Mechanistic Models of Deformation Twinning and Martensitic Transformations

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Acknowledge: John Hirth

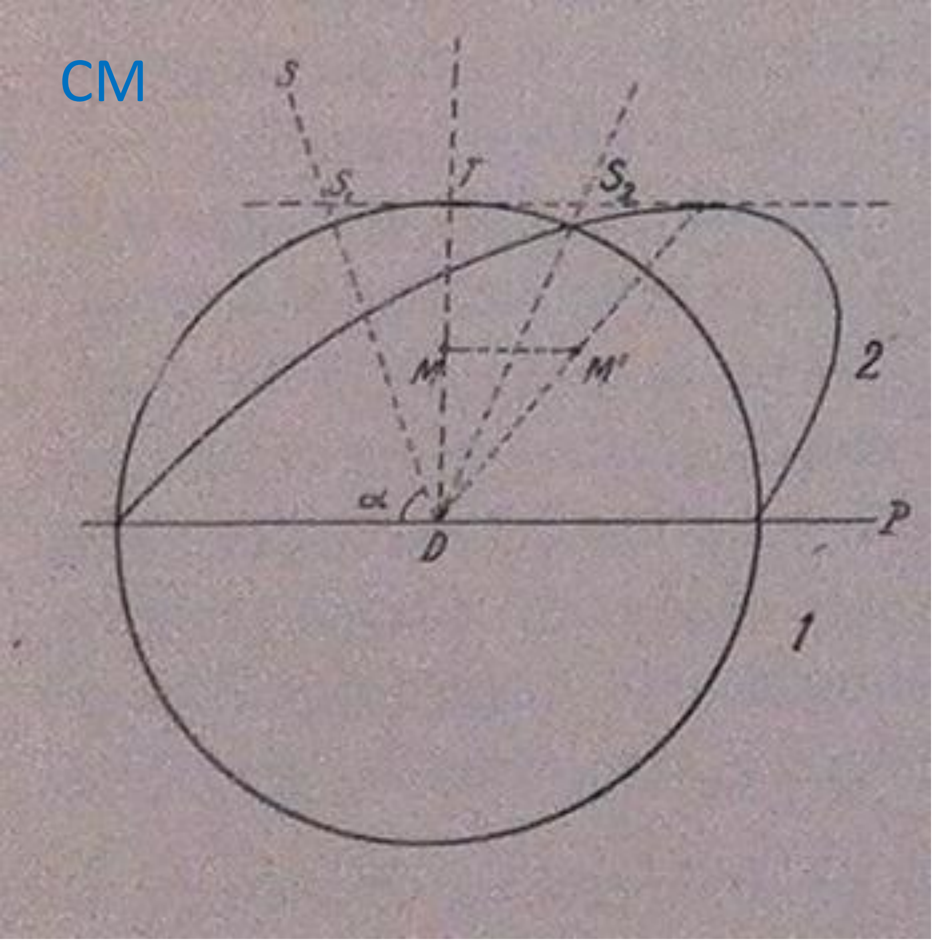
Classical Model (CM)

Geometrical
– invariant plane

Topological Model (TM)

Mechanistic
– coherent interfaces, interfacial line-defects

CM

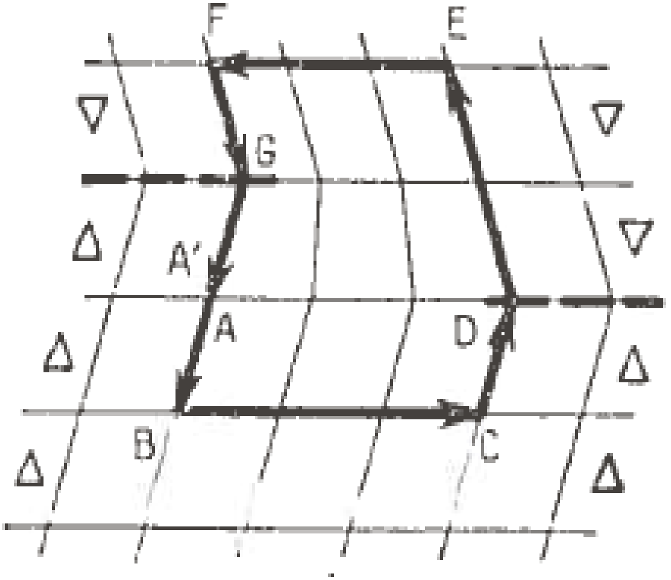


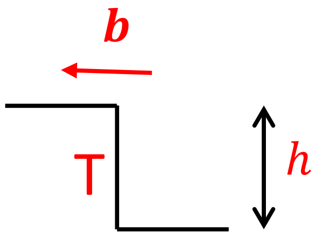
Twinning : e.g. G. Friedel, 1926

PTMC : WLR and BM, 1953

s

TM





$\gamma = b/h$

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

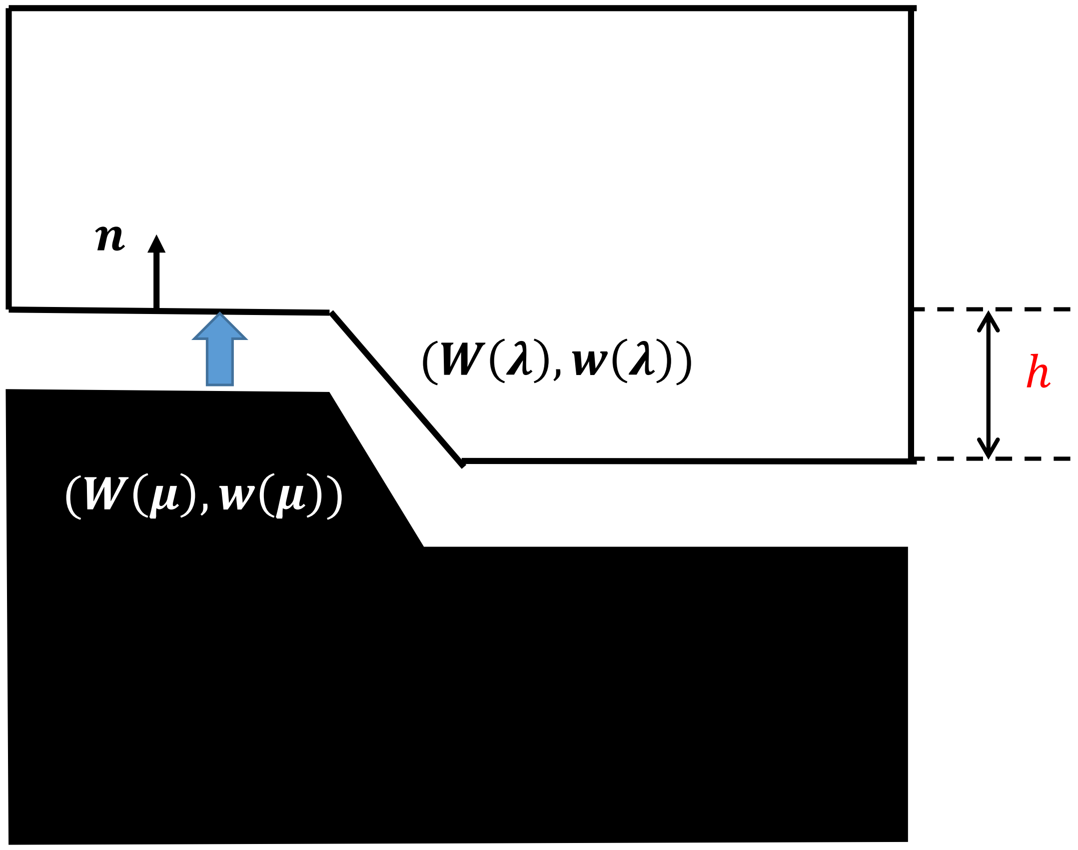
Bilby & Crocker, 1965

Martensitic Transformations
Pond and Hirth, 2003

Interfacial defect character and kinetics

Admissible interfacial defects

white crystal
$\boldsymbol{\lambda}$



black crystal
μ

bicrystal

Operation characterising defect

$$(\boldsymbol{W}(\boldsymbol{\lambda}), \boldsymbol{w}(\boldsymbol{\lambda}))(\boldsymbol{W}(\boldsymbol{\mu}), \boldsymbol{w}(\boldsymbol{\mu}))^{-1}$$

Interfacial dislocations

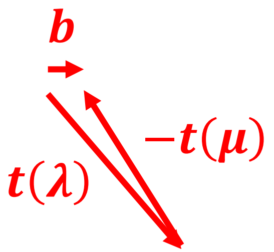
$$(\boldsymbol{I}, \boldsymbol{b})$$

Twinning disconnections

$$\boldsymbol{b} = \boldsymbol{t}(\boldsymbol{\lambda}) - \boldsymbol{P}\boldsymbol{t}(\boldsymbol{\mu})$$

$$h = \boldsymbol{n} \cdot \boldsymbol{t}(\boldsymbol{\lambda})$$

$$\gamma = b/h$$



Pond, 1989

Thermally activated disconnections

- activation energy at fixed stress ~ 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

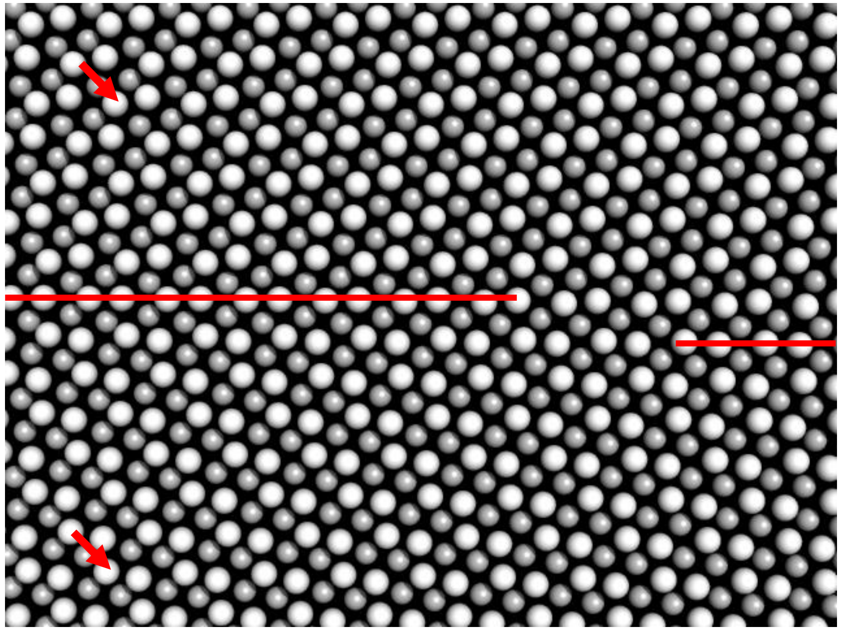
➢ simple shuffles

Motion of a twinning disconnection in a $(10\bar{1}2)$ twin

$\boldsymbol{t}(\boldsymbol{\lambda})$
$[10\bar{1}0]$

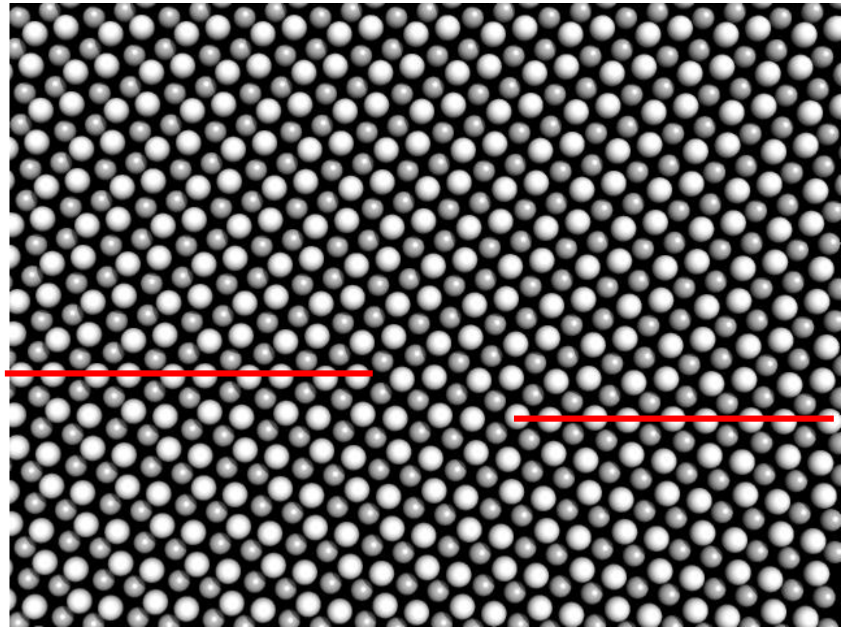
$E_i =$
$0.26\ Jm^{-2}$

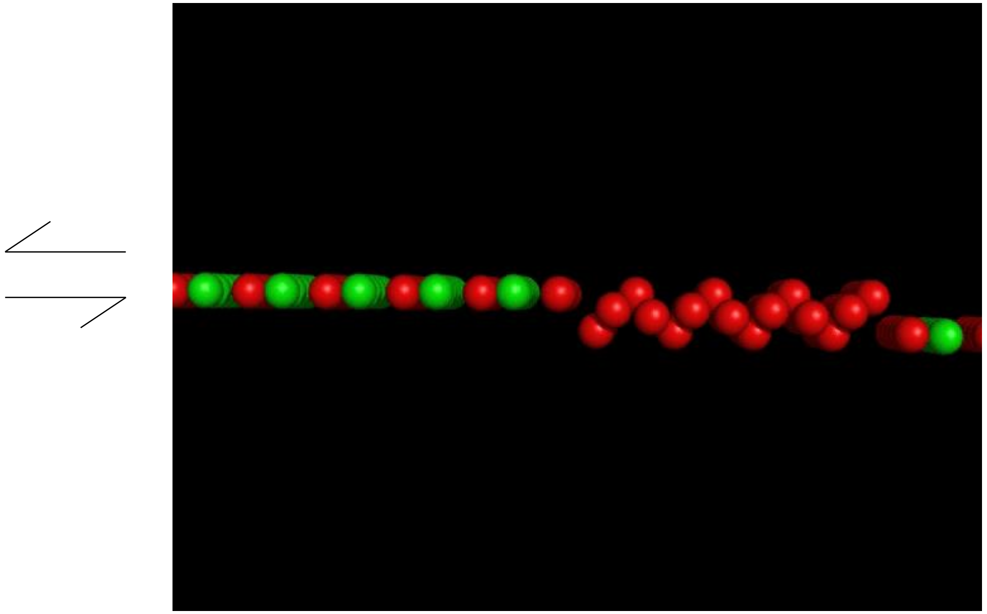
$\boldsymbol{t}(\boldsymbol{\mu})$
$[0001]$



h

$\perp$
$\vec{\mathbf{b}}$





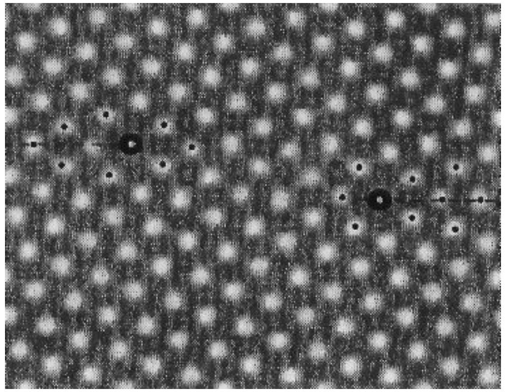
$|\boldsymbol{b}| = 0.062\ nm$

$h = 2d_{(10\bar{1}2)}$
$= 0.376\ nm$

$\gamma = b/h$

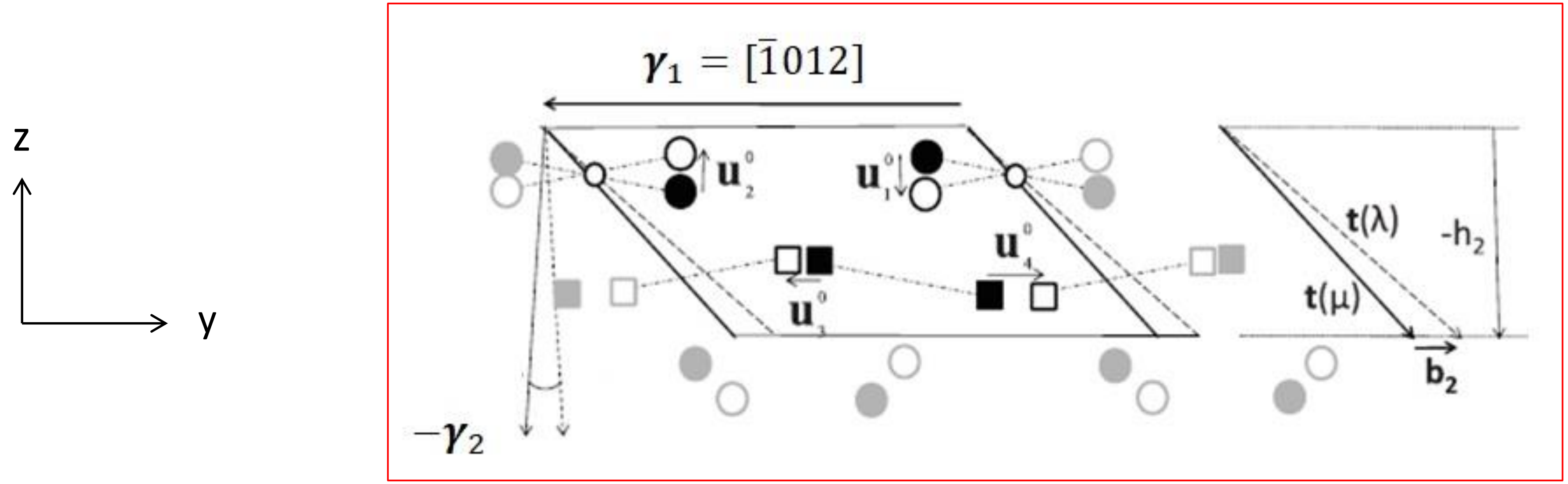
$w \sim 6a$

$\sigma_P^d = 1\ MPa$



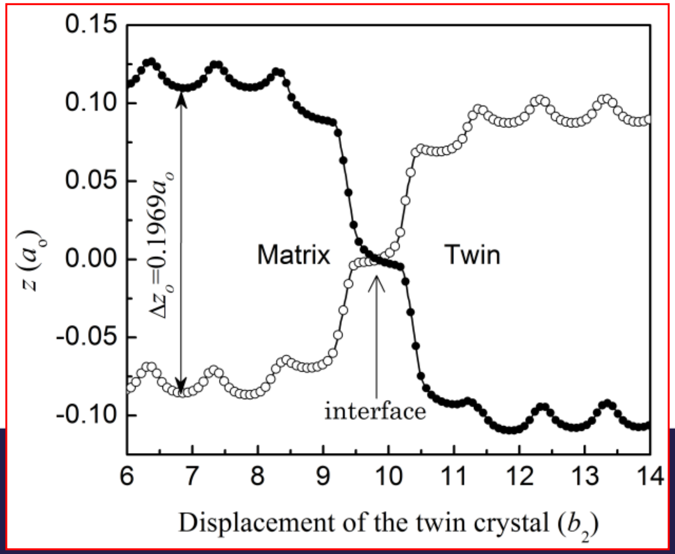
$\alpha - Ti$
$Braisaz\ et\ al.\ 1966$

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

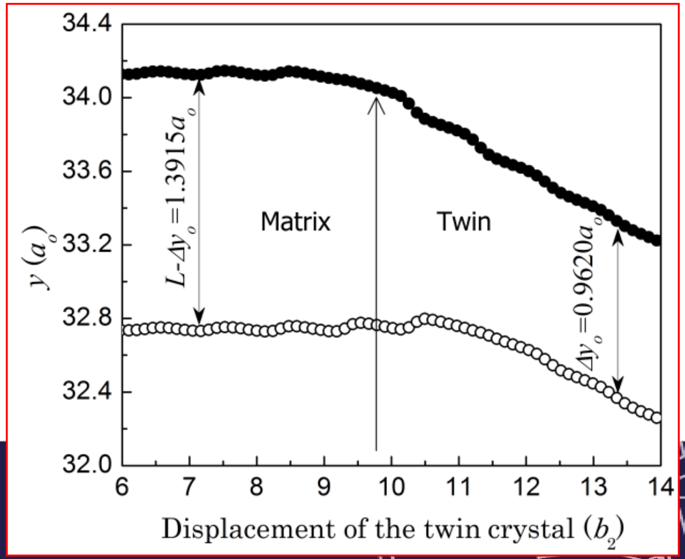


4 distinct atoms

"rocking"

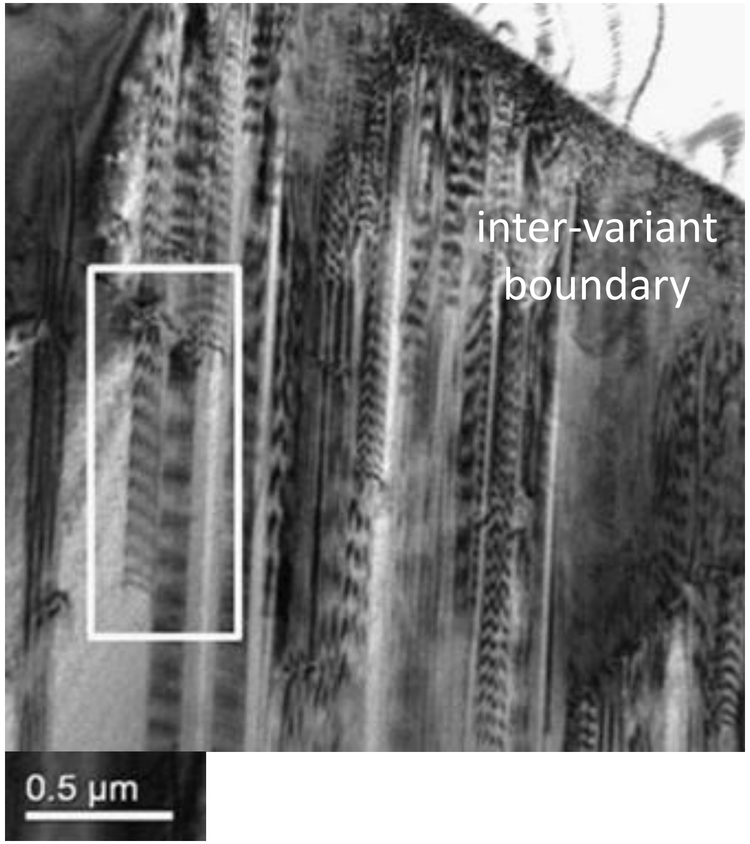


"swapping"

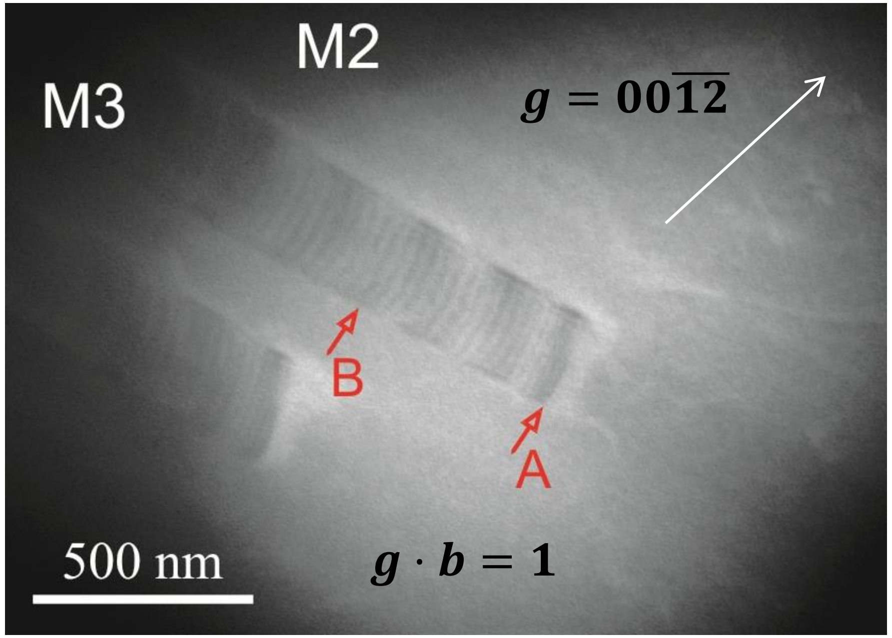


Pond et al., 2013

Deformation twins in Ni_2MnGa



Pond et al. 2012



Zarubova et al. 2012

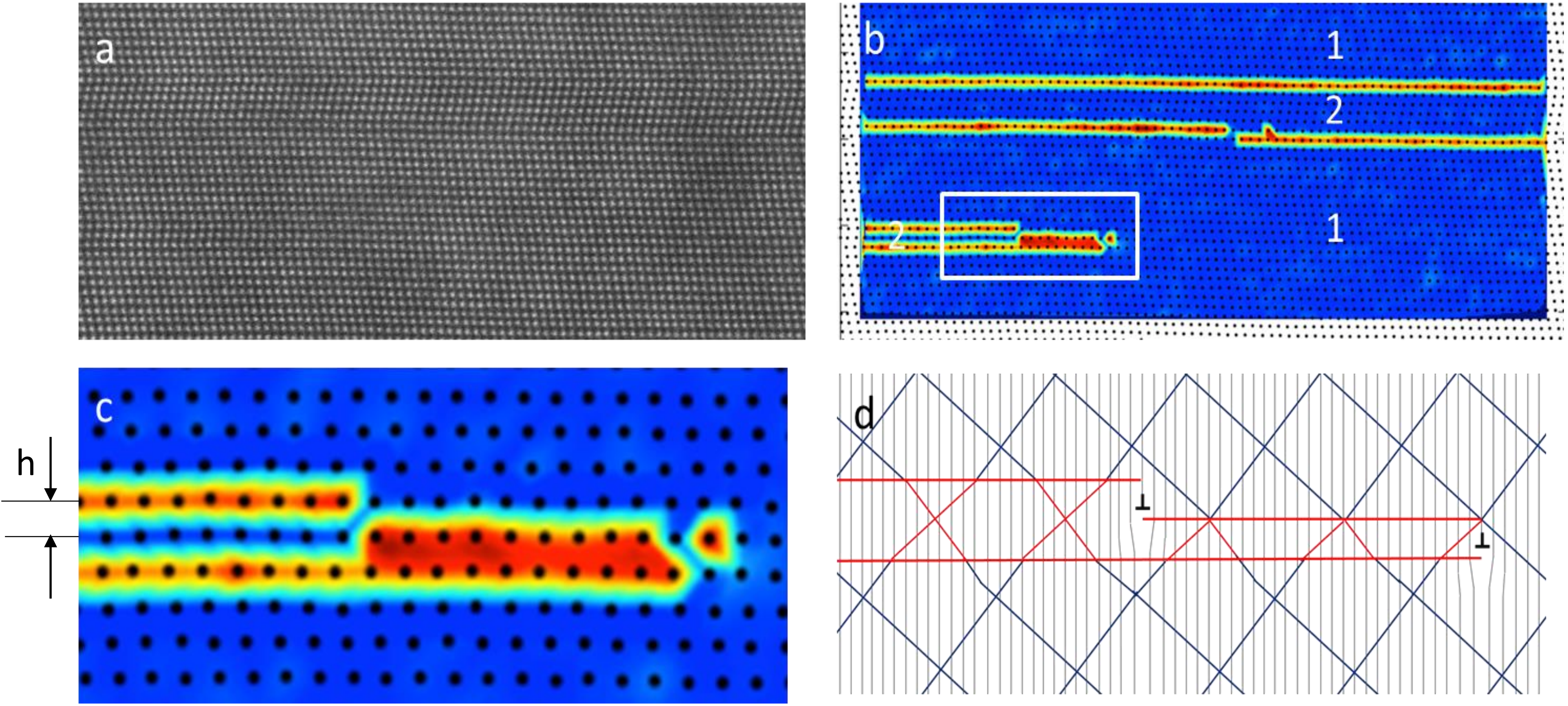
Disconnection

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

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

$$\gamma = \frac{b}{h} = 0.34$$

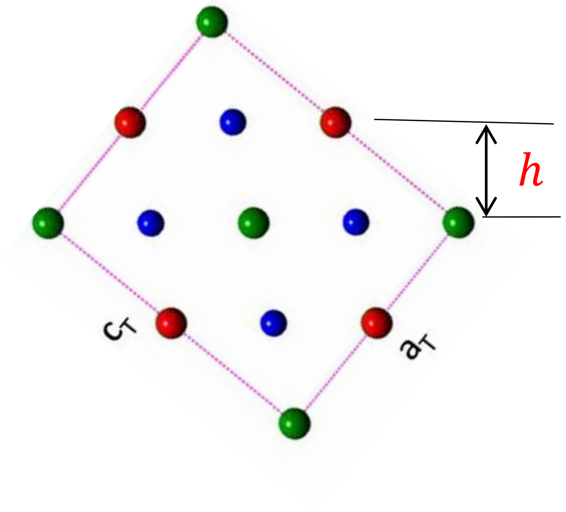
Twin tip in Ni_2MnGa



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

4 distinct atoms

no shuffling



$g = 20\bar{2}$

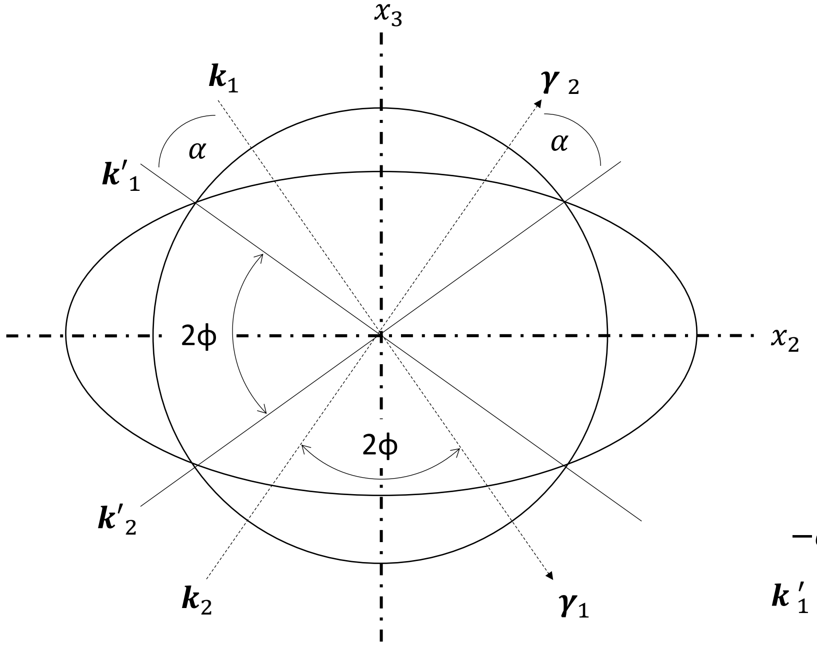
Muntifering et al. 2014

HAADF STEM (Titan PNNL)

SF

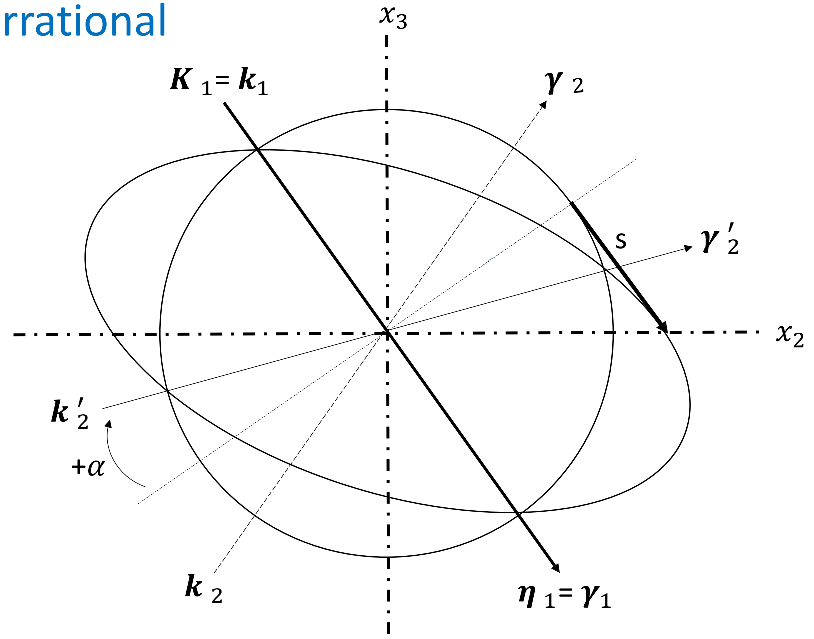
Topological model for type II twinning

Classical Model: irrational plane of shear



Type I

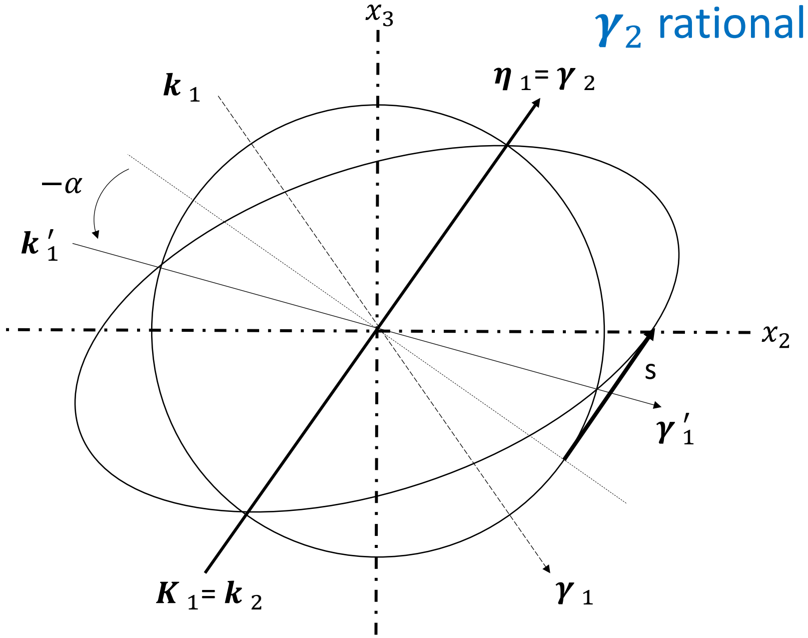
$\boldsymbol{k}_1$ rational
$\boldsymbol{\gamma}_1$ irrational

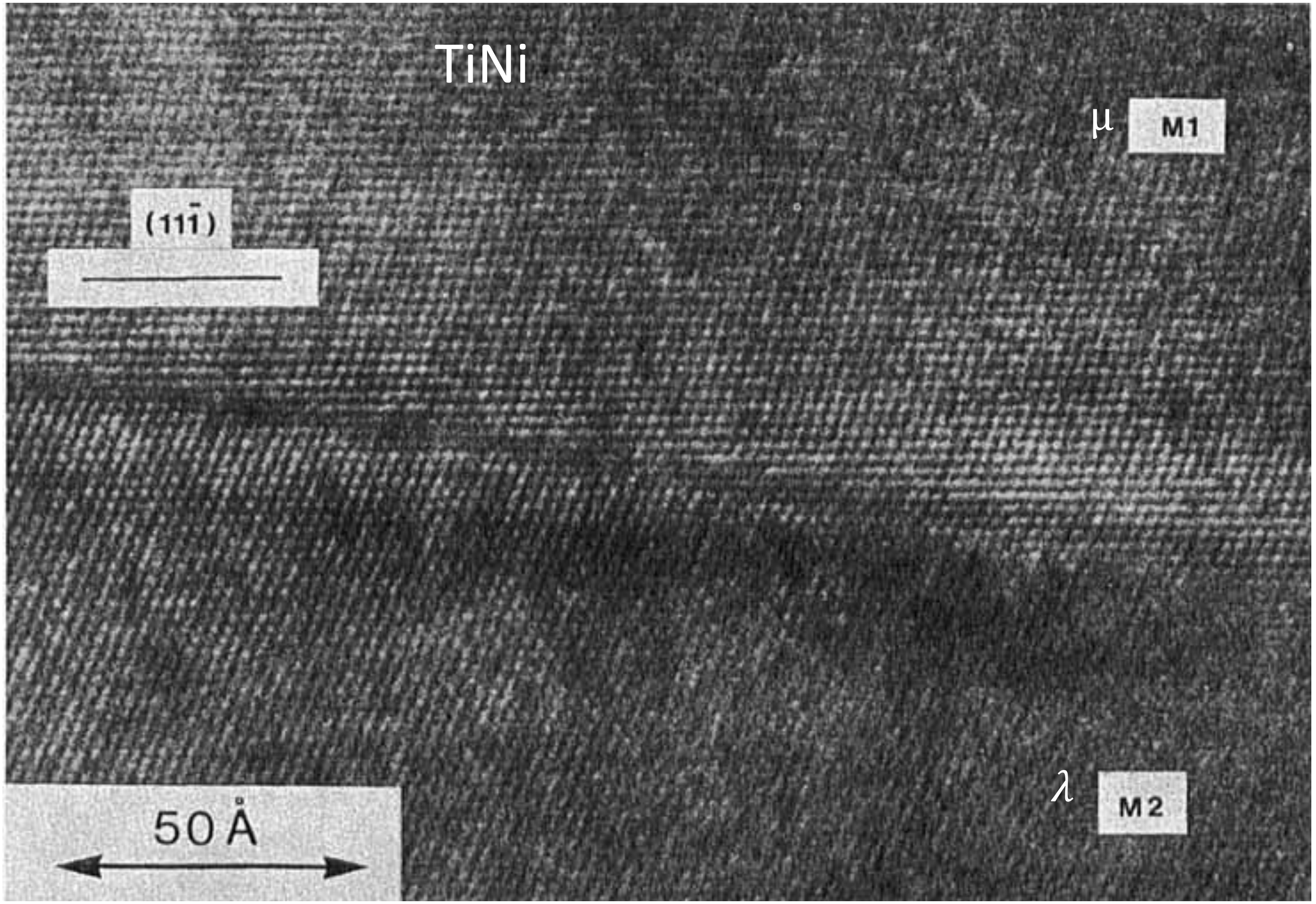


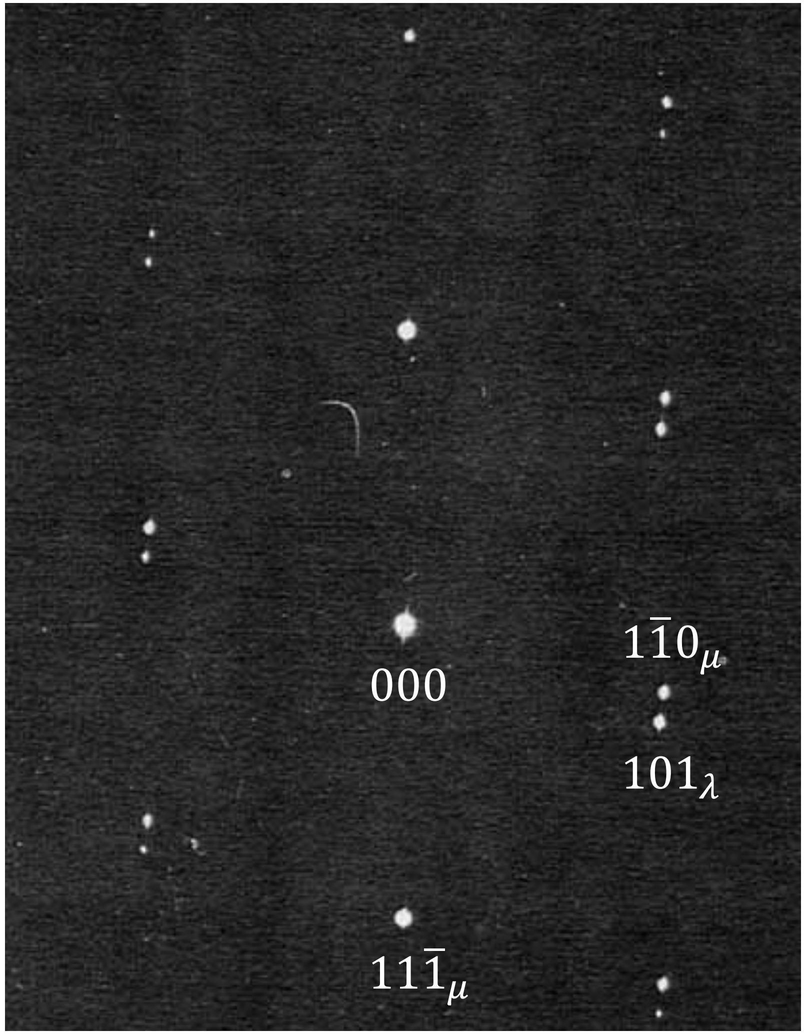
$$s = 2tan\alpha$$

Type II

$\boldsymbol{k}_2$ irrational
$\boldsymbol{\gamma}_2$ rational





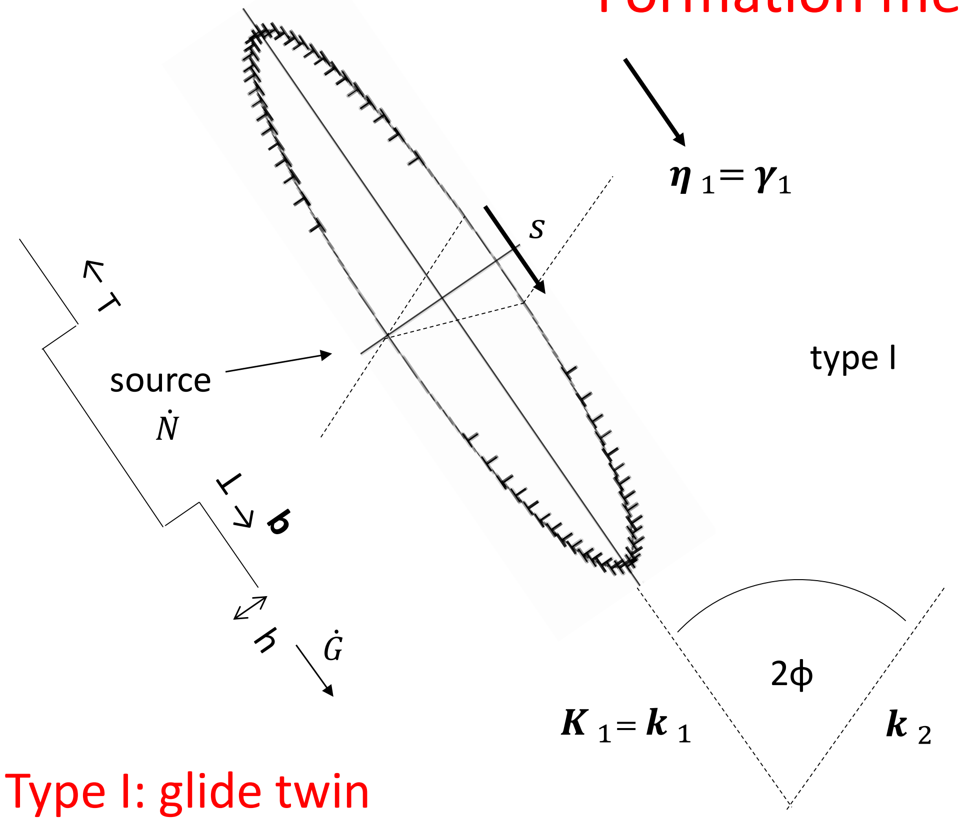


Knowles, 1982

(a)

(b)

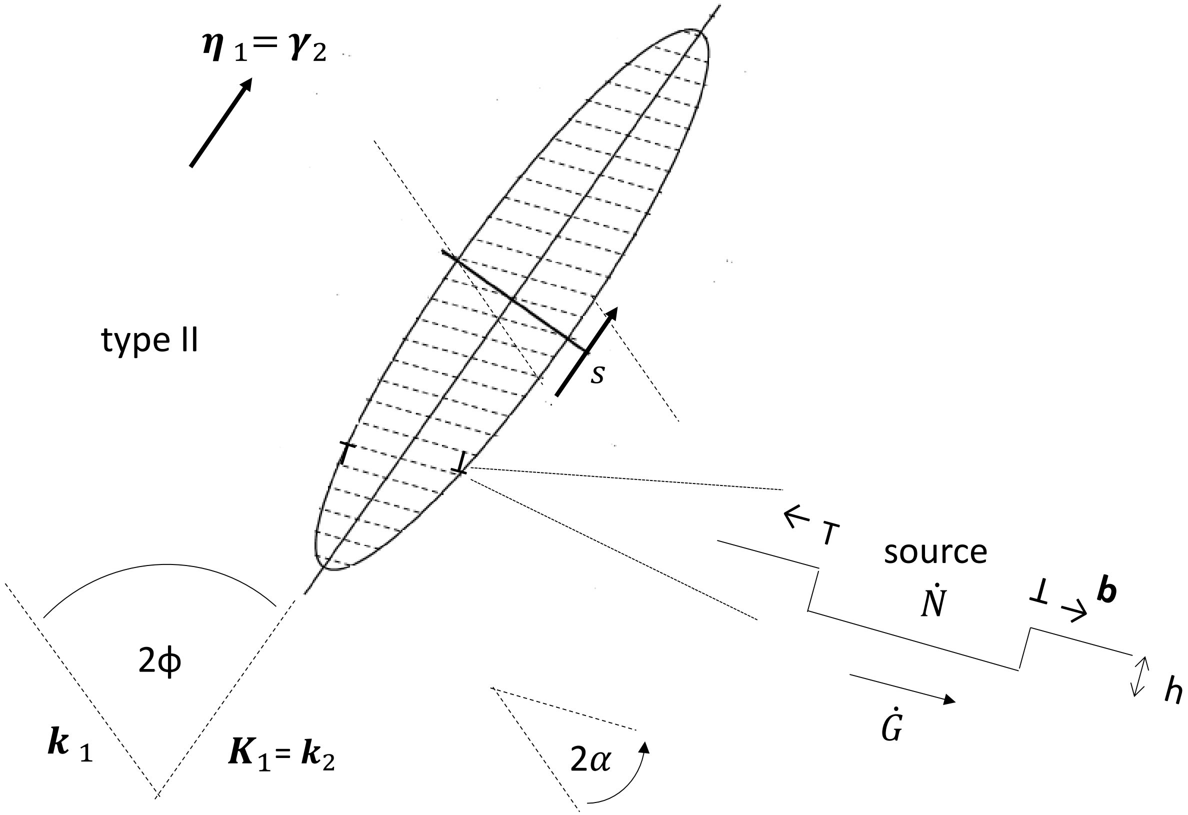
Formation mechanisms for type I and II twins



Type I: glide twin

$\gamma = b/h$

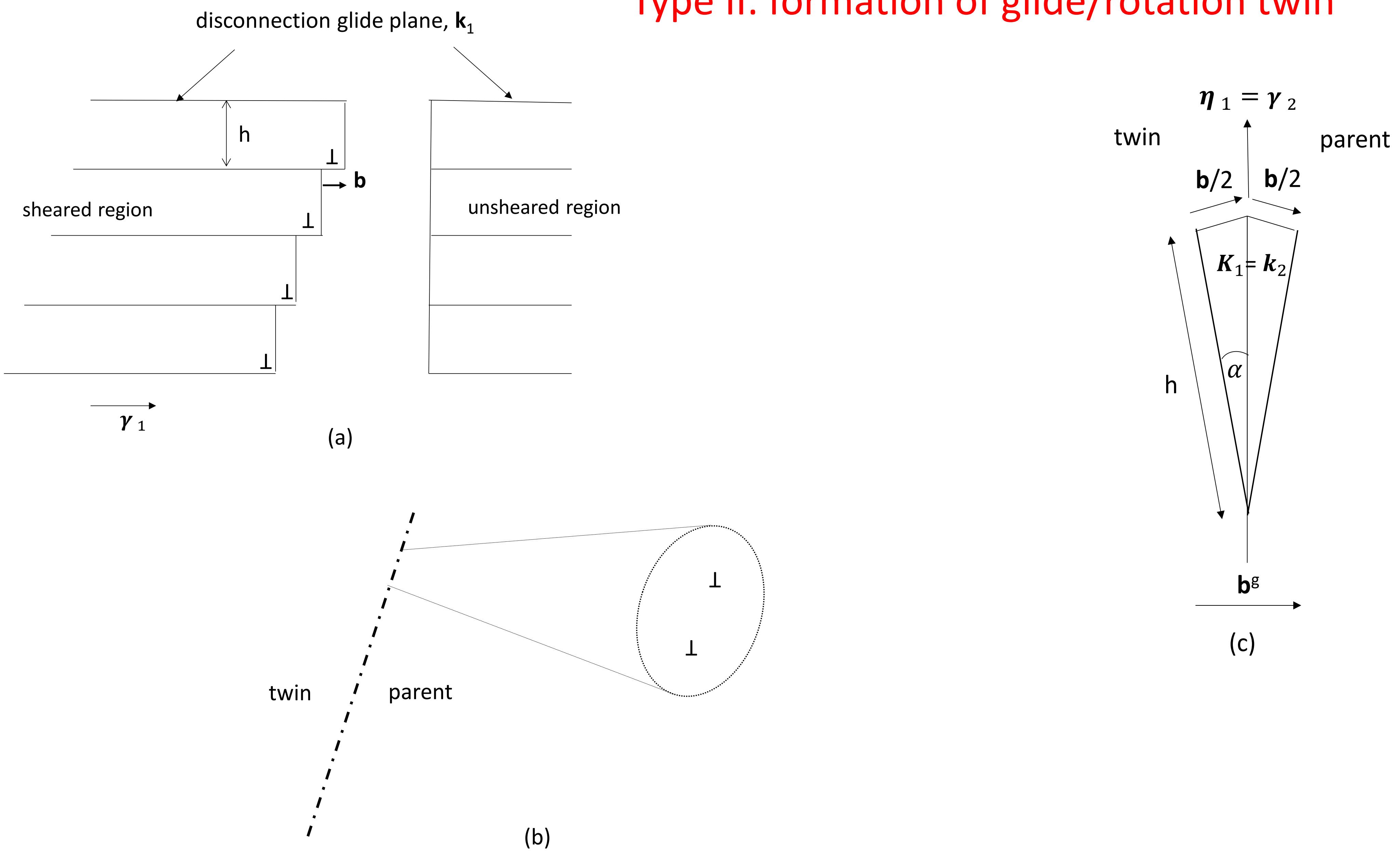
Type II: glide/rotation twin



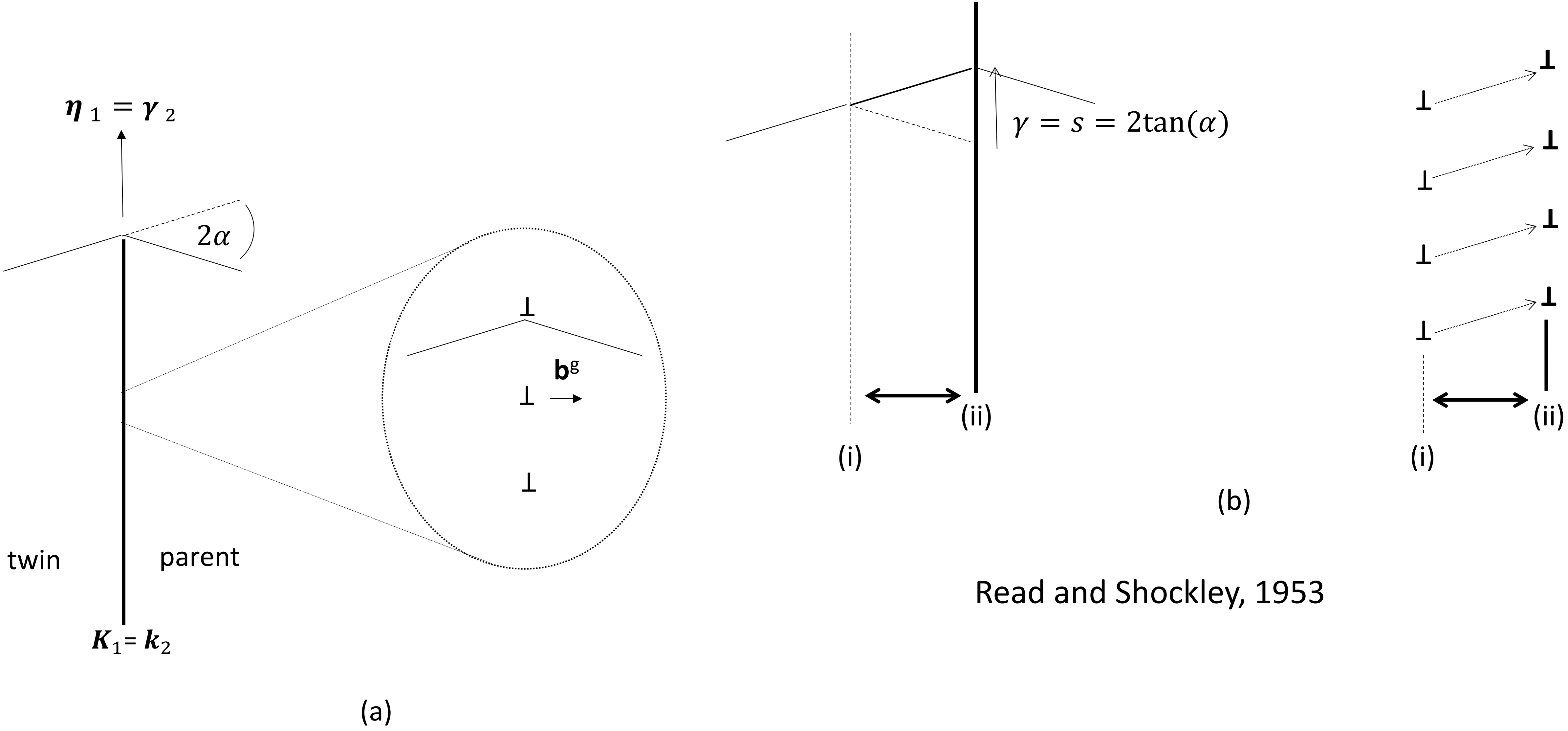
competitive mechanisms: High $\dot{G}/\dot{N}$ favours type I

Low $\dot{G}/\dot{N}$ favours type II

Type II: formation of glide/rotation twin



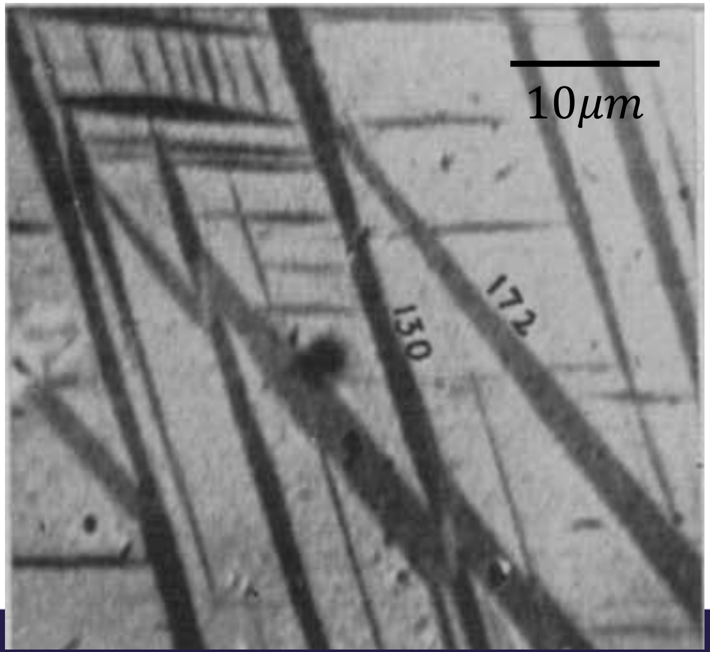
Type II: growth



Read and Shockley, 1953

Experimental observations: e.g. $\alpha - U$

K_1	K_2	η_1	type	b nm	h nm	γ	No. dist. atoms	$\dot{G}/\dot{N}$
"$\{17\bar{6}\}$"	$\{111\}$	$1/2 < 512 >$	II	0.098	0.456	0.216	4	low
"$\{1\bar{7}2\}$"	$\{112\}$	$1/2 < 312 >$	II	0.081	0.356	0.228	4	low
$\{1\bar{3}0\}$	$\{110\}$	$1/2 < 310 >$	compound	0.048	0.161	0.299	2	high



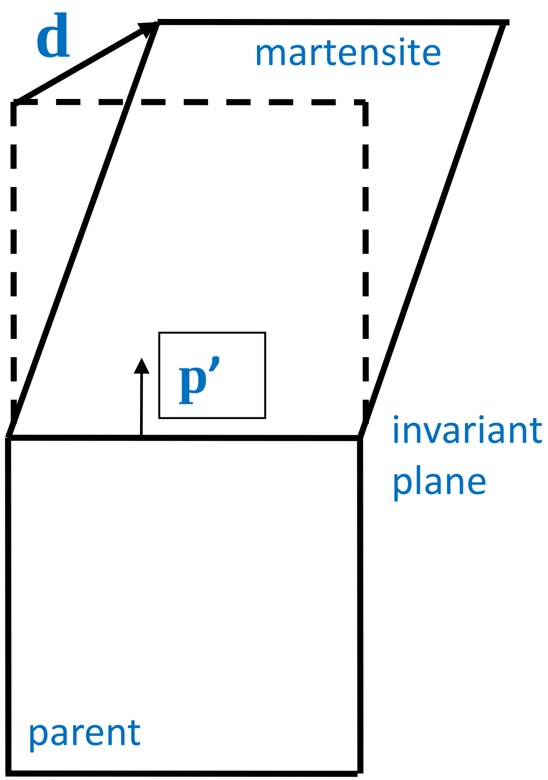
$\alpha - U, Cahn$ 1953

Type II Twinning in Other Systems

NiTi
CuAlNi
TiPd
devitrite

Topological model of martensitic transformations

PTMC

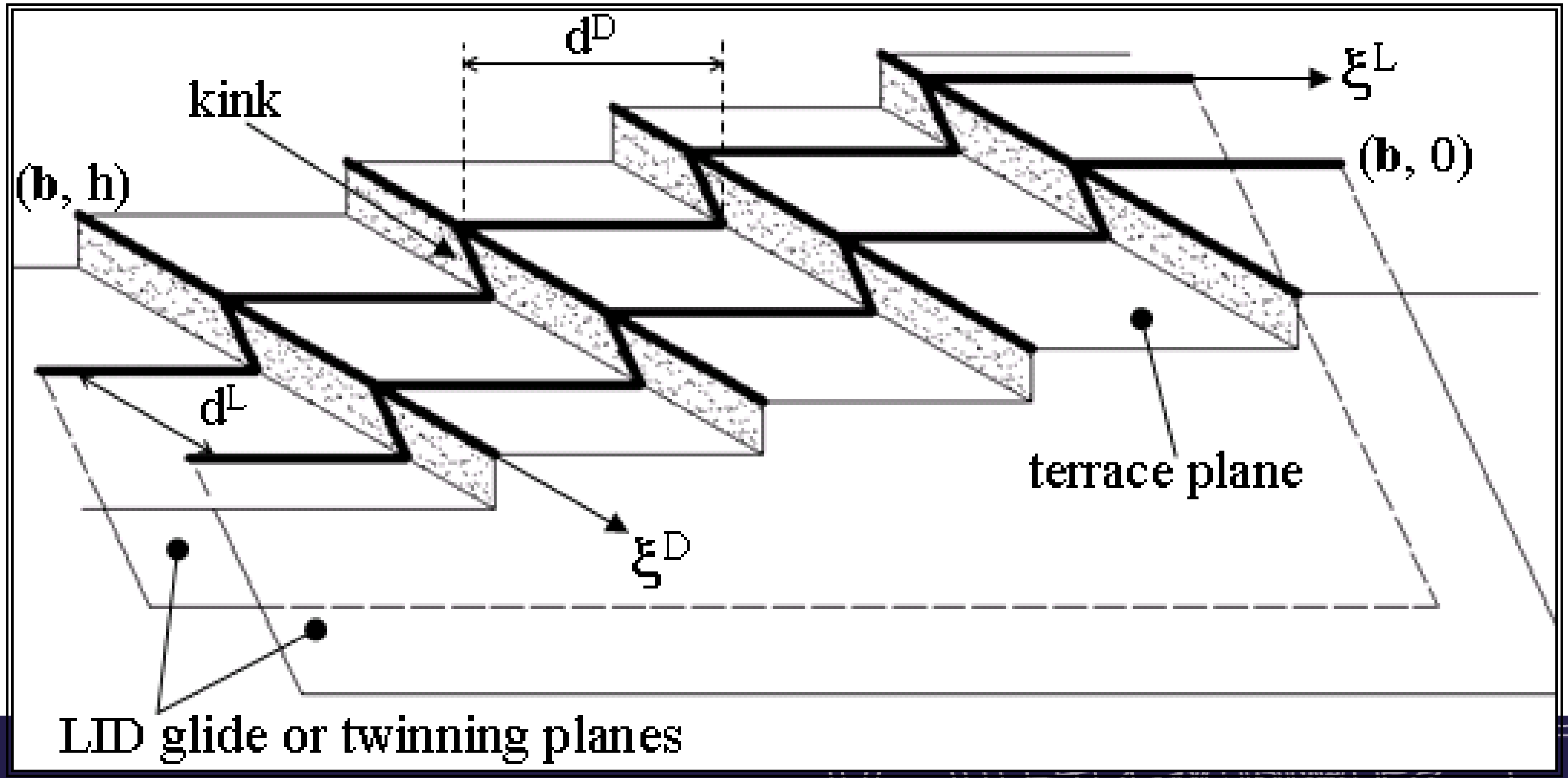


Shape deformation

$$P_1 = RBP_2 = (I + dp')$$

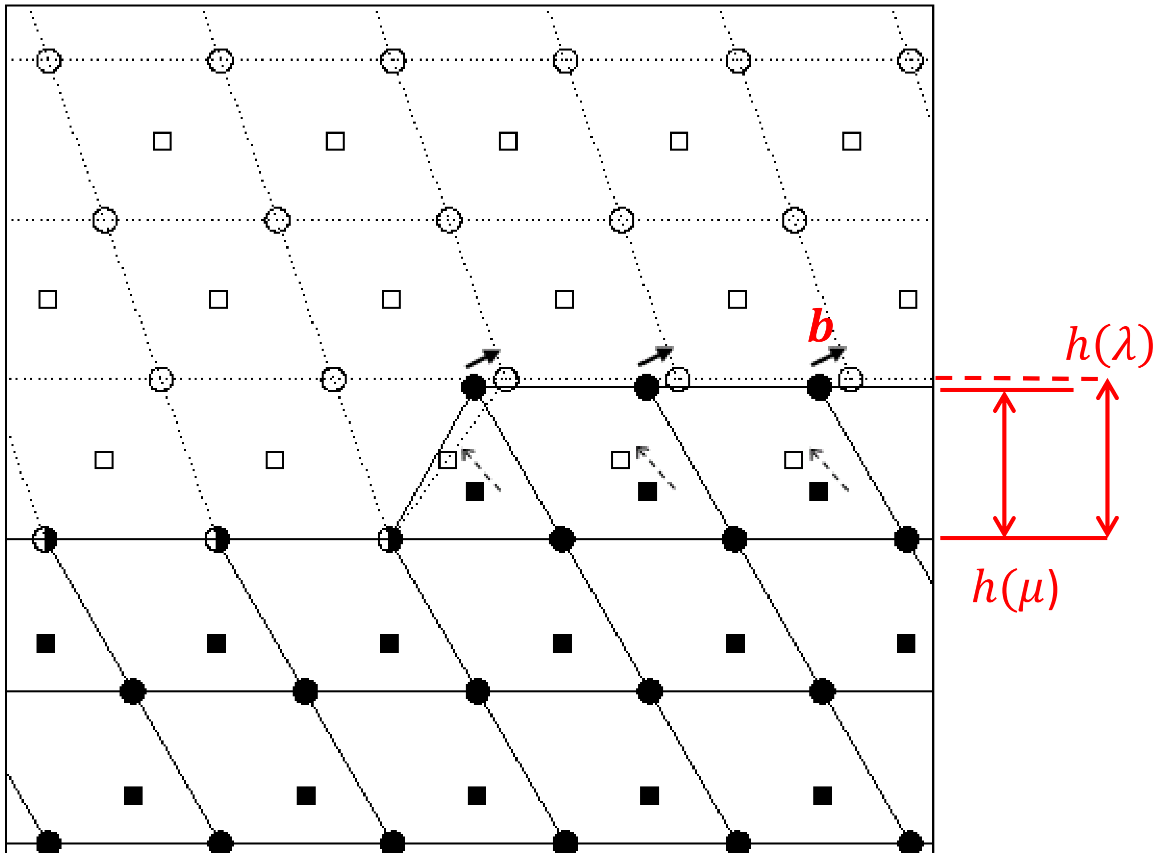
TM

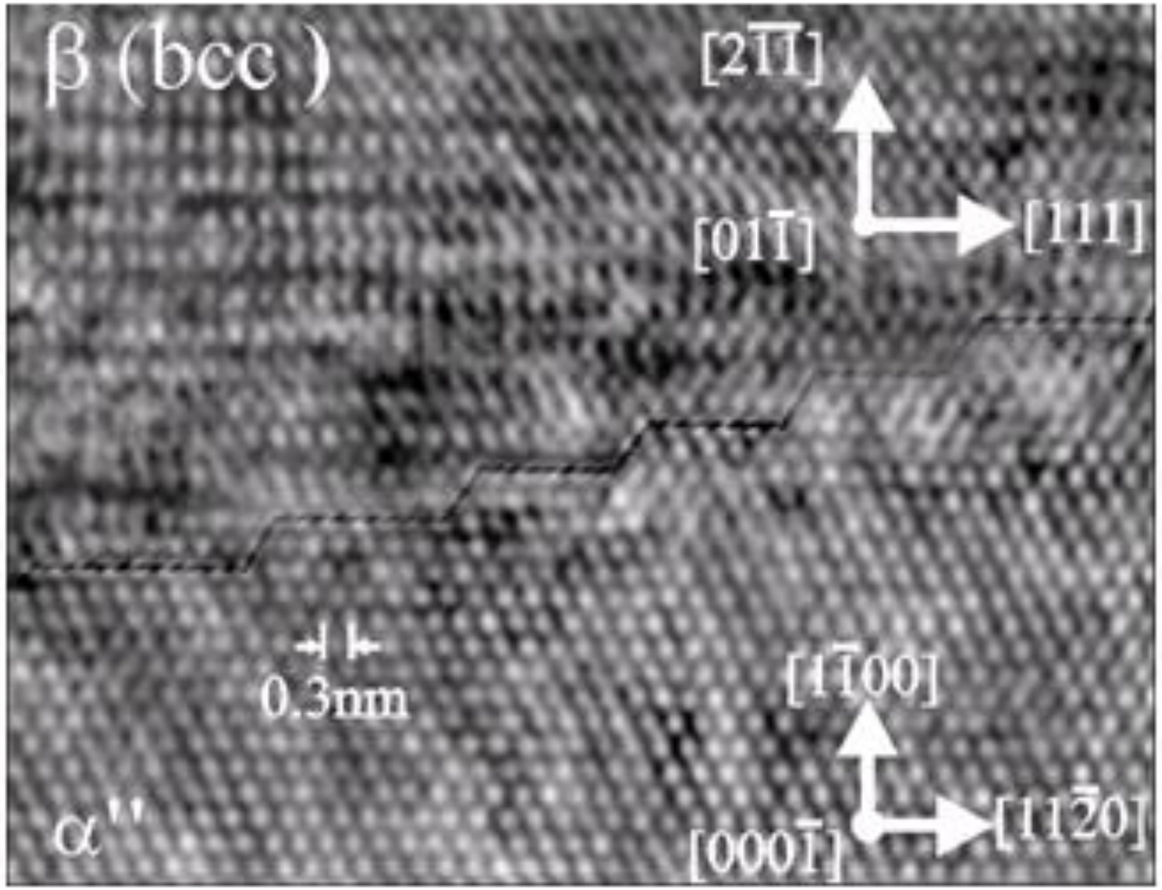
- low energy terraces (coherently strained epitaxial)
- two defect arrays: disconnections & LID
- distortion field of defect network accommodates coherency strains
- motion of all defects produces shape deformation

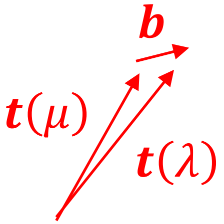


Glissile Disconnections

Ti 10 wt % Mo   Klenov 2002



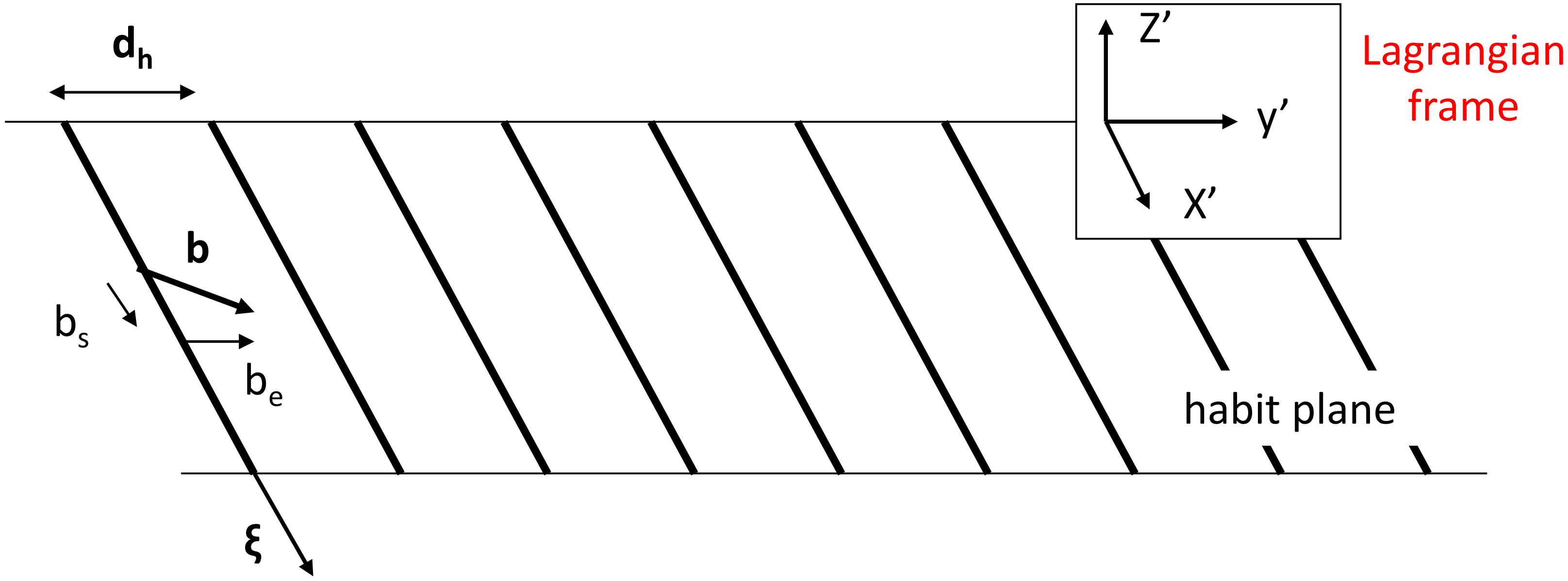




$\boldsymbol{b}_n = h(\lambda) - h(\mu)$

- 2 distinct atoms
- steps cause habit plane to be inclined to terrace plane
- $\boldsymbol{b}_n$ also produces rotational distortions
- motion causes one-to-one atomic exchange between phases with different densities

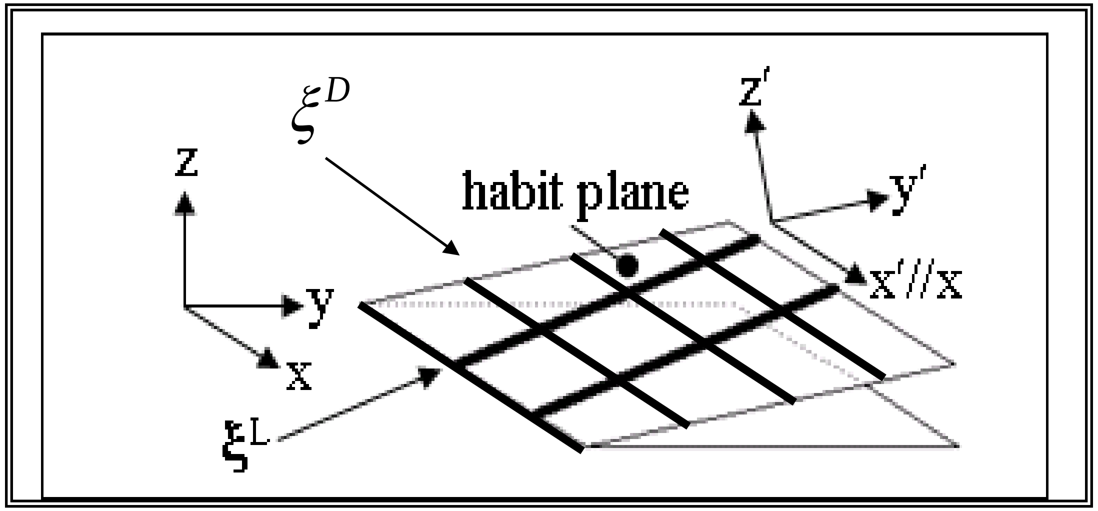
Distortion field of a Defect Array



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

$$\epsilon'_{xx} = b_x/d \qquad \omega'_{yz} = b_z/2d$$

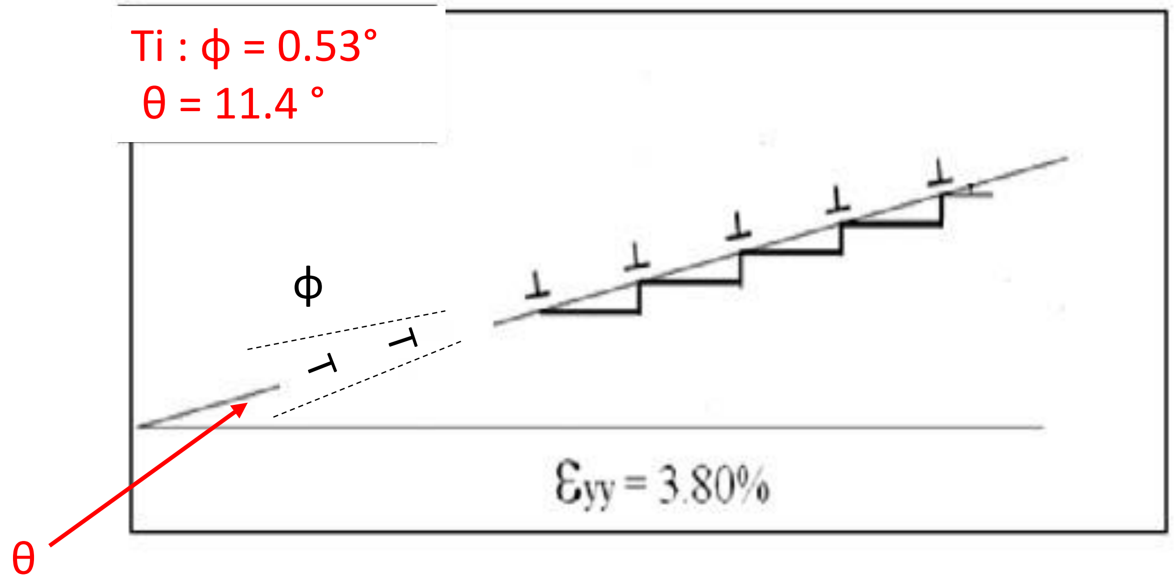
Equilibrium: superposed coherency and defect array distortion fields



$$\boldsymbol{D}_{ij}'^{m} = \begin{pmatrix} D_{xx}'^{m} & D_{xy}'^{m} & D_{xz}'^{m} \\ D_{xy}'^{m} & D_{yy}'^{m} & D_{yz}'^{m} \\ D_{xz}'^{m} & D_{yz}'^{m} & D_{zz}'^{m} \end{pmatrix} = -\boldsymbol{D}_{ij}'^{c}$$

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

Habit plane orientation



β crystal: Θ - ϕ

α crystal: Θ + ϕ

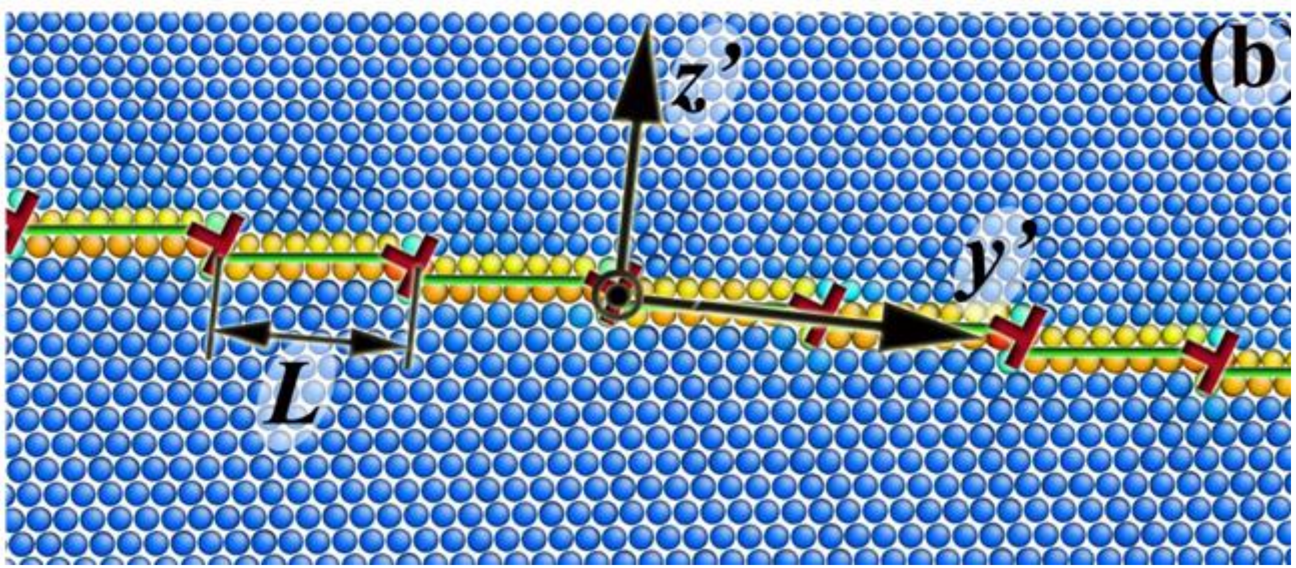
homogeneous
isotropic
approximation

inhomogeneous anisotropic case
rotations partitioned according to relative elastic compliances

TM solutions for habit plane orientation differ slightly from PTMC, unless $\boldsymbol{b}_n = 0$

Partitioning of rotations

Cu



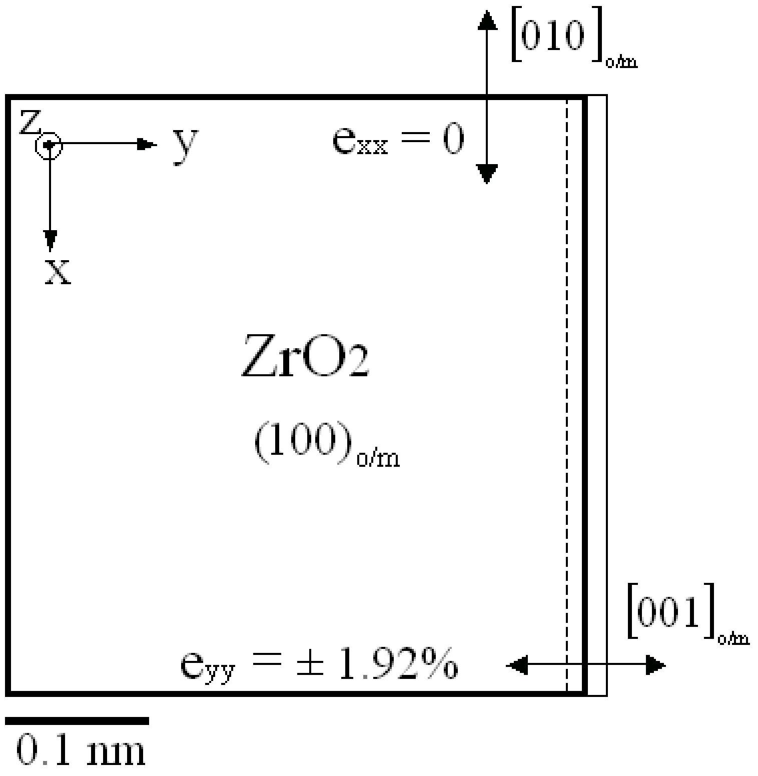
Ag

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

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

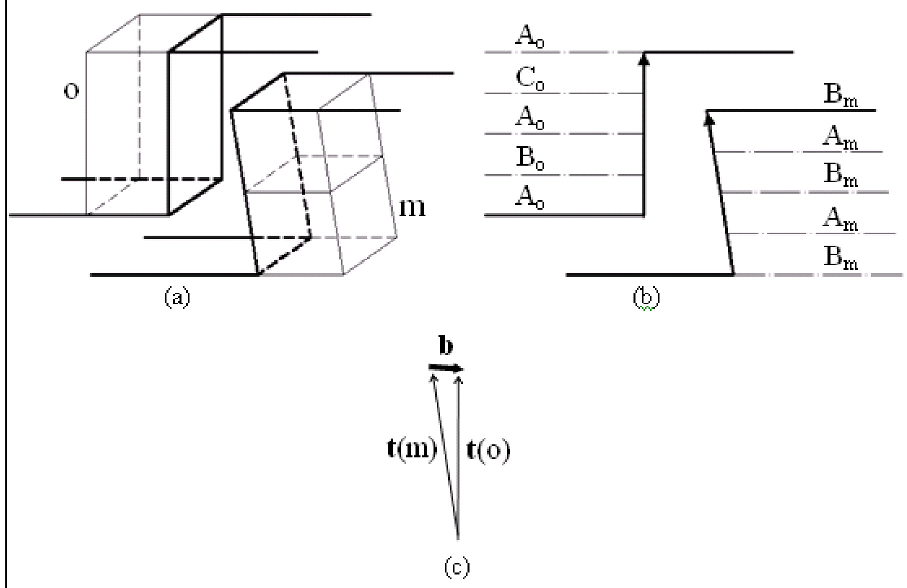
Case	φ_{Cu}	φ_{Ag}	φ	$-\varphi_{Ag}/\varphi_{Cu}$
Isotropic, inhomogeneous	0.449	-0.698	1.15	1.55
Anisotropic	0.504	-0.853	1.36	1.69
MD	0.483	-0.929	1.41	1.92
MD (Artificial)	0.665	-0.659	1.312	0.97

Orthorhombic to Monoclinic Transformation in ZrO_2



Principal strains on terrace plane

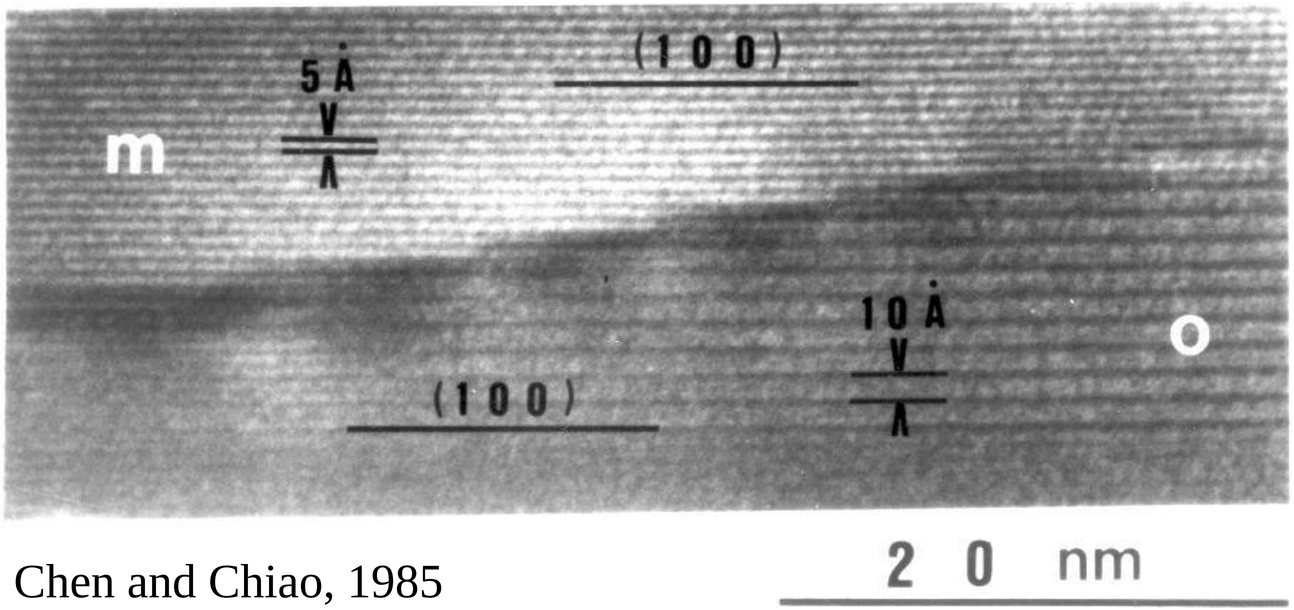
$\varepsilon_{xx} = 0$ $\varepsilon_{yy} = 3.8\%$



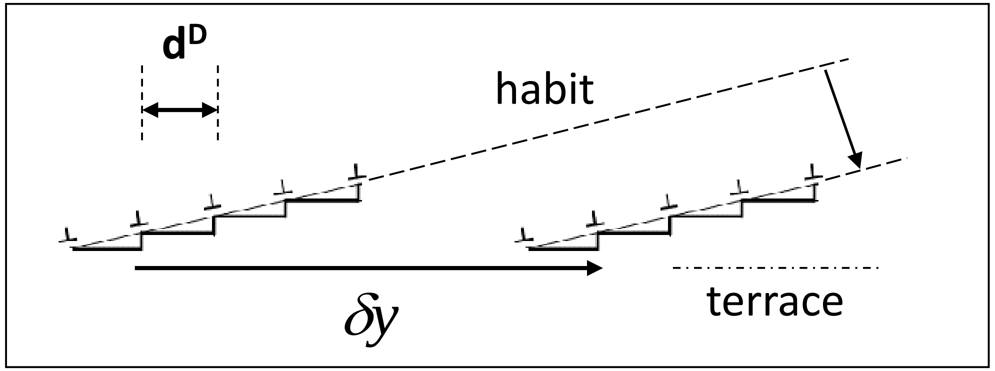
considerable shuffling:

8 Zr & 16 O distinct ions

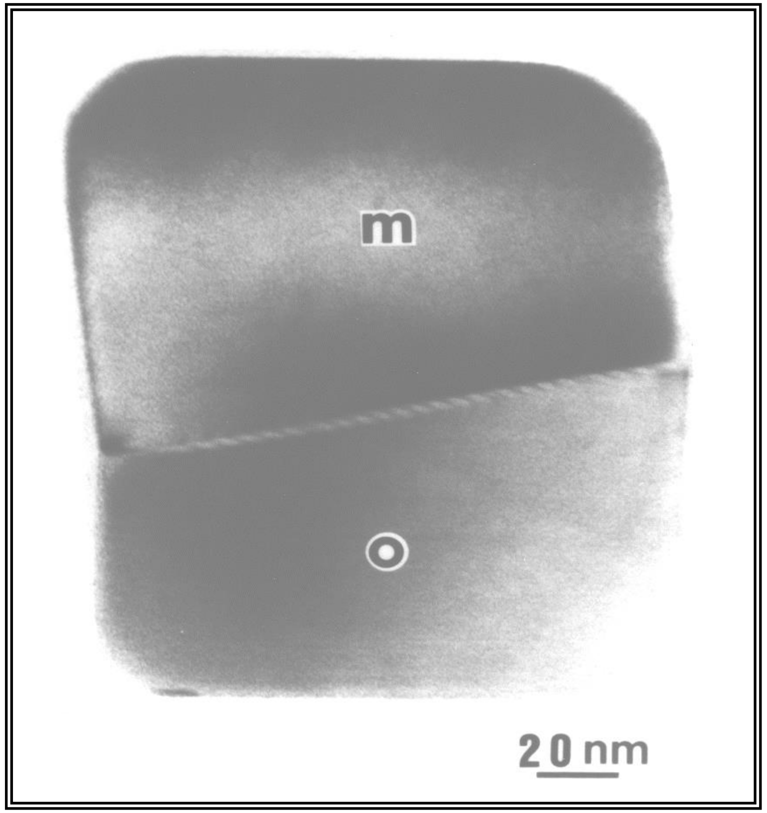
synchronous motion of disconnections



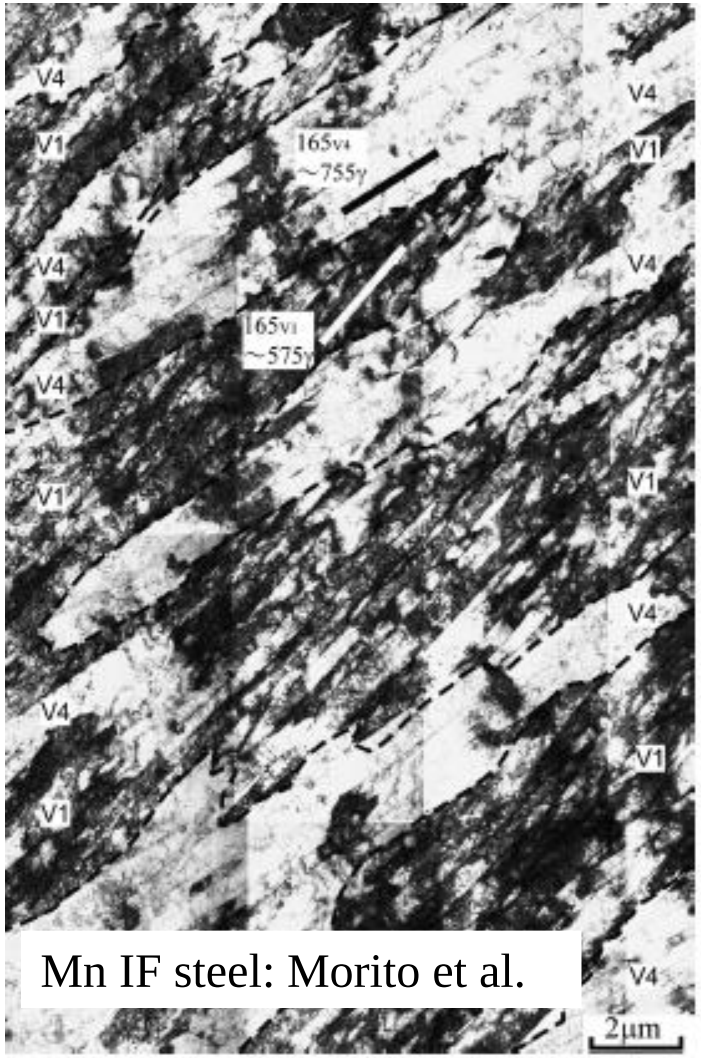
Chen and Chiao, 1985



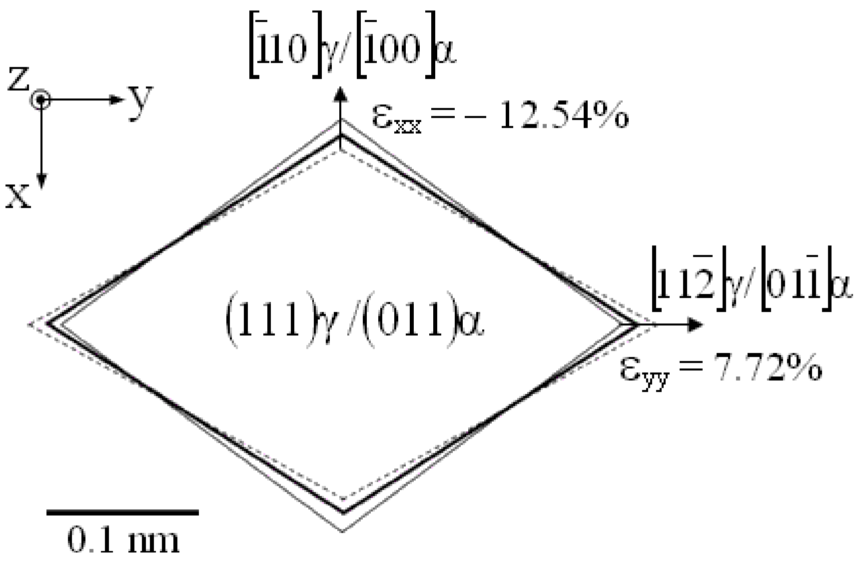
$$\Gamma_m^D = \begin{pmatrix} 0 & 0 & \gamma_{xz} \\ 0 & 0 & \gamma_{yz} \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix} = \frac{\delta y}{d^D} \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix}^D \begin{pmatrix} 0 & 0 & n_z \end{pmatrix}$$



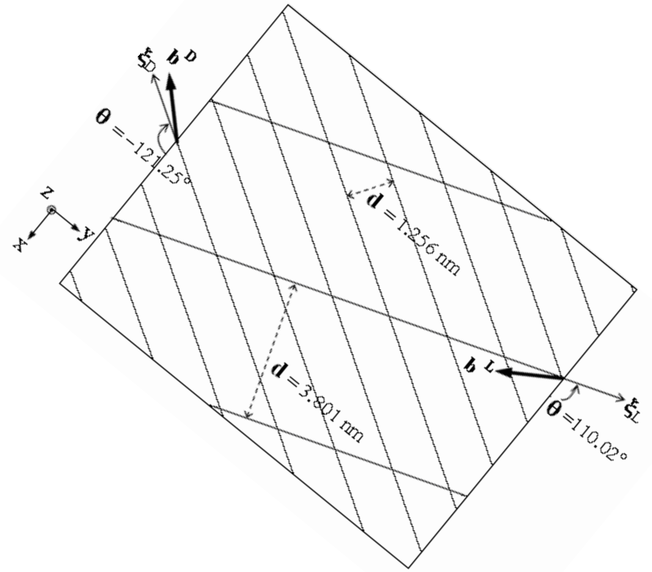
Lath martensite in ferrous alloys



Mn IF steel: Morito et al.



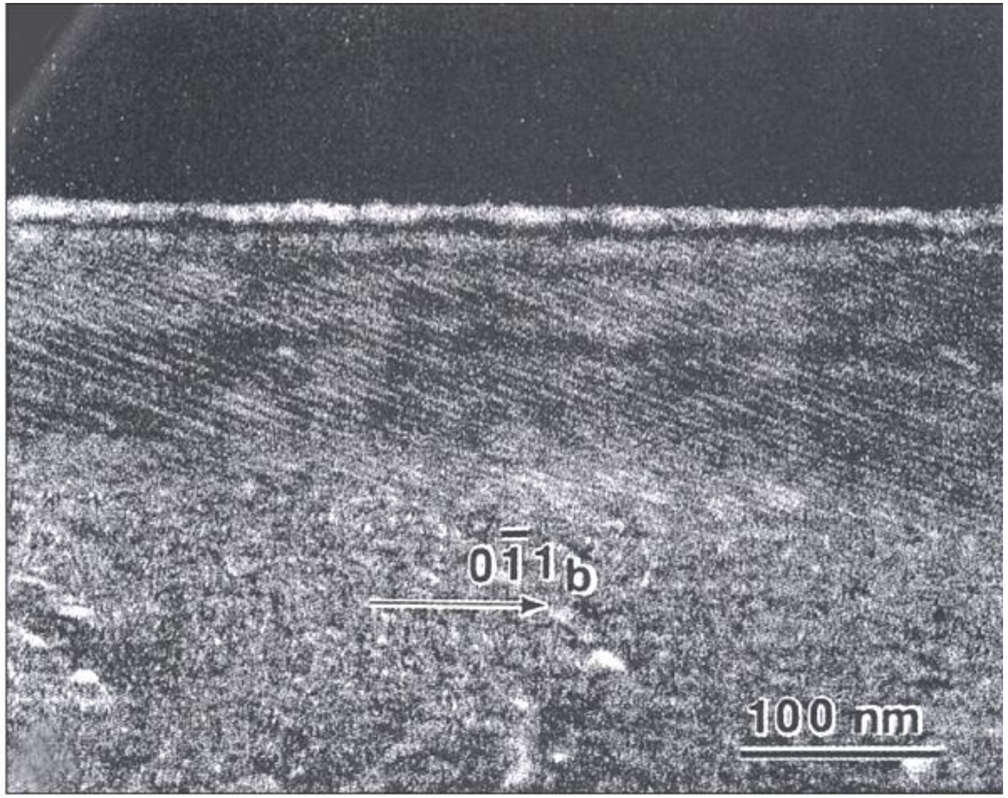
"N-W OR"



~{575}

G-T OR

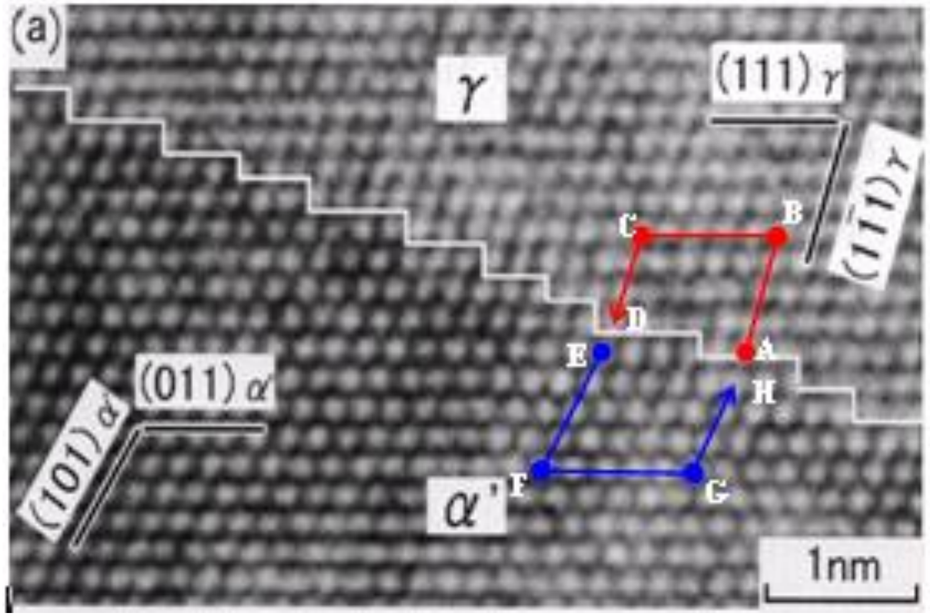
TEM: LID slip dislocations

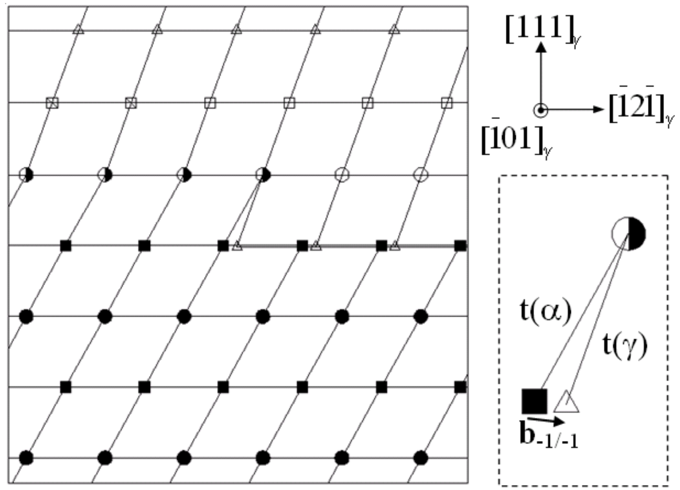


$1/2[1\bar{1}1]_\alpha$ dislocations, ~10° from screw, with spacing 2.8 -6.3 nm

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

TEM: Disconnections in near screw orientation



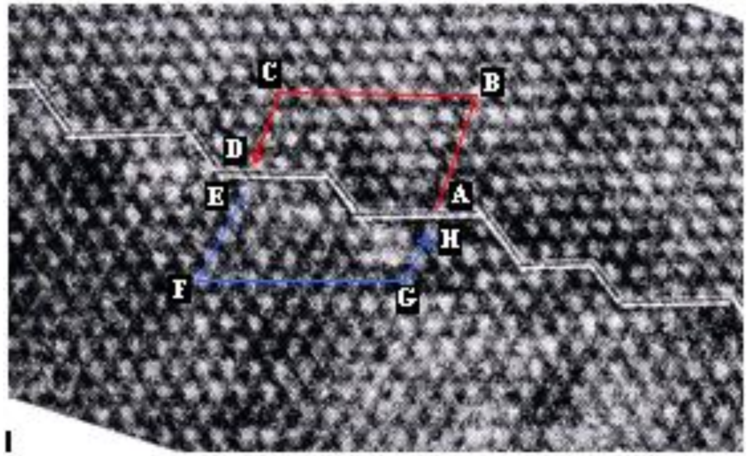


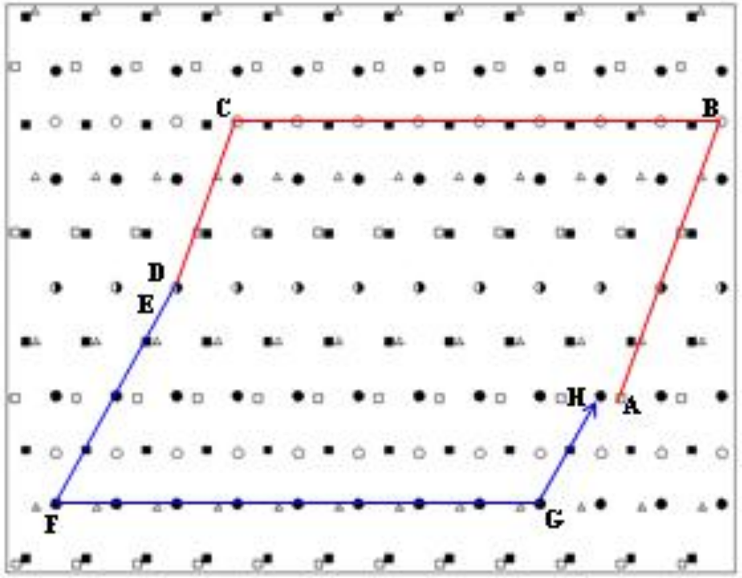
Moritani et al. Fe-Ni-Mn

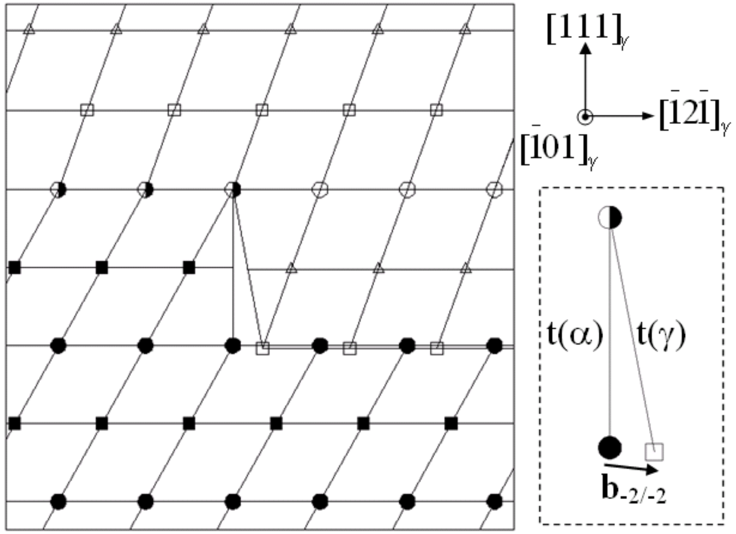
$[-101]_\gamma$ projection

Plate Martensite

~{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.