Mechanistic Models of Deformation Twinning and Martensitic Transformations

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Acknowledge: John Hirth
Classical Model (CM)

Geometrical
– invariant plane

Topological Model (TM)

Mechanistic
– coherent interfaces, interfacial line-defects
Twinning: e.g. G. Friedel, 1926

PTMC: WLR and BM, 1953

Twinning dislocation: e.g. F.C. Frank, 1949 (disconnection)

Bilby & Crocker, 1965

Martensitic Transformations
Pond and Hirth, 2003

\[ \gamma = \frac{b}{h} \]
Interfacial defect character and kinetics
Admissible interfacial defects

Operation characterising defect

\[(W(\lambda), w(\lambda))(W(\mu), w(\mu))^{-1}\]

Interfacial dislocations
\[(I, b)\]

Twinning disconnections
\[b = t(\lambda) - Pt(\mu)\]
\[h = n \cdot t(\lambda)\]

\[\gamma = \frac{b}{h}\]

Pond, 1989
Thermally activated disconnections

• activation energy at fixed stress $\sim b^2$

- loop nucleation rate, $\dot{N}$, reasonable for small $b$

• defect mobility, $\dot{G}$

- enhanced by larger core width, $w$, which is promoted by small $h$

- simple shuffles
Motion of a twinning disconnection in a (10\overline{1}2) twin

- $t(\lambda)_{[10\overline{1}0]}$
- $t(\mu)_{[0001]}
- \|b\| = 0.062 \text{ nm}$
- $|b| = 0.062 \text{ nm}$
- $h = 2d_{(10\overline{1}2)}$
- $h = 0.376 \text{ nm}$
- $\gamma = b/h$
- $w \sim 6a$
- $\sigma_b^d = 1 \text{ MPa}$

$E_i = 0.26 Jm^{-2}$

Braisaz et al. 1966

$\alpha - Ti$
Atom Tracking: Shear and Shuffle Displacements in \((10\bar{1}2)\) Twin

\[ \gamma_1 = [\bar{1}012] \]

4 distinct atoms

“rocking”

“swapping”

Pond et al., 2013
Deformation twins in Ni$_2$MnGa

Disconnection

$b = \frac{1}{12} [10\bar{1}] = 0.072 \text{ nm}$

$h = d_{(202)} = 0.211 \text{ nm}$

$\gamma = \frac{b}{h} = 0.34$
Twin tip in $\text{Ni}_2\text{MnGa}$

$E_i = 0.01 \text{Jm}^{-2}$

4 distinct atoms

no shuffling

$g = 20 \bar{2}$

Muntifering et al. 2014
Topological model for type II twinning
Classical Model: irrational plane of shear

Type I

$k_1$ rational
$\gamma_1$ irrational

$s = 2\tan(\alpha)$

Type II

$k_2$ irrational
$\gamma_2$ rational

$s = 2\tan(\alpha)$
Formation mechanisms for type I and II twins

Type I: glide twin

\[ \gamma = \frac{b}{h} \]

competitive mechanisms:
- High \( \dot{G}/\dot{N} \) favours type I
- Low \( \dot{G}/\dot{N} \) favours type II
Type II: formation of glide/rotation twin

![Diagram of Type II: formation of glide/rotation twin](image)

- disconnection glide plane, $k_1$
- sheared region
- unsheared region
- twin parent
- $\eta_1 = \gamma_2$
- $b/2$
- $K_1 = k_2$
- $h$
- $\alpha$
- $b^g$
- twin
- parent

(a) 
(b) 
(c)
Type II: growth

\[ \eta_1 = \gamma_2 \]

\[ \gamma = s = 2\tan(\alpha) \]

Read and Shockley, 1953
Experimental observations: e.g. $\alpha - U$

<table>
<thead>
<tr>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$\eta_1$</th>
<th>type</th>
<th>$b$ nm</th>
<th>$h$ nm</th>
<th>$\gamma$</th>
<th>No. dist. atoms</th>
<th>$\dot{G}/\dot{N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;{176}&quot;</td>
<td>{111}</td>
<td>1/2 $&lt; 512 &gt;$</td>
<td>II</td>
<td>0.098</td>
<td>0.456</td>
<td>0.216</td>
<td>4</td>
<td>low</td>
</tr>
<tr>
<td>&quot;{172}&quot;</td>
<td>{112}</td>
<td>1/2 $&lt; 312 &gt;$</td>
<td>II</td>
<td>0.081</td>
<td>0.356</td>
<td>0.228</td>
<td>4</td>
<td>low</td>
</tr>
<tr>
<td>{130}</td>
<td>{110}</td>
<td>1/2 $&lt; 310 &gt;$</td>
<td>compound</td>
<td>0.048</td>
<td>0.161</td>
<td>0.299</td>
<td>2</td>
<td>high</td>
</tr>
</tbody>
</table>

Type II Twinning in Other Systems

- NiTi
- CuAlNi
- TiPd
- devitrite

$\alpha - U, \text{ Cahn 1953}$
Topological model of martensitic transformations
Shape deformation

\[ P_1 = RBP_2 = (I + dp') \]

PTMC

\[ d \]

parent

\[ \text{martensite} \]

\[ \text{invariant plane} \]

\[ p' \]

TM

- low energy terraces (coherently strained epitaxial)
- two defect arrays: disconnections & LID
- distortion field of defect network accommodates coherency strains
- motion of all defects produces shape deformation
Glissile Disconnections

- 2 distinct atoms
- steps cause habit plane to be inclined to terrace plane
- $b_n$ also produces rotational distortions
- motion causes one-to-one atomic exchange between phases with different densities

$bt = h(\lambda) - h(\mu)$

Ti 10 wt % Mo  Klenov 2002
Distortion field of a Defect Array

\[ D^m(x',y',z') = \begin{pmatrix} \epsilon'_{xx} & \epsilon'_{xy} & \epsilon'_{xz} \\ \epsilon'_{xy} & \epsilon'_{yy} & \epsilon'_{yz} \\ \epsilon'_{xz} & \epsilon'_{yz} & \epsilon'_{zz} \end{pmatrix} + \begin{pmatrix} 0 & -\omega'_{xy} & \omega'_{xz} \\ \omega'_{xy} & 0 & -\omega'_{yz} \\ -\omega'_{xz} & \omega'_{yz} & 0 \end{pmatrix} \]

\[ \epsilon'_{xx} = \frac{b_x}{d} \quad \omega'_{yz} = \frac{b_z}{2d} \]
Equilibrium: superposed coherency and defect array distortion fields

Solve the Frank-Bilby Equation for the defect array with long-range distortion matrix, $D_{ij}^{\prime m}$, which compensates $D_{ij}^{\prime c}$. 

\[
D_{ij}^{\prime m} = \begin{pmatrix}
D_{xx}^{\prime m} & D_{xy}^{\prime m} & D_{xz}^{\prime m} \\
D_{xy}^{\prime m} & D_{yy}^{\prime m} & D_{yz}^{\prime m} \\
D_{xz}^{\prime m} & D_{yz}^{\prime m} & D_{zz}^{\prime m}
\end{pmatrix} = -D_{ij}^{\prime c}
\]
Habit plane orientation

$\theta$ = 11.4°

$\phi$ = 0.53°

$\alpha$ crystal: $\Theta + \phi$

$\beta$ crystal: $\Theta - \phi$

homogeneous isotropic approximation

inhomogeneous anisotropic case rotations partitioned according to relative elastic compliances

TM solutions for habit plane orientation differ slightly from PTMC, unless $b_n = 0$
Partitioning of rotations

molecular dynamic simulation of static Cu(111)/Ag(111) interface, Wang et al. 2011

$\epsilon_{yy}^{c} = 12.33\%$

<table>
<thead>
<tr>
<th>Case</th>
<th>$\phi_{Cu}$</th>
<th>$\phi_{Ag}$</th>
<th>$\phi$</th>
<th>$-\phi_{Ag}/\phi_{Cu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic, inhomogeneous</td>
<td>0.449</td>
<td>-0.698</td>
<td>1.15</td>
<td>1.55</td>
</tr>
<tr>
<td>Anisotropic</td>
<td>0.504</td>
<td>-0.853</td>
<td>1.36</td>
<td>1.69</td>
</tr>
<tr>
<td>MD</td>
<td>0.483</td>
<td>-0.929</td>
<td>1.41</td>
<td>1.92</td>
</tr>
<tr>
<td>MD (Artificial)</td>
<td>0.665</td>
<td>-0.659</td>
<td>1.312</td>
<td>0.97</td>
</tr>
</tbody>
</table>
Orthorhombic to Monoclinic Transformation in ZrO$_2$

Principal strains on terrace plane

$\varepsilon_{xx} = 0 \quad \varepsilon_{yy} = 3.8\%$

considerable shuffling:

8 Zr & 16 O distinct ions
synchronous motion of disconnections

\[
\Gamma_m^D = \begin{pmatrix} 0 & 0 & \gamma_{xz} \\ 0 & 0 & \gamma_{yz} \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix} = \frac{\delta y}{d^D} \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} D \begin{pmatrix} 0 & 0 & n_z \end{pmatrix}
\]
Lath martensite in ferrous alloys

Mn IF steel: Morito et al.

1: terrace plane

\[ [\text{110}]_\gamma / [\text{100}]_\alpha \]

\[ \varepsilon_{xx} = -12.54\% \]

\[ (111)_\gamma / (011)_\alpha \]

\[ \varepsilon_{yy} = 7.72\% \]

“N-W OR”
dislocations, \(\sim 10^\circ\) from screw, with spacing 2.8 -6.3 nm

Fe-20Ni-5Mn (Sandvik and Wayman, 1983)

TEM: LID slip dislocations

1/2[\(\bar{1}1\)]_\alpha \) dislocations, \(\sim 10^\circ\) from screw, with spacing 2.8 -6.3 nm
TEM: Disconnections in near screw orientation

Moritani et al. Fe-Ni-Mn

[-101]γ projection
Plate Martensite
\[\sim\{121\}\]

Ogawa and Kajiwara, 2004
Fe-Ni-Mn
Conclusions

Topological modelling provides insights into mechanisms and kinetics.

Twinning:

- proposed new model of type II twin formation.

Martensite:

- predicted interface structures consistent with observations,
- predicted habits differ slightly from PTMC.