The deformation can be represented with the DEFORMATION TENSOR (F)

$F \rightarrow 3\times 3$ matrix

such that

$$F\vec{a} = \vec{A}$$
$$F\vec{b} = \vec{B}$$
$$F\vec{c} = \vec{C}$$

$\vec{a}, \vec{b}, \vec{c}$ can be collected within a matrix:

$$\mathcal{L} = [\vec{a}, \vec{b}, \vec{c}] = \begin{bmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{bmatrix}$$

similarly

$$\mathcal{L}' = [\vec{A}, \vec{B}, \vec{C}]$$

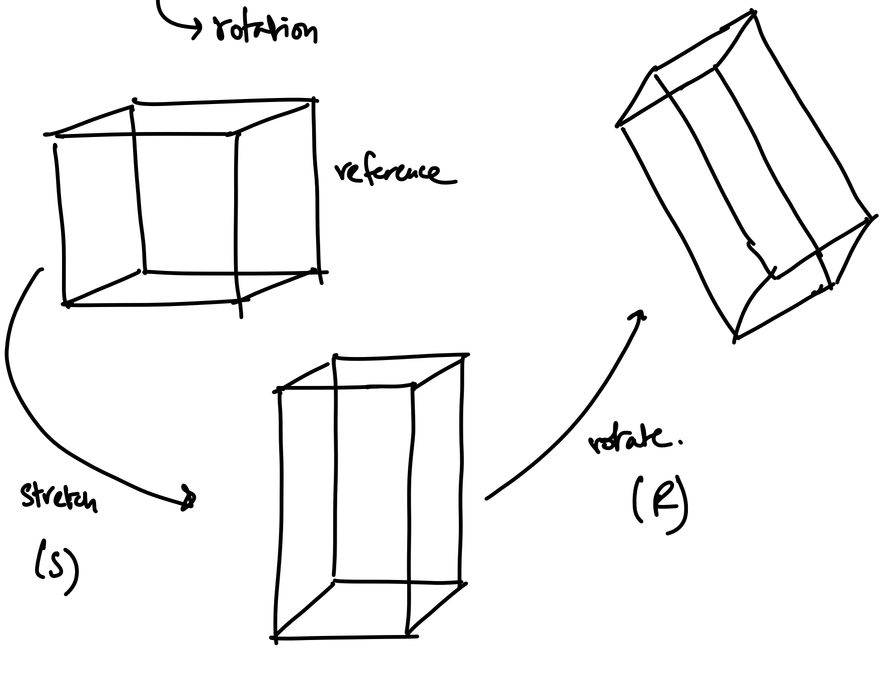
$$F[\vec{a}, \vec{b}, \vec{c}] = [\vec{A}, \vec{B}, \vec{C}]$$

1 $\boxed{F\mathcal{L} = \mathcal{L}'}$

if we have $\mathcal{L}, \mathcal{L}' \rightarrow F = \mathcal{L}'\mathcal{L}^{-1}$ 2 if we would like to impose a particular strain $F\mathcal{L} = \mathcal{L}'$

We can decompose F as

$$F = \underbrace{R}_{\text{rotation}} \cdot \overbrace{S}^{\text{stretch.}}$$



$R \longrightarrow$ rotation matrix $\longrightarrow$ unitary

$$\Rightarrow R^T R = I$$

Consider:

$$F^T F = (RS)^T (RS) = S^T \underbrace{R^T R}_{I} S = S^T S$$

$F^T F \longrightarrow$ invariant to rigid rotations!

Can we use $F^T F$ as a metric of strain?

say $F = I \Rightarrow F\mathcal{L} = \mathcal{L}' \Rightarrow \mathcal{L} = \mathcal{L}' \Rightarrow$ the crystal is not deformed $\Rightarrow$ Strain should be zero.

$$F^T F = I^T I = I \neq 0$$

One metric that is convenient:

$$E = \text{Green-Lagrange strain} = \frac{1}{2}(F^T F - I) = \frac{1}{2}(S^T S - I) \longrightarrow E \text{ is symmetric}$$

when the deformations are small:

$$E \simeq \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix}$$

- FREE ENERGY & STRAIN:

The free energy of a phase will ingeneral depend on the state of strain

$$H(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{yz}, \varepsilon_{yx}, \varepsilon_{xz}, c_i, \eta_j, T)$$

In general ε_{ij} should be replaced with E_{ij}, we will continue to use ε_{ij} for clarity.

Say the reference crystal has a volume V_0:

$$h = \frac{H}{V_0} = \text{free energy density.}$$

Taylor expand h around $\varepsilon_{ij} = 0$

$$h(\underline{\underline{\varepsilon}}) = \underbrace{h(0)}_{\text{free energy of the reference crystal}} + \sum_{\alpha\beta} \underbrace{\left.\frac{\partial h}{\partial \varepsilon_{\alpha\beta}}\right|_{\varepsilon=0}} \varepsilon_{\alpha\beta} + \sum_{\alpha\beta\gamma\delta} \left.\frac{\partial^2 h}{\partial \varepsilon_{\alpha\beta}\partial \varepsilon_{\gamma\delta}}\right|_{\varepsilon=0} \varepsilon_{\alpha\beta}\varepsilon_{\gamma\delta} + \cdots$$

free energy of the reference crystal

$$\frac{\partial h}{\partial \varepsilon_{\alpha\beta}} = -\sigma^0_{\alpha\beta}$$

stress we need to impose to keep the crystal in the reference state

elastic moduli

$$C_{\alpha\beta\gamma\delta} = \frac{\partial^2 h}{\partial \varepsilon_{\alpha\beta}\partial \varepsilon_{\gamma\delta}}$$

Symmetries of $C_{\alpha\beta\gamma\delta}$:

① $\varepsilon \longrightarrow$ symmetric matrix.

$$\varepsilon_{\alpha\beta} = \varepsilon_{\beta\alpha} \Rightarrow C_{\alpha\beta\gamma\delta} = C_{\beta\alpha\delta\gamma} = C_{\alpha\beta\delta\gamma} = C_{\beta\alpha\gamma\delta}$$

② Maxwell relations.

$$\frac{\partial^2 h}{\partial \varepsilon_{\alpha\beta}\partial \varepsilon_{\gamma\delta}} = \frac{\partial^2 h}{\partial \varepsilon_{\gamma\delta}\partial \varepsilon_{\alpha\beta}} \Rightarrow C_{\alpha\beta\gamma\delta} = C_{\gamma\delta\alpha\beta}$$

③ Crystal symmetry: $\longrightarrow$ Additional constraints:

(eg) cubic

$$C_{1111} = C_{2222} = C_{3333} = C_{11}$$

$$C_{1122} = C_{1133} = C_{2233} = C_{12}$$

$$C_{1212} = C_{1313} = C_{2323} = C_{44}$$

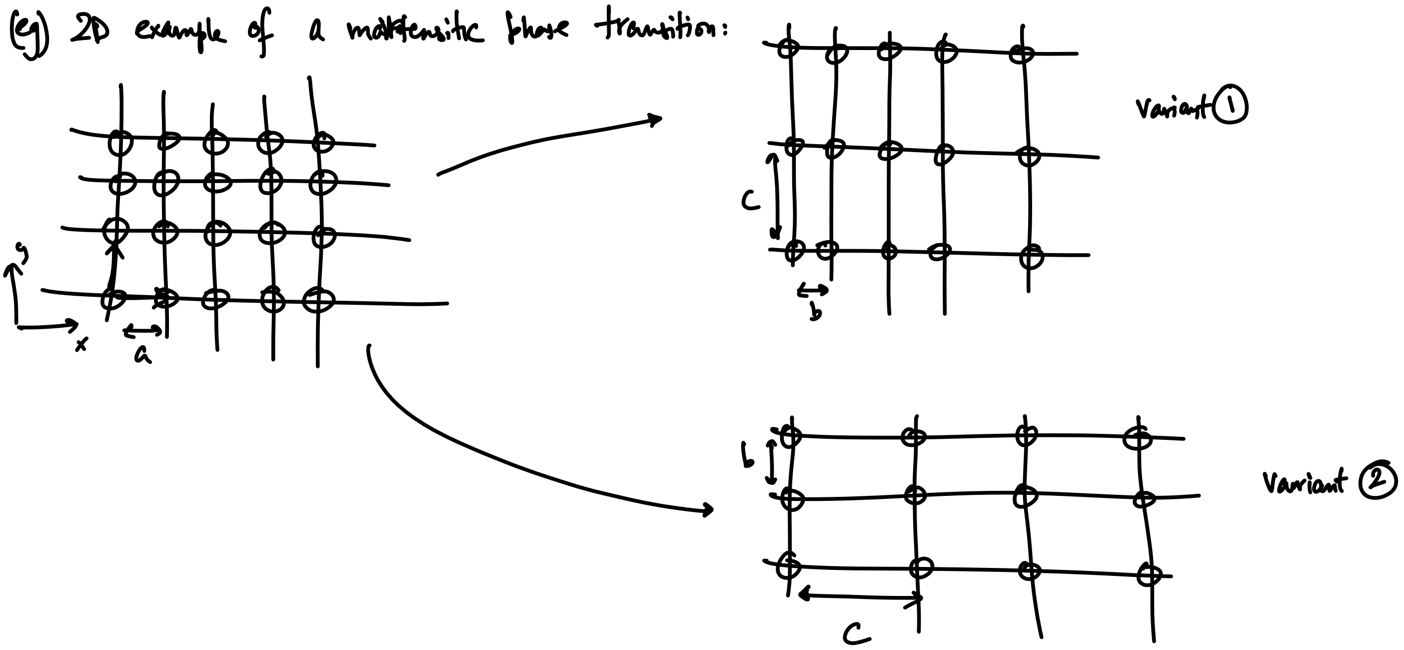
MARTENSITIC PHASE TRANSITIONS:

- Athermal phase transitions, typically occur at the speed of sound.

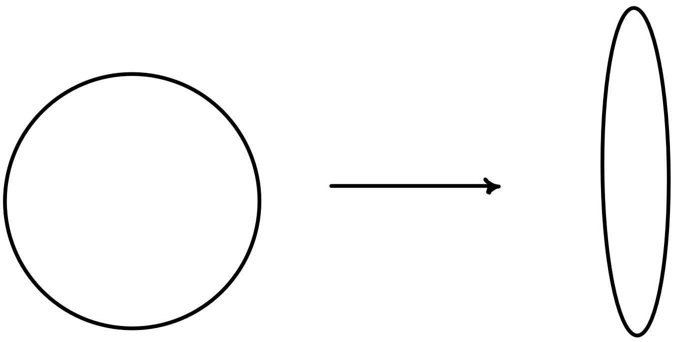
(eg) Fe-C, Ni-Ti (SMAs), Ti-alloys, ferroelectric materials, YSZ, battery materials.
(austenite (fcc) ⟷ martensite (bct))

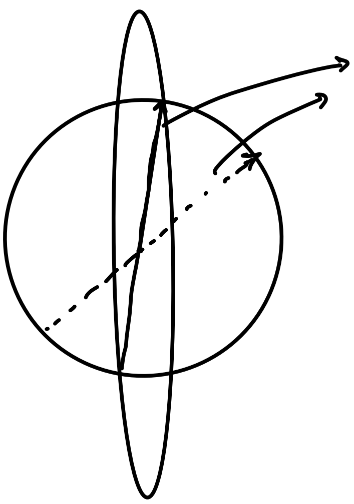
- diffusionless phase transition
- microstructure is chosen to eliminate strain energy all together.

(eg) 2D example of a martensitic phase transition:

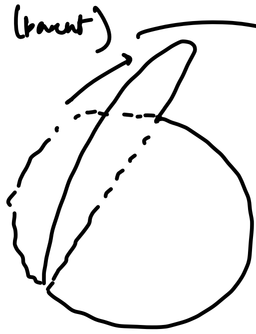


* Eliminating strain with a strain invariant plane:





these lengths match in both the "austenite" and "martensite" phases.
(parent)



shear

★ **Finding The Invariant Plane:**

Say the austenite phase has a lattice $\mathcal{L} = [\vec{a}\ \vec{b}\ \vec{c}]$

martensite phase $M = [\vec{A}\ \vec{B}\ \vec{C}]$

We will call the deformation tensor : F

$$\boxed{F\mathcal{L} = M} \Rightarrow \boxed{F = M\mathcal{L}^{-1}}$$

<u>To compute:</u>

$\hat{n} \longrightarrow$ normal vector to the plane that remains unchanged between austenite & martensite.

<u>Given:</u> $(\mathcal{L}, M)$

$\longrightarrow$ Recall: $F = \underset{\text{rotation}}{R}\,\overset{\text{stretch}}{U} \Rightarrow \left.F^TF = U^TU\right]$ no rotation matrices are found in F^TF

Let us diagonalize $(F^TF) = \lambda_1^2 \overbrace{\hat{e}_1\hat{e}_1^T}^{\text{tensor product}} + \lambda_2^2\hat{e}_2\hat{e}_2^T + \lambda_3^2\hat{e}_3\hat{e}_3^T$

eigenvalues of F^TF: $(\lambda_1^2, \lambda_2^2, \lambda_3^2)$

eigenvectors of F^TF: $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$

$\hat{e}_1, \hat{e}_2, \hat{e}_3 \longrightarrow$ orthogonal unit vectors

$$\hat{e}_1 = \begin{bmatrix} e_1^x \\ e_1^y \\ e_1^z \end{bmatrix} \Rightarrow \begin{aligned} \hat{e}_1^T\hat{e}_1 &= 1 \\ \hat{e}_1^T\hat{e}_2 &= 0 \end{aligned}$$

<u>Notice:</u> $U = \lambda_1\hat{e}_1\hat{e}_1^T + \lambda_2\hat{e}_2\hat{e}_2^T + \lambda_3\hat{e}_3\hat{e}_3^T$

$U \longrightarrow$ also a deformation tensor (except without the rotation)

Say $\vec{r}$ is a vector that we deform with U

$$U\vec{r} = \vec{r}\,' = \lambda_1(\hat{e}_1^T\vec{r})\hat{e}_1 + \lambda_2(\hat{e}_2^T\vec{r})\hat{e}_2 + \lambda_3(\hat{e}_3^T\vec{r})\hat{e}_3$$

if $\vec{r} = \hat{e}, \hat{e}_2, \hat{e}_3 \longrightarrow$ only deform by $\lambda_1, \lambda_2, \lambda_3$] $\longrightarrow$ Eigenstrains or principal strains (usually defined as $\sqrt{\lambda_i^2 - 1}$)

Consider:

$$F^TF = I + (\lambda_1^2-1)\hat{e}_1\hat{e}_1^T + (\lambda_2^2-1)\hat{e}_2\hat{e}_2^T + (\lambda_3^2-1)\hat{e}_3\hat{e}_3^T$$

If $\lambda_1^2 < 1$, $\lambda_2^2 = 1$, $\lambda_3^2 > 1$

$\Rightarrow$ principal strain along $\hat{e}_2 = 0$

any vector $\vec{r} = r\hat{e}_2$ after deformation is transformed to $\vec{r}' = r\hat{e}_2$

$\boxed{\hat{e}_2 \longrightarrow \text{Strain invariant direction}}$

We need to find one more direction to find a strain invariant plane:

$$\boxed{U = \lambda_1\hat{e}_1\hat{e}_1^T + \hat{e}_2\hat{e}_2^T + \lambda_3\hat{e}_3\hat{e}_3^T}$$

Consider:

$$\hat{p} = \sqrt{\frac{1-\lambda_1^2}{\lambda_3^2-\lambda_1^2}}\,\hat{e}_3 - \sqrt{\frac{\lambda_3^2-1}{\lambda_3^2-\lambda_1^2}}\,\hat{e}_1$$

$|\hat{p}| = 1$

$\hat{p}\cdot\hat{e}_2 = 0$ [$\hat{p}$ lies in the plane spanned by $\hat{e}_1, \hat{e}_3$]

$U\hat{p} = \hat{p}'$

$$(\lambda_1\hat{e}_1\hat{e}_1^T + \hat{e}_2\hat{e}_2^T + \lambda_3\hat{e}_3\hat{e}_3^T)(\hat{p}) = \lambda_3\sqrt{\frac{1-\lambda_1^2}{\lambda_3^2-\lambda_1^2}}\,\hat{e}_3 - \lambda_1\sqrt{\frac{\lambda_3^2-1}{\lambda_3^2-\lambda_1^2}}\,\hat{e}_1 = \hat{p}'$$

$$|\hat{p}'| = \frac{\lambda_3^2 - \lambda_3^2\lambda_1^2 + \lambda_1^2\lambda_3^2 - \lambda_1^2}{\lambda_3^2-\lambda_1^2} = 1$$

$\Rightarrow |\hat{p}| = |\hat{p}'|$ & $\boxed{R\hat{p} = \hat{p}'}$ $\hat{p}$ is only rotated!

As $\hat{p}$ and $\hat{e}_2$ remain undeformed upon the application of U

$\Rightarrow \boxed{\hat{n} = \hat{p}\times\hat{e}_2} \longrightarrow$ normal to the strain invariant plane

$$\boxed{\hat{n} = \sqrt{\frac{\lambda_3^2 - 1}{\lambda_3^2 - \lambda_1^2}}\,\hat{e}_3 + \sqrt{\frac{1 - \lambda_1^2}{\lambda_3^2 - \lambda_1^2}}\,\hat{e}_1}$$