$$a^{Slip\leftarrow Xtal}_{ij} = \begin{bmatrix} t_1 & b_1 & n_1 \\ t_2 & b_2 & n_2 \\ t_3 & b_3 & n_3 \end{bmatrix}$$

$$a^{Xtal\leftarrow Slip}_{ij} = \begin{bmatrix} t_1 & t_2 & t_3 \\ b_1 & b_2 & b_3 \\ n_1 & n_2 & n_3 \end{bmatrix}$$

$$\boxed{\tau^{s}_{RSS} = \boldsymbol{\sigma}^{(Slip\ Axes)}\cdot\mathbf{n}^{s,(Slip\ Axes)}\cdot\mathbf{b}^{s,(Slip\ Axes)}}$$ Will give the same answer

Schmid factor and alternative ways

$$\boxed{\tau^{s}_{\mathrm{RSS}} = \sigma^{\mathrm{macoscopic\ uni}} \cdot \mathbf{n}^{s} \cdot \mathbf{b}^{s}}$$

This equation is widely used in MSE community to calculate the Schmid factor of individual grains:

The hidden assumption is that you know the stress state of grain, and it should be 'uniaxial' stress value σ

The fact is, in many cases, you really don't know the stress state of grain, even if you know the macroscopic stress. Even if the sample is under uniaxial loading, the stress state of individual strain can be very different from that of specimen because of 'interactions' with the neighbor grains – some grains may be stiff than others and vice versa.

- We do not know the exact stress state of individual grains, even if we know the stress given to the entire sample.
- One might assume the stress state of individual grain is equivalent to that of macroscopic loading (Sachs)
- This assumption may look very primitive s, but many pioneers have done it in early 20th century.
- We will look at Taylor, Sachs and self-consistent approach on this problem.