An Introduction to Austenite-Martensite Phase-Transition in Crystalline Solids

— Ajeet Kumar

- A Solid to Solid phase transition where lattice or molecular structure changes abruptly at transition temperature.
- no diffusion occurs during transition
- first order (abrupt change in lattice parameter)
- Austenite: High temperature phase
  Martensite: Low temp. phase

An Experiment with shape memory alloy shown below :-

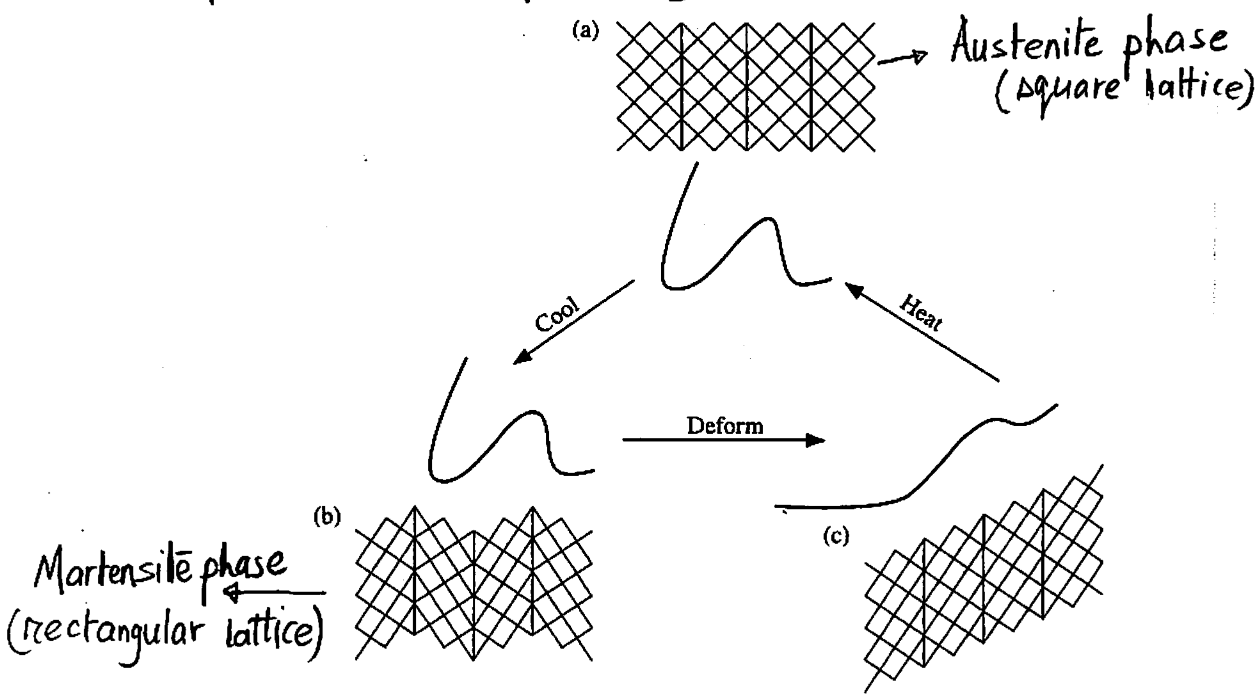


FIG. 1.6. The shape-memory effect, and its schematic explanation in terms of the martensitic phase transformation. A piece of wire that is deformed while cold ((b)–(c)) recovers the deformation on heating ((c)–(a)). Cooling ((a)–(b)) does not change the shape. If we look closely in one region, we find the austenite lattice in (a), which transforms on cooling to a self-accommodated microstructure of martensite in (b). One variant converts to another during deformation and we obtain a different arrangement of martensite variants in (c).

(taken from reference II)

Observation during experiment :-

1. Abrupt change from square to rectangular lattice $(a \rightarrow b)$ while cooling
2. Two variants present at low temperature phase (b)
3. The variants orient themselves in such a way that (i) deformation is continuous at the <u>interface</u> and (ii) macroscopic shape remains the same (self accomodation)
4. $b \rightarrow c$, (under application of force)
   - 'b' & 'c' at same energy level
   - no recoiling from $c \rightarrow b$ when force is removed
5. 'c' returns to 'a' when heated.
   - shape memory effect.

Our Goal: To make an attempt to understand above observation

A Discrete Bravais Lattice:-

$$\mathbb{L} = \{ \underset{\sim}{x} \in \mathbb{E}^3 : \underset{\sim}{x} = n_i \underset{\sim}{a}_i \;\; \forall n_i \in \mathbb{Z} \}$$, $\underset{\sim}{a}_i$'s are called Lattice bases.

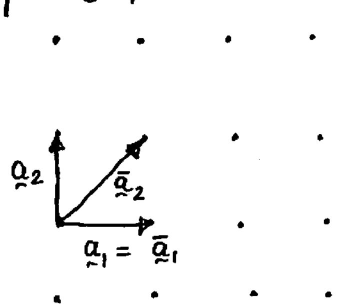
Remark: Bases for a lattice is not unique.

Two bases must be related as follows:

$$\bar{\underset{\sim}{a}}_i = m_i^j \underset{\sim}{a}_j \, , \quad m_i^j \in \mathbb{Z} \text{ and } \det[m_i^j] = 1$$

$\bar{\underset{\sim}{a}}_i$ is another bases.

An Example:-(square lattice)



$$\bar{\underset{\sim}{a}}_1 = 1 \cdot \underset{\sim}{a}_1 + 0 \cdot \underset{\sim}{a}_2$$
$$\bar{\underset{\sim}{a}}_2 = 1 \cdot \underset{\sim}{a}_1 + 1 \cdot \underset{\sim}{a}_2$$

$$[m_i^j] = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$$

Also denotes finite shear.

Free energy function for lattice :-

$$\Psi(\underbrace{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3,}_{\text{bases}} \underset{\downarrow\\ \text{temperature}}{\theta})$$

Objectivity : $\Psi(\mathbf{Q}\mathbf{a}_1, \mathbf{Q}\mathbf{a}_2, \mathbf{Q}\mathbf{a}_3, \theta) = \Psi(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \theta) \quad \forall \mathbf{Q} \in SO(3)$

Deformation of Lattice, Lattice - Continuum link :

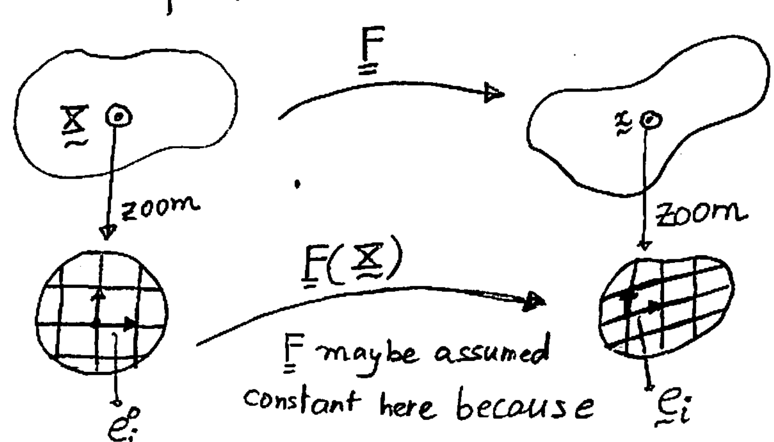
In continuum theory, we have infinitesimal line elements and they deform under deformation gradient as follows: $d\mathbf{x} = \mathbf{F}(\mathbf{X})\, d\mathbf{X}$

But, in lattice structures, we have no such line element.

Cauchy Born Hypothesis bridges gap between lattice & continuum.

It says, bases vectors of Lattice behave like infinitesimal line elements.

So, $\underset{\substack{\downarrow \\ \text{basis vector after} \\ \text{deformation}}}{\mathbf{e}_i(\mathbf{X})} = \mathbf{F}(\mathbf{X})\, \underset{\substack{\downarrow \\ \text{basis vector before} \\ \text{deformation.}}}{\mathbf{e}_i^{\circ}(\mathbf{X})}$



$\mathbf{F}$ maybe assumed constant here because we are looking at a very small region.

With this, continuum energy density follows:

$$W(\mathbf{F}, \theta) \equiv \Psi(\mathbf{F}\mathbf{e}_i^{\circ}, \theta) \equiv \Psi(\mathbf{e}_i, \theta), \quad \underline{\text{MO}}: W(\mathbf{F}, \theta) = W(\mathbf{R}\mathbf{F}, \theta), \ \forall \mathbf{R} \in SO(3)$$

- See Ericksen, 2008 for more details

Symmetry group of Lattice (Material Symmetry)

We have seen, Ψ (free energy) is a function of bases of lattice.
But from page ② a lattice does not have a unique basis.

So, $\Psi(\underset{\sim}{a}_1, \underset{\sim}{a}_2, \underset{\sim}{a}_3, \theta) = \Psi(\bar{\underset{\sim}{a}}_1, \bar{\underset{\sim}{a}}_2, \bar{\underset{\sim}{a}}_3, \theta)$ $\forall$ other bases.

Observe that $\bar{\underset{\sim}{a}}_i$ can be interpreted as image of $\underset{\sim}{a}_i$ under deformation

$\underset{=}{F}$: $F_{ij} \in \mathbb{Z}$ and $\det[\underset{=}{F}] = 1$.

We say, $\underset{=}{F} \in \mathcal{G}$, symmetry group of lattice.

<u>Note</u>: $\mathcal{G}$ also contains elements related to finite shear (example in page ②)
This is a huge group: discrete, infinite, non-compact.

<u>Material Symmetry</u>:- Doing our Arm-chair experiment,

we see, $W(\underset{=}{F}\underset{=}{H}) = W(\underset{=}{F}) \quad \forall \underset{=}{H} \in \mathcal{G}$

Ericksen-Pitteri Neighborhood:

- In general, symmetry group of a lattice changes when a deformation is applied to it.

Let $\underset{\sim}{e}_i^0$ be the reference basis. The idea is to define a "neighbourhood", $\mathcal{N}(\underset{\sim}{e}_i^0)$ and a symmetry group for the neighbourhood (not just for reference basis), $\mathcal{P}(\underset{\sim}{e}_i^0)$ so that for $\forall\, \underset{=}{F} \in \mathcal{P}(\underset{\sim}{e}_i^0)$ and $\forall\, \underset{\sim}{e}_i \in \mathcal{N}(\underset{\sim}{e}_i^0) \Rightarrow \underset{=}{F}\underset{\sim}{e}_i \in \mathcal{N}(\underset{\sim}{e}_i^0)$.

So, $\mathcal{N}(\underset{\sim}{e}_i^0)$ is invariant under symmetry group $\mathcal{P}(\underset{\sim}{e}_i^0)$.

Properties that fall out under these restrictions:-

1. $\mathcal{P}(\underset{\sim}{e}_i^0)$ does not contain elements corresponding to finite shear in $\mathcal{G}$.
2. $\forall \underset{=}{F} \in \mathcal{P}(\underset{\sim}{e}_i^0)$, $\mathcal{P}(\underset{=}{F}\underset{\sim}{e}_i^0) \subsetneq \mathcal{P}(\underset{\sim}{e}_i^0)$. It is necessary to see shape memory effect.

$\mathcal{P}$ is also called point group.

<u>How to define $\mathcal{N}(\underset{\sim}{e}_i^0)$</u>:

Define: $C_{ij} = \underset{\sim}{e}_i \cdot \underset{\sim}{e}_j$

$$\|\underset{\approx}{C}\| = \sqrt{C_{ij}C_{ij}} = (\mathrm{tr}\,\underset{\approx}{C}^2)^{1/2}$$

$$\mathcal{N}(\underset{\sim}{e}_i^\circ) = \left\{\{\underset{\sim}{e}_i\} : \|[\underset{\sim}{e}_i\cdot\underset{\sim}{e}_j] - [\underset{\sim}{e}_i^\circ\cdot\underset{\sim}{e}_j^\circ]\| \le \epsilon\right\}$$

ϵ is chosen judiciously to satisfy properties listed on page (4)

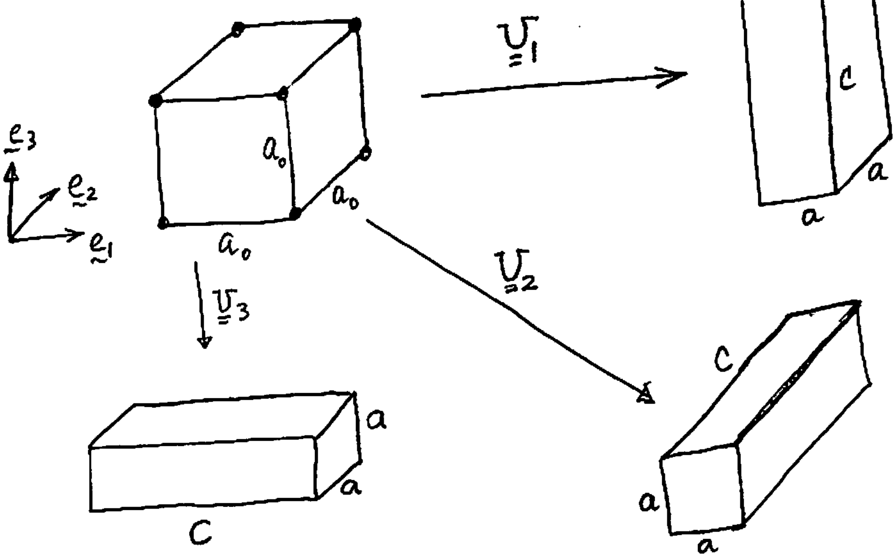
- For detailed discussion, see section 3.5 from reference II

Symmetry related variants of Martensite :-

We can define: Austenite - Reference configuration ($\underset{\approx}{I}$)
Martensite - Deformed " ($\underset{\approx}{F}$)

For convenience, we always take $\underset{\approx}{F}$ to be sym, +ve definite.

Let us take an example of Cubic to Tetragonal transformation.



$$U_1 = \begin{bmatrix} a/a_0 & 0 & 0 \\ 0 & a/a_0 & 0 \\ 0 & 0 & c/a_0 \end{bmatrix}$$

$$U_2 = \begin{bmatrix} a/a_0 & 0 & 0 \\ 0 & c/a_0 & 0 \\ 0 & 0 & a/a_0 \end{bmatrix}$$

$\underset{\approx}{U}_2$ can also be realised as: $\underset{\approx}{U}_2 = \underset{\approx}{R}^T \underset{\approx}{U}_1 \underset{\approx}{R}$, $\underset{\approx}{R}$: rotation about $\underset{\sim}{e}_1$ by 90°

Note $\underset{\approx}{R} \in \mathcal{P}(\underset{\sim}{e}_i^\circ)$ for cubic lattice.

So, $\underset{\approx}{U}_2$ & $\underset{\approx}{U}_1$ are called symmetry related variants.

Now, #elements $(\mathcal{P}(\underset{\sim}{e}_i^\circ)$ for cubic lattice$) = 24$.

Q. Do we have 24 variants of Martensite ??

Claim:- $\underline{\underline{U}}_1 = \underline{\underline{R}}\,\underline{\underline{U}}_1\,\underline{\underline{R}}^T$ iff $\underline{\underline{R}}$ also belongs to symmetry group of tetragonal lattice.

Proof:

($\Rightarrow$) $\quad \underline{\underline{U}}_1 = \frac{a}{a_0}\underline{\underline{I}} + \frac{c-a}{a_0}\, \underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3$

or, $\cancel{\frac{a}{a_0}\underline{\underline{I}}} + \frac{c-a}{a_0}\, \underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3 = \cancel{\frac{a}{a_0}\underline{\underline{I}}} + \frac{c-a}{a_0}\, \underline{\underline{R}}\,\underset{\sim}{e}_3 \otimes \underline{\underline{R}}\,\underset{\sim}{e}_3$

$\Rightarrow \underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3 = \underline{\underline{R}}\,\underset{\sim}{e}_3 \otimes \underline{\underline{R}}\,\underset{\sim}{e}_3$

$\Rightarrow (\underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3)\underset{\sim}{v} = (\underline{\underline{R}}\,\underset{\sim}{e}_3 \otimes \underline{\underline{R}}\,\underset{\sim}{e}_3)\underset{\sim}{v} \;\forall\, \underset{\sim}{v} \in \mathbb{E}^3$

$\Rightarrow (\underset{\sim}{e}_3 \cdot \underset{\sim}{v})\,\underset{\sim}{e}_3 = (\underline{\underline{R}}\,\underset{\sim}{e}_3 \cdot \underset{\sim}{v})\,\underline{\underline{R}}\,\underset{\sim}{e}_3$

$\Rightarrow$ $\underline{\underline{R}}\,\underset{\sim}{e}_3$ & $\underset{\sim}{e}_3$ must be colinear

$\Rightarrow \underline{\underline{R}}\,\underset{\sim}{e}_3 = \pm\,\underset{\sim}{e}_3$

$\Rightarrow$ $\underline{\underline{R}}$ lies in symmetry group of tetragonal lattice

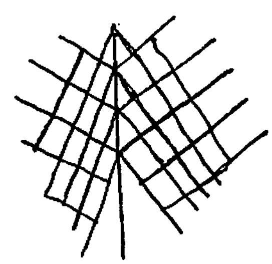
Similarly, ($\Leftarrow$) can be proved.

This gives a formula:

$$\#\text{ variants of Martensite} = \frac{\text{number of rotation elements in } \mathcal{G}_a}{\text{number of rotation elements in } \mathcal{G}_m}$$

Also, $W(\underline{\underline{U}}_1, \theta) = W(\underline{\underline{U}}_2, \theta) \cdots\cdots = W(\underline{\underline{U}}_N, \theta)$ $\forall\, \underline{\underline{U}}_i$'s which are symmetry related.

Twinning in Martensite :-



To satisfy boundary conditions and also minimize the overall energy, microstructures are developed in martensite phase with two different variants existing together with an interface in between. This is called twinning. There is a jump in deformation gradient across the interface but the deformation must be continuous. We will derive equation for twinning in the coming sections and also look for their solution.

Deformation gradient "$\underset{\sim}{F}$" in presence of single variant

Let, $\nabla \underset{\sim}{f} = \underline{\underline{R}}(\underset{\sim}{X})\,\underline{\underline{U}}$, where $\underline{\underline{U}}$ is constant since we have single variant.

Let, $\underline{\underline{U}} = \underline{\underline{I}}$

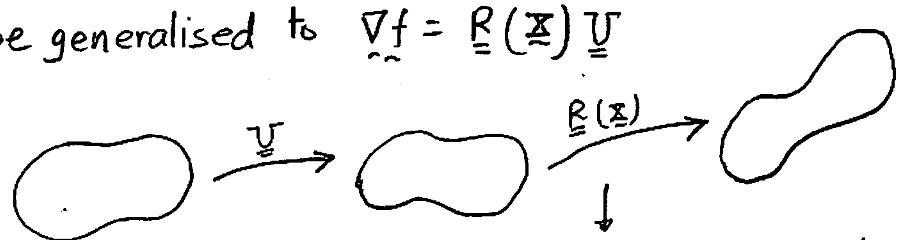
$\Rightarrow \nabla \underset{\sim}{f} = \underline{\underline{R}}(\underset{\sim}{X})$, $\underline{\underline{R}} \in SO(3)$

According to theorem ,

$$\nabla \underset{\sim}{f} = \underline{\underline{R}} = \text{constant}$$

(See Reshetnyak '67 for $\underset{\sim}{f} \in W^{1,\infty}(\Omega, \mathbb{R}^3)$)

This can be generalised to $\nabla \underset{\sim}{f} = \underline{\underline{R}}(\underset{\sim}{X})\,\underline{\underline{U}}$



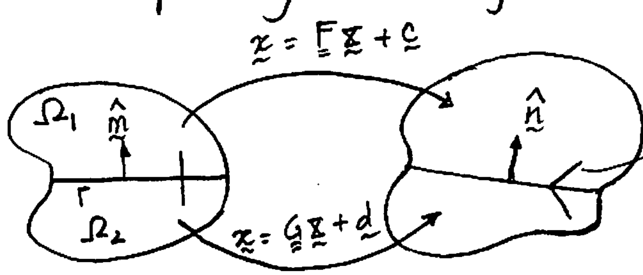
$\underline{\underline{R}}$ must be constant from previous result

$\Rightarrow \nabla \underset{\sim}{f} = \underline{\underline{R}}\,\underline{\underline{U}} = \text{constant}.$

So, in presence of single variant, deformation must be homogeneous.

So, in twinning, deformation gradient is different but constant on two sides of interface.

Kinematic compatibility at Interface :



continuous line element but with a kink (coherent interface)

Γ is the interface plane with normal $\hat{\underset{\sim}{m}}$

Compatibility condition:-

- Deformation continuous at the interface.
- any infinitesimal line element lying in the interface surface must deform the same way from the two sides of interface.

$$\Rightarrow \underline{\underline{F}}\,\underline{v} = \underline{\underline{G}}\,\underline{v} \;, \forall\, \underline{v} \perp \hat{\underline{m}} \quad \cdots \text{(i)}$$

Claim: (i) is equivalent to $\underline{\underline{F}} - \underline{\underline{G}} = \underline{a} \otimes \hat{\underline{m}}$ for some $\underline{a}$

Proof: Take any vector $\underline{v}$ in the interface plane ($\underline{v} \perp \hat{\underline{m}}$) and operate it on both sides.

$$\Rightarrow \underline{\underline{F}}\,\underline{v} - \underline{\underline{G}}\,\underline{v} = \underline{a}\,\cancelto{0}{(\hat{\underline{m}}\cdot\underline{v})}$$

$$\Rightarrow \underline{\underline{F}}\,\underline{v} = \underline{\underline{G}}\,\underline{v} \;, \forall\, \underline{v} \perp \hat{\underline{m}}$$

In case of twinning,

$$\underline{\underline{F}} = \underline{\underline{Q}}_1 \underline{\underline{U}}_1 \;, \quad \underline{\underline{G}} = \underline{\underline{Q}}_2 \underline{\underline{U}}_2$$

$$\Rightarrow \underline{\underline{Q}}_1 \underline{\underline{U}}_1 - \underline{\underline{Q}}_2 \underline{\underline{U}}_2 = \underline{b} \otimes \hat{\underline{m}}$$

$$\text{or, } \boxed{\underline{\underline{Q}}\,\underline{\underline{U}}_1 - \underline{\underline{U}}_2 = \underline{a} \otimes \hat{\underline{m}}} \;, \quad \underline{a} = \underline{\underline{Q}}_2^{\,\prime}\, \underline{b} \,, \quad \underline{\underline{Q}} = \underline{\underline{Q}}_2^{\,\prime}\, \underline{\underline{Q}}_1$$

$\downarrow$

twinning equation (rank one connectivity)

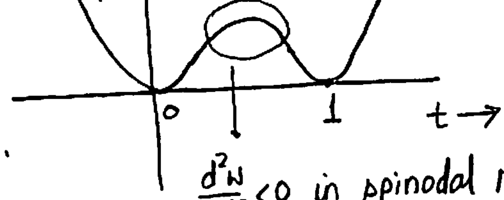
A deviation: Is the free energy function rank-1 convex ??

Let $\underline{\underline{F}}_1 = \underline{\underline{Q}}_1 \underline{\underline{U}}_1$ & $\underline{\underline{F}}_2 = \underline{\underline{Q}}_2 \underline{\underline{U}}_2$ be rank-1 connected

$$\text{or, } \underline{\underline{F}}_2 = \underline{\underline{F}}_1 + \underline{a} \otimes \hat{\underline{m}}$$

$$\text{Let, } \underline{\underline{F}} = \underline{\underline{F}}_1 + t\, \underline{a} \otimes \hat{\underline{m}}$$

So, $\underline{\underline{F}}(0)$ & $\underline{\underline{F}}(1)$ are local minima of energy function.



$\frac{d^2 W}{dt^2} < 0$ in spinodal region

$$\Rightarrow \left.\frac{dW}{dt}\right|_{t=0,1} = 0$$

Let us suppose, $\frac{dW}{dt} > 0$ at $t = a \in (0,1)$ and consider the interval $(a,1)$
(if $\frac{dW}{dt} < 0$, chose the interval $(0,a)$)

So, $\frac{dW}{dt}(a) > 0$, $\frac{dW}{dt}(1) = 0$

Use mean value theorem in the interval $(a,1)$

$$\Rightarrow \left.\frac{d^2W}{dt^2}\right|_{t=b\in(a,1)} = \frac{\frac{dW}{dt}(1) - \frac{dW}{dt}(a)}{1-a} < 0$$

So, $\underset{\sim}{a} \otimes \hat{\underset{\sim}{m}} \cdot \frac{d^2W}{d\underset{=}{F}^2}\left(\underset{=}{F}_1 + b\,\underset{\sim}{a} \otimes \hat{\underset{\sim}{m}}\right)[\underset{\sim}{a} \otimes \hat{\underset{\sim}{m}}] < 0$
$\Rightarrow$ violates ellipticity

Failure of ellipticity $\Rightarrow$ Energy functional is not semi-lower continuous with respect to weak convergence in sobolev space $W^{1,p}(\Omega, R^3)$
(Youngs'52, Ball & James'87)

- This leads to formation of fine micro-structures.

Austenite/Martensite interface

Austenite: $\underset{=}{I}$
Martensite: $\underset{=}{R}\,\underset{=}{U}$

In order to form twins, they must be rank-1 connected.

$$\Rightarrow \underset{=}{R}\,\underset{=}{U} - \underset{=}{I} = \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}}, \text{ for some } \underset{\sim}{a} \text{ and } \hat{\underset{\sim}{n}}$$

$$\Rightarrow \underset{=}{R}\,\underset{=}{U} = \underset{=}{I} + \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}}$$

$$\Rightarrow \underset{=}{U}^2 = (\underset{=}{R}\,\underset{=}{U})^T(\underset{=}{R}\,\underset{=}{U}) = (\underset{=}{I} + \hat{\underset{\sim}{n}} \otimes \underset{\sim}{a})(\underset{=}{I} + \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}})$$
$$= \underset{=}{I} + |\underset{\sim}{a}|^2\, \hat{\underset{\sim}{n}} \otimes \hat{\underset{\sim}{n}} + \hat{\underset{\sim}{n}} \otimes \underset{\sim}{a} + \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}}$$

Take $\underset{\sim}{v} = \underset{\sim}{a} \times \hat{\underset{\sim}{n}}$ or, $\underset{\sim}{v} \perp \underset{\sim}{a}$, $\underset{\sim}{v} \perp \hat{\underset{\sim}{n}}$

$$\Rightarrow \underset{=}{U}^2\underset{\sim}{v} = \underset{=}{I}\underset{\sim}{v} + |\underset{\sim}{a}|^2\, \hat{\underset{\sim}{n}}\,\cancelto{0}{(\hat{\underset{\sim}{n}}\cdot\underset{\sim}{v})} + \hat{\underset{\sim}{n}}\,\cancelto{0}{(\underset{\sim}{a}\cdot\underset{\sim}{v})} + \underset{\sim}{a}\,\cancelto{0}{(\hat{\underset{\sim}{n}}\cdot\underset{\sim}{v})}$$

or, $\underset{=}{U}^2\underset{\sim}{v} = \underset{\sim}{v}$

So, $\underline{\underline{U}}^2$ has one of eigenvalues equal to 1.

or, $\underline{\underline{U}}$ has one of its eigenvalues equal to 1.

But, $\underline{\underline{U}}$ having eigenvalue = 1 is very non-generic.

So, Austenite and Martensite do not form such twins. Their interface is much more complicated.

Appendix:-

Interpretation of a twin (Martensite-Martensite interface)

A twin is a planar defect in a crystal with the following properties:-

1. The lattice on one side can be obtained by a simple shear of lattice on other side.
2. The two variants are also related through rotation.

Let, $\underset{\sim}{e}_i^a$ be austenite basis.

$\underset{\sim}{f}_i = \underline{\underline{Q}}\,\underline{\underline{U}}_I\,\underset{\sim}{e}_i^a$, $\underset{\sim}{g}_i = \underline{\underline{U}}_J\,\underset{\sim}{e}_i^a$ be the bases of two martensite variants.

Twinning eq:- $\underline{\underline{Q}}\,\underline{\underline{U}}_I = \underline{\underline{U}}_J + \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}} = \left(\underline{\underline{I}} + \underset{\sim}{a} \otimes \left(\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right)\right)\underline{\underline{U}}_J$ -- (i)

Multiply by $\underset{\sim}{e}_i^a$ on both sides

$\Rightarrow \underset{\sim}{f}_i = \left(\underline{\underline{I}} + \underset{\sim}{a} \otimes \left(\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right)\right)\underset{\sim}{g}_i$ -- (ii)

Claim:- $\underline{\underline{I}} + \underset{\sim}{a} \otimes \left(\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right)$ denotes simple shear.

Take the determinant of expression (i) on both sides,

$\Rightarrow \det \underline{\underline{Q}} \cdot \det \underline{\underline{U}}_I = \det\left(\underline{\underline{I}} + \underset{\sim}{a} \otimes \left(\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right)\right) \det \underline{\underline{U}}_J$

But, $\det \underline{\underline{U}}_I = \det \underline{\underline{U}}_J$ (symmetry related variants)

$\Rightarrow \det\left(\underline{\underline{I}} + \underset{\sim}{a} \otimes \left(\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right)\right) = 1$ --- (iii)

Let us represent $\underline{\underline{I}} + \underset{\sim}{a} \otimes \underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}$ in matrix form in the following orthonormal bases $\left(\dfrac{\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}}{|\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}|}\right.$, two other vectors$\left.\right)$

$$\begin{bmatrix} (1+\underset{\sim}{a}\cdot\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}) & 0 & 0 \\ x & 1 & 0 \\ x & 0 & 1 \end{bmatrix} \Rightarrow \det\left(\underline{\underline{I}} + \underset{\sim}{a} \otimes \underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}}\right) = 1 + \underset{\sim}{a}\cdot\underline{\underline{U}}_J^{-1}\hat{\underset{\sim}{n}} \quad \text{--- (iv)}$$

From (iii) & (iv), $\underset{\sim}{a} \cdot \underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}} = 0 \Rightarrow \underset{\sim}{a} \perp \underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}$

Let us again represent $\underset{\approx}{I} + \underset{\sim}{a} \otimes \underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}$ in the following orthonormal basis:-

$$\frac{\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}}{|\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}|}, \quad \frac{\underset{\sim}{a}}{|\underset{\sim}{a}|}, \quad \text{third orthonormal vector}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ |\underset{\sim}{a}||\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}| & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\left(\underset{\approx}{I} + \underset{\sim}{a} \otimes \underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}\right) \frac{\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}}{|\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}|} = \frac{\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}}{|\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}|} + |\underset{\sim}{a}||\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}| \frac{\underset{\sim}{a}}{|\underset{\sim}{a}|}$$

$$\left(\underset{\approx}{I} + \underset{\sim}{a} \otimes \underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}\right) \frac{\underset{\sim}{a}}{|\underset{\sim}{a}|} = \frac{\underset{\sim}{a}}{|\underset{\sim}{a}|}$$

The above matrix reminds us of <u>simple shear</u>

with, $s = |\underset{\sim}{a}||\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}|$

direction of shear $= \dfrac{\underset{\sim}{a}}{|\underset{\sim}{a}|}$, twin plane normal: $\dfrac{\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}}{|\underset{\approx}{U}_J^{-1} \hat{\underset{\sim}{n}}|}$

Now, $\underset{\approx}{U}_I = \underset{\approx}{R}^T \underset{\approx}{U}_J \underset{\approx}{R}$, where $\underset{\approx}{R}$: $\underset{\approx}{R} \underset{\sim}{e}_i^a = \mu_i^j \underset{\sim}{e}_j^a$

So, $\underset{\sim}{f}_i = \underset{\approx}{Q} \underset{\approx}{U}_I \underset{\sim}{e}_i^a = \underset{\approx}{Q} \underset{\approx}{R}^T \underset{\approx}{U}_J \underset{\approx}{R} \underset{\sim}{e}_i^a$

$$= \underset{\approx}{Q}' \underset{\approx}{U}_J \mu_i^j \underset{\sim}{e}_j^a$$

$$= \mu_i^j \underset{\approx}{Q}' \underset{\approx}{U}_J \underset{\sim}{e}_j^a = \mu_i^j \underset{\approx}{Q}' \underset{\sim}{g}_j$$

$\Rightarrow$ $\underset{\sim}{f}_i$ and $\underset{\approx}{Q}' \underset{\sim}{g}_j$ describe the same lattice and they are related through rotation $\underset{\approx}{Q}'$.

<u>Solution of Twinning equation</u> :-

$$\underset{\approx}{Q} \underset{\approx}{F} - \underset{\approx}{G} = \underset{\sim}{a} \otimes \hat{\underset{\sim}{n}}$$

1. Calculate $\underset{\approx}{C} = \underset{\approx}{G}^{-T} \underset{\approx}{F}^T \underset{\approx}{F} \underset{\approx}{G}^{-1}$
2. If $\underset{\approx}{C} = \underset{\approx}{I}$, no solution (this corresponds to single variant)
3. If $\underset{\approx}{C} \neq \underset{\approx}{I}$, we have a solution iff eigenvalues of $\underset{\approx}{C}$ satisfy $\lambda_1 \leq 1$, $\lambda_2 = 1$, $\lambda_3 \geq 1$.

Proof:- ($\Rightarrow$)

$$\underset{\approx}{Q} \underset{\approx}{F} \underset{\approx}{G}^{-1} = \underset{\approx}{I} + \underset{\sim}{a} \otimes \underset{\approx}{G}^{-T} \hat{\underset{\sim}{n}}$$

$$\Rightarrow \underline{\underline{C}} = (\underline{\underline{Q}}\,\underline{\underline{F}}\,\underline{\underline{G}}^{-1})^T(\underline{\underline{Q}}\,\underline{\underline{F}}\,\underline{\underline{G}}^{-1})$$

$$= (\underline{\underline{I}} + \underline{\underline{G}}^{-T}\hat{\underline{n}} \otimes \underline{a})(\underline{\underline{I}} + \underline{a} \otimes \underline{\underline{G}}^{-T}\hat{\underline{n}})$$

$$\Rightarrow \underline{\underline{C}} - \underline{\underline{I}} = \underline{c} \otimes \underline{d} + \underline{d} \otimes \underline{c} \quad , \quad \underline{c} = \underline{a} + \tfrac{1}{2}|\underline{a}|^2 \underline{\underline{G}}^{-T}\hat{\underline{n}}$$

$$\underline{d} = \underline{\underline{G}}^{-T}\hat{\underline{n}}$$

Clearly, $\underline{\underline{C}} - \underline{\underline{I}}$ has one eigenvalue $= 0$ (eigenvector $\perp$ to both $\underline{c}$ & $\underline{d}$)

Also, $\hat{\underline{e}} \cdot (\underline{\underline{C}} - \underline{\underline{I}})\hat{\underline{e}} = 2(\underline{c} \cdot \hat{\underline{e}})(\underline{d} \cdot \hat{\underline{e}})$

With a proper choice of $\hat{\underline{e}}$, RHS can be made +ve or −ve

So, $\mu_1 = \min_{\hat{\underline{e}}} \hat{\underline{e}} \cdot (\underline{\underline{C}} - \underline{\underline{I}})\hat{\underline{e}} \leq 0 \leq \max_{\hat{\underline{e}}} \hat{\underline{e}} \cdot (\underline{\underline{C}} - \underline{\underline{I}})\hat{\underline{e}} = \mu_2$

So, eigenvalues of $\underline{\underline{C}} - \underline{\underline{I}}$: $\mu_1 \leq \mu_2 = 0 \leq \mu_3$

So, eigenvalues of $\underline{\underline{C}}$: $\boxed{\lambda_1 \leq 1 = \lambda_2 \leq \lambda_3}$

$\Leftarrow$ can be proved similary (Ball & James' 87)

References :-

I. Lecture Notes on "Austenite-Martensite Phase Transition" of Prof. Healey

II. Microstructure of Martensite - Kaushik Bhattacharya

III. Fine phase mixtures as minimizers of Energy: Ball & James' 87