Examples of Einstein summation

$$a_i = b_{ij}c_jd_j$$
 LHS 그리고 RHS 모두 i 만 free index; (Correctly used notation)

$$a_ib_j=c_{ik}d_{kj}$$
 LHS 그리고 RHS 모두 i,j 가 free index; (Correctly used notation) Index j is repeated in $m{c}$ and $m{d}$. So, Einstein Summation Convention is implied

$$a_i b_j = c_{ik} d_{kj} + e_i f_j + g_i p_{jj} + q_l r_{ij}$$

LHS has two free index i and j. In RHS, in the third term the same j is used as if it is non free index; (Conflicts). Also, the fourth term has an extra index l.

When Einstein summation convention is implied, we call the index (over which summation is performed) dummy as it is not important what letter is given.

For instance, $a_i b_i = a_k b_k = a_l b_l \dots etc$

Examples of Einstein summation

$$a_i = b_{ij}c_jd_j$$
 LHS 그리고 RHS 모두 i 만 free index; (Correctly used notation)

$$a_ib_j=c_{ik}d_{kj}$$
 LHS 그리고 RHS 모두 i,j 가 free index; (Correctly used notation) Index j is repeated in $m{c}$ and $m{d}$. So, Einstein Summation Convention is implied

$$a_i b_j = c_{ik} d_{kj} + e_i f_j + g_i p_{jj} + q_l r_{ij}$$

LHS has two free index i and j. In RHS, in the third term the same j is used as if it is non free index; (Conflicts). Also, the fourth term has an extra index l.

When Einstein summation convention is implied, we call the index (over which summation is performed) dummy as it is not important what letter is given.

For instance, $a_i b_i = a_k b_k = a_l b_l \dots etc$

• 3차원 공간에서의 물리량으로 이루어진 다음 expression을 Einstein summation convention을 사용하여 나타내시오.

$$\boldsymbol{b} = \boldsymbol{x} + \boldsymbol{C} \cdot \boldsymbol{y}$$

 $C \cdot y$ 은 내적이며 C가 2^{nd} order tensor (3x3 matrix) 이고 y는 벡터이다. 따라서 그 결과는

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} C_{11}y_1 + C_{12}y_2 + C_{13}y_3 \\ C_{21}y_2 + C_{22}y_2 + C_{23}y_3 \\ C_{31}y_1 + C_{32}y_2 + C_{33}y_3 \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{3} C_{2j}y_j \\ \sum_{j=1}^{3} C_{2j}y_j \\ \sum_{j=1}^{3} C_{3j}y_j \end{bmatrix}$$

$$c \cdot y \in \text{ 내적이며 } c \text{가 2}^{\text{nd}} \text{ order tensor (3x3 matrix)} \text{ 이고 } y \in \text{ 벡터이다. 따라서 } \text{ 그 결과는 }$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} C_{11}y_1 + C_{12}y_2 + C_{13}y_3 \\ C_{21}y_2 + C_{22}y_2 + C_{23}y_3 \\ C_{31}y_1 + C_{32}y_2 + C_{33}y_3 \end{bmatrix} = \begin{bmatrix} \sum_{j=3}^{3} c_{2j}y_j \\ \sum_{j=3}^{3} c_{3j}y_j \end{bmatrix}$$

$$b_i = x_i + \sum_{j=3}^{3} c_{1j}y_j \quad \text{for } i = 1,2,3$$

$$b_i = x_i + C_{ij}y_j \quad \text{or } i = 1,2,3$$

$$b_i = x_i + C_{ij}y_j \quad \text{or } i = 1,2,3$$

벡터 (vector) operations

• Dot product aka inner dot product (내적):

$$d = \boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{b} \cdot \boldsymbol{a}$$
 or $d = \sum_{i=1}^{3} a_{i} b_{i} \rightarrow \text{(Einstein)}$: $d = a_{i} b_{i}$

Alternative form:

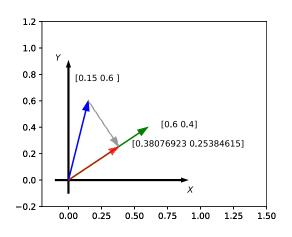
$$\boldsymbol{a} \cdot \boldsymbol{b} = |\boldsymbol{a}| |\boldsymbol{b}| \cos \theta$$

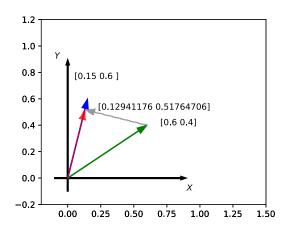
 θ 는 두 벡터 (\boldsymbol{a} and \boldsymbol{b}) 사이의 각이다. 또한 두 내적인 다음과 같이 연산할 수도 있다. $\boldsymbol{a} \cdot \boldsymbol{b} = (a_x \boldsymbol{i} + a_y \boldsymbol{j} + a_z \boldsymbol{k}) \cdot (b_x \boldsymbol{i} + b_y \boldsymbol{j} + b_z \boldsymbol{k})$

i, j, k 는 참조하는 좌표계의 세 베이시스 벡터 $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ 를 의미한다.

• Inner product of different basis vector leads in zero, while that of the same basis vectors lead to 1: $\mathbf{i} \cdot \mathbf{j} = 0$ and $\mathbf{i} \cdot \mathbf{i} = 1$

 $ightarrow \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ (Kronecker delta)





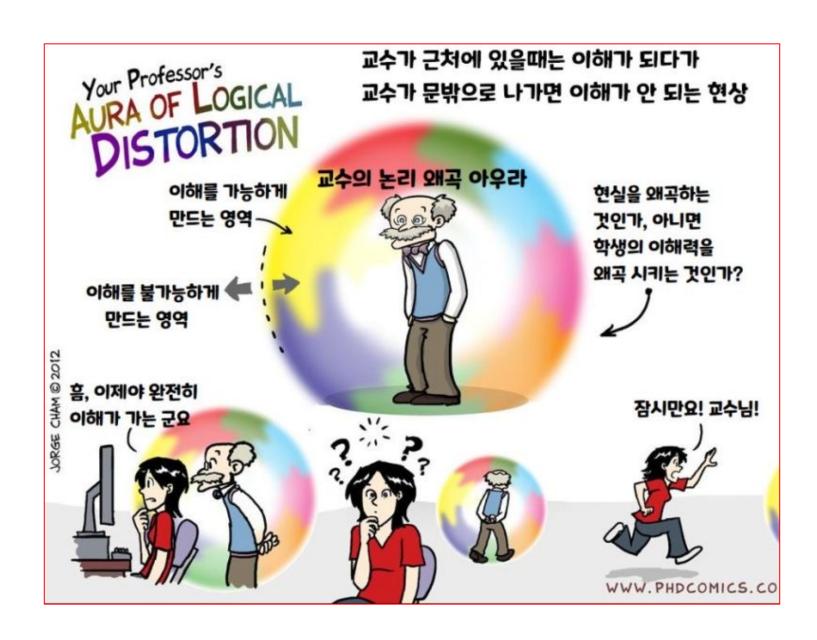
Either way, the dot product amounts to ~42.27

summary

- Nomenclature
 - 굵은 글씨 문자 (예 a)는 벡터, 혹은 행렬을 뜻함.
 - 굵지 않은 글씨 문자는 (예 a, a_i, b_{ij}) 등은 scalar (혹은 벡터 행렬의 구성성분)를 뜻함
- 벡터 a의 크기 (magnitude)는 |a| 로 표기하고 다음과 같이 정의됨 $|a| = (a_1^2 + a_2^2 + a_3^2)^{0.5}$
- 벡터 a의 단위 벡터는 다음과 같이 정의됨 $\frac{a}{|a|}$
- 벡터는 더하기, 빼기, dot product, cross product, double dot product, dyadic product 등의 연산을 가짐.
- 주어진 좌표계의 basis vector를 사용해서 벡터를 다음과 같이 표기할 수 있음.

$$\boldsymbol{a} = a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3$$

• 인덱스 표기법 및 Einstein 축약표기법은 벡터 연산을 표기하는데 매우 유용하며 익숙해져야 한다.



예제)

• Q1) 다음은 Miller index로 나타낸 BCC 결정 구조내의 면과 방향이다: (110), [110]두 방향사이의 끼인각은?

• Q2) 다음 결정면 n 과 방향 b으로 이루어진 slip system이 FCC 결정내 존재할까 ?

$$\mathbf{n} = (1, \overline{1}, 1)$$
$$\mathbf{b} = [1, \overline{1}, 0]$$

• Q3) 벡터 a = (1, -0.5,3)과 c = [1,2,0]을 이용해 다음 연산의 답을 구하시오.

$$a_k b_k = ?$$

• Q4) 위 Q3)의 벡터를 활용하여 예상되는 a_ib_k 와 a_ib_i 의 차이를 설명하시오.

벡터 (vector) dyadic operations

• Dyadic product:

$$\mathbf{a} \otimes \mathbf{b} = (a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3) \otimes (b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2 + b_3 \mathbf{e}_3)$$

where \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 are unit vectors along the axes 1,2,3, respectively.

$$\mathbf{a} \otimes \mathbf{b} = a_1 b_1 (\mathbf{e}_1 \otimes \mathbf{e}_1) + a_1 b_2 (\mathbf{e}_1 \otimes \mathbf{e}_2) + a_1 b_3 (\mathbf{e}_1 \otimes \mathbf{e}_3) + a_2 b_1 (\mathbf{e}_2 \otimes \mathbf{e}_1) + a_2 b_2 (\mathbf{e}_2 \otimes \mathbf{e}_2) + a_2 b_3 (\mathbf{e}_2 \otimes \mathbf{e}_3) + a_3 b_1 (\mathbf{e}_3 \otimes \mathbf{e}_1) + a_3 b_2 (\mathbf{e}_3 \otimes \mathbf{e}_2) + a_3 b_3 (\mathbf{e}_3 \otimes \mathbf{e}_3)$$

Also equivalently,

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{bmatrix}$$

If n^s and b^s are slip system s consisting of (unit) plane normal and (unit) slip direction vectors, $n^s \otimes b^s$ corresponds to Schmid tensor such that $M^s = n^s \otimes b^s$ or $M^s_{ij} = n^s_i b^s_j$ (no dummy index)

벡터 (vector) dyadic operations

• Dyadic product:

$$\mathbf{a} \otimes \mathbf{b} = (a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3) \otimes (b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2 + b_3 \mathbf{e}_3)$$

where \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 are unit vectors along the axes 1,2,3, respectively.

$$\mathbf{a} \otimes \mathbf{b} = a_1 b_1 (\mathbf{e}_1 \otimes \mathbf{e}_1) + a_1 b_2 (\mathbf{e}_1 \otimes \mathbf{e}_2) + a_1 b_3 (\mathbf{e}_1 \otimes \mathbf{e}_3) + a_2 b_1 (\mathbf{e}_2 \otimes \mathbf{e}_1) + a_2 b_2 (\mathbf{e}_2 \otimes \mathbf{e}_2) + a_2 b_3 (\mathbf{e}_2 \otimes \mathbf{e}_3) + a_3 b_1 (\mathbf{e}_3 \otimes \mathbf{e}_1) + a_3 b_2 (\mathbf{e}_3 \otimes \mathbf{e}_2) + a_3 b_3 (\mathbf{e}_3 \otimes \mathbf{e}_3)$$

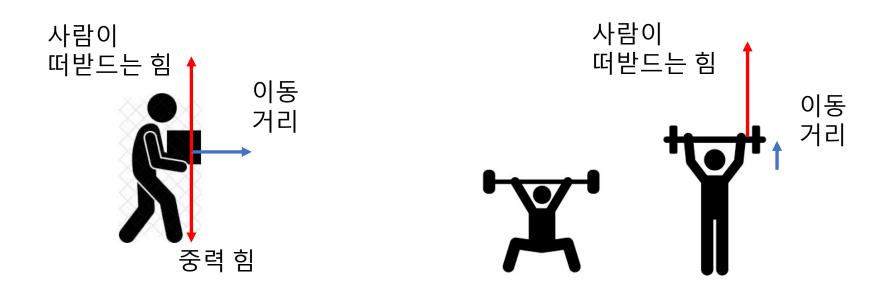
Also equivalently,

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{bmatrix}$$

If n^s and b^s are slip system s consisting of (unit) plane normal and (unit) slip direction vectors, $n^s \otimes b^s$ corresponds to Schmid tensor such that $M^s = n^s \otimes b^s$ or $M^s_{ij} = n^s_i b^s_j$ (no dummy index)

Examples: 사물에 준 일(work)

• 사물에 준 일: 가해진 힘벡터와 이동 벡터의 내적



$$w = \mathbf{F} \cdot \mathbf{r}$$
 \rightarrow $w(t) = w(0) + \int_{r_1}^{r_2} \mathbf{F} \cdot d\mathbf{r}$

Schmid tensor and resolved shear stress

•
$$n^{s} = \frac{(1,1,1)}{|(1,1,1)|}$$
 and $b^{s} = \frac{(1,0,-1)}{|(1,0,-1)|}$

Say, the crystal is subjected to stress tensor of

$$\boldsymbol{\sigma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The resolved shear stress (RSS) amounts to

$$\tau^{S} = \boldsymbol{\sigma} \cdot \boldsymbol{n}^{S} \cdot \boldsymbol{b}^{S} = \boldsymbol{\sigma} : \boldsymbol{M}^{S} = \sigma_{ij} M_{ij}^{S}$$

$$\tau^{s} = \begin{pmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{6}} \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \cdot \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Recall the Schmid law: $\tau^s = \sigma \cos \phi \cos \lambda$

** Caution, direct use of miller index for crystal plane normal and direction should be careful.

Crystal coordinate system of cubic (FCC, BCC) are equivalent to Cartesian. Less symmetric

Structures (such as triclinic) would require change of the miller indices to relevant components in Cartesian coordinates.

Schmid tensor and resolved shear stress

•
$$n^{s} = \frac{(1,1,1)}{|(1,1,1)|}$$
 and $b^{s} = \frac{(1,0,-1)}{|(1,0,-1)|}$

Say, the crystal is subjected to stress tensor of

$$\boldsymbol{\sigma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The resolved shear stress (RSS) amounts to

$$\tau^{S} = \boldsymbol{\sigma} \cdot \boldsymbol{n}^{S} \cdot \boldsymbol{b}^{S} = \boldsymbol{\sigma} : \boldsymbol{M}^{S} = \sigma_{ij} M_{ij}^{S}$$

$$\tau^{s} = \begin{pmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{6}} \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \cdot \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Recall the Schmid law: $\tau^s = \sigma \cos \phi \cos \lambda$

** Caution, direct use of miller index for crystal plane normal and direction should be careful.

Crystal coordinate system of cubic (FCC, BCC) are equivalent to Cartesian. Less symmetric

Structures (such as triclinic) would require change of the miller indices to relevant components in Cartesian coordinates.

Pressure independence of slip

•
$$n^S = \frac{(1,1,1)}{|(1,1,1)|}$$
 and $b^S = \frac{(1,0,-1)}{|(1,0,-1)|}$

Say, the crystal is subjected to stress tensor of

$$\boldsymbol{\sigma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \boldsymbol{\sigma} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \boldsymbol{\sigma} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

Q) Calculate the resolved shear stress for each stress tensor above, and discuss what you observed.