An Advanced Perspective on Twin Growth and Slip in NiTi

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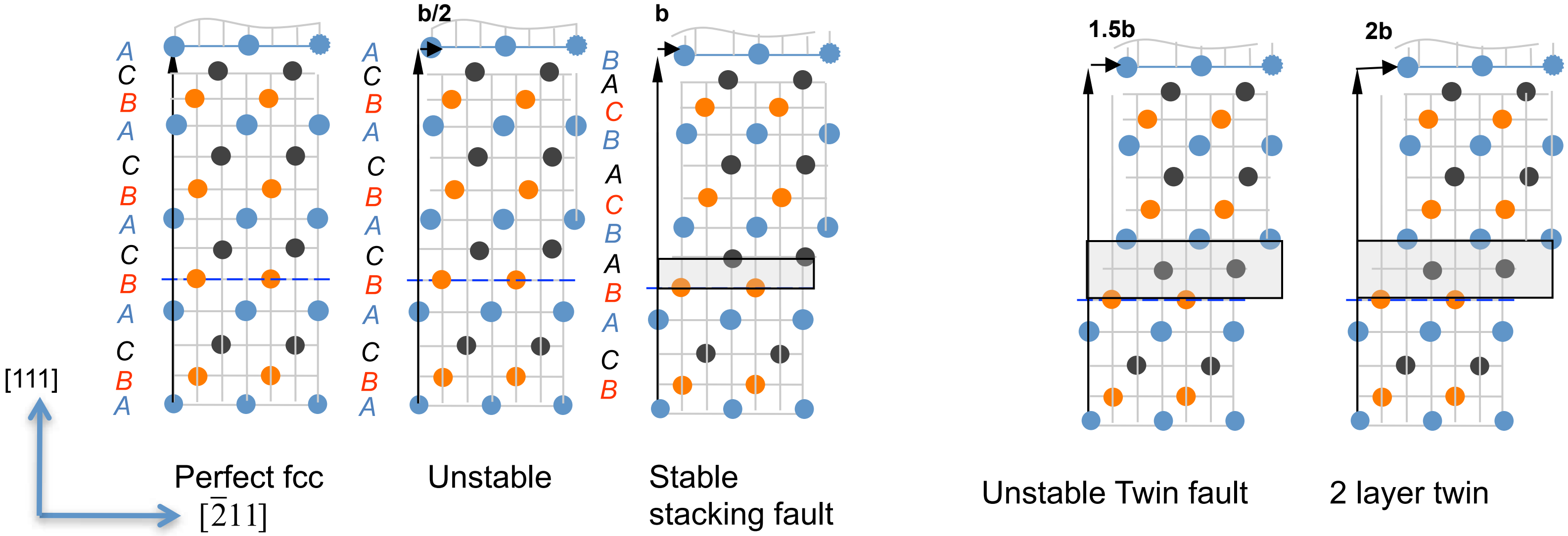
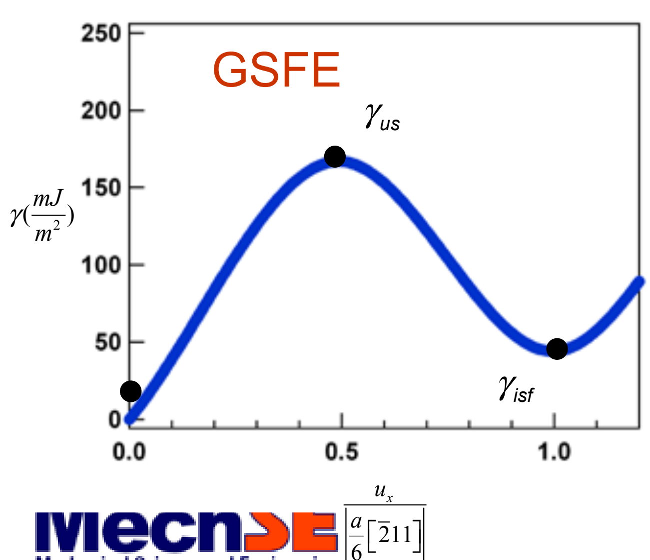
Presentation Outline

- Detwinning mechanism of Type II-1 twin in Martensitic NiTi
- Compound twinning in Martensite (001), (100) and $(20\bar{1})$ Modes
- Twinning in Austenite (112) and (114) Modes
- Slip in B2 NiTi

Fault Energy Measurement: Example with FCC

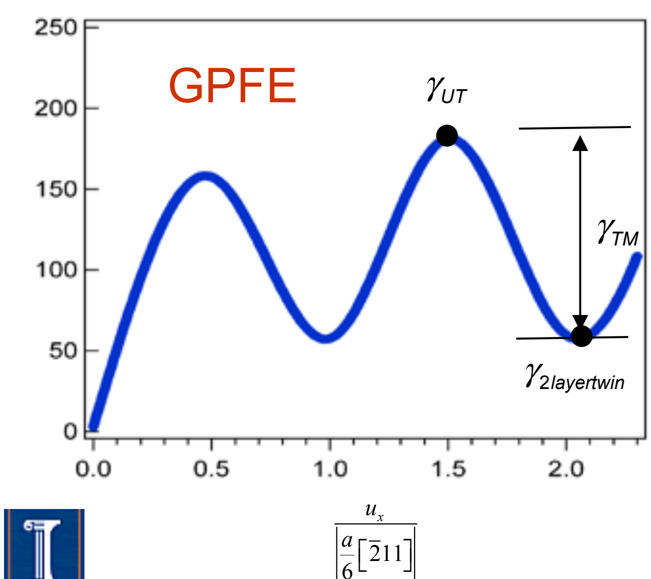


FCC is the Simplest!



γ_{us}

is linked to Dislocation Nucleation



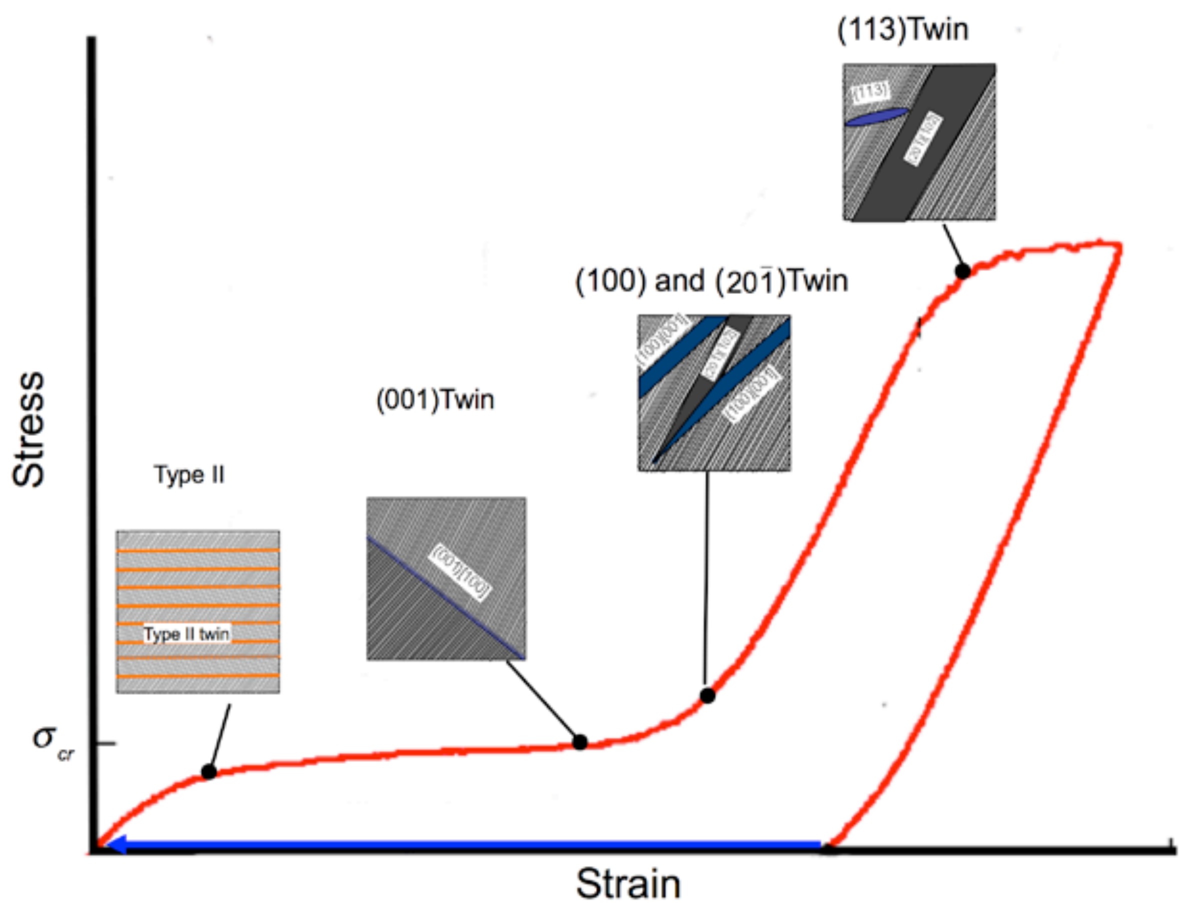
γ_{UT}

is the energy barrier to overcome during Twin Nucleation

γ_{TM}

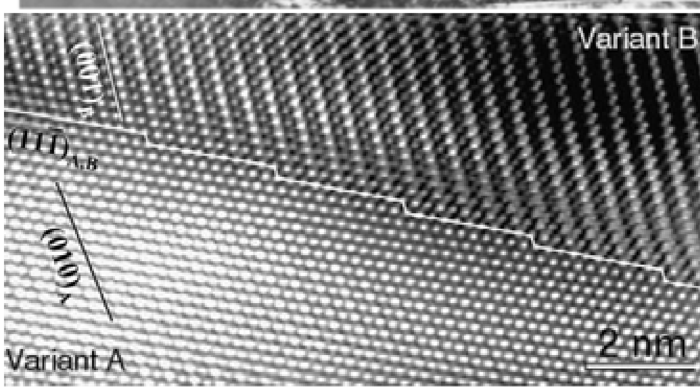
is the barrier to overcome during Twin growth

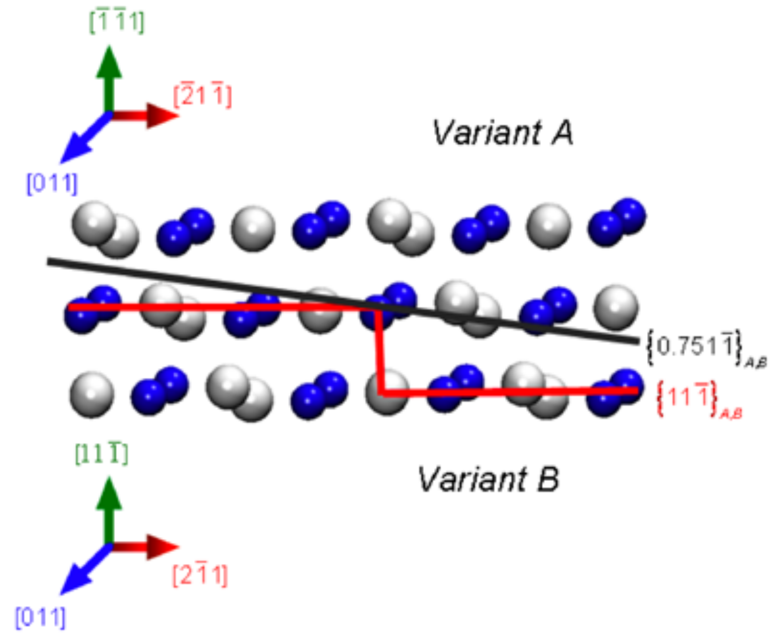
Detwinning and Twinning of NiTi Martensite



Adapted from Ishida et al.,2006

Type II-1 twins





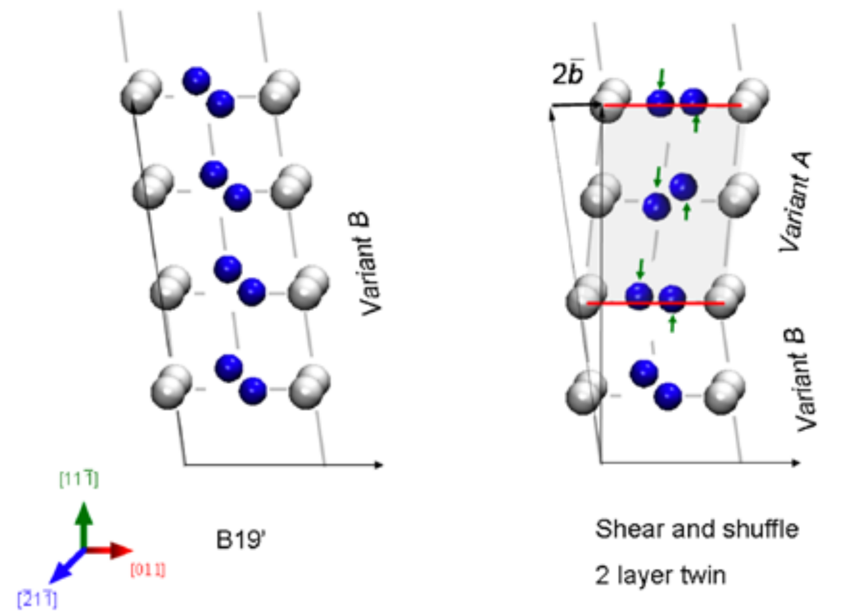
Phenomenological Theory provides twinning plane to be irrational $(0.7205\ 1\ \bar{1})$

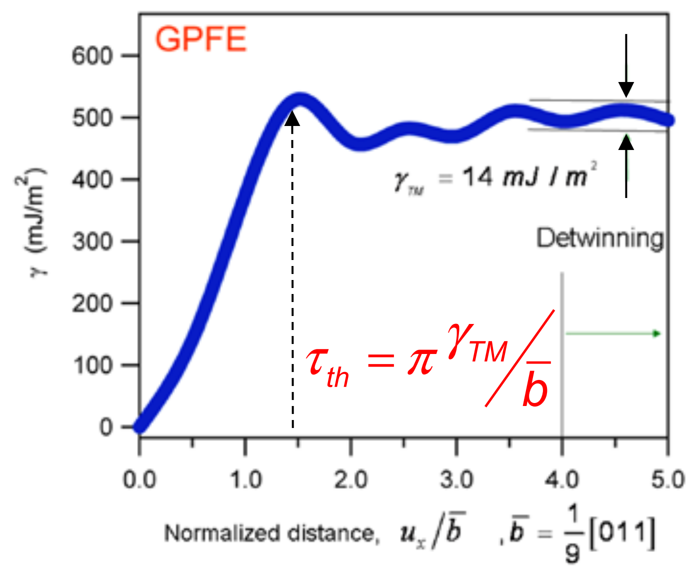
Experimentally evidence of rational $(1\ 1\ \bar{1})$

ledges and steps

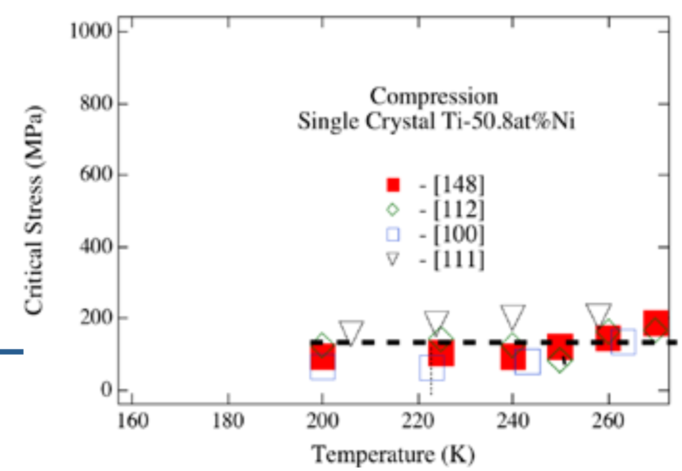
Liu, Van Humbeeck, 46, 1998, Acta Mat.
Xie,Liu,84,3497,2004, Acta Mat.

Fault Energy in Type II twin





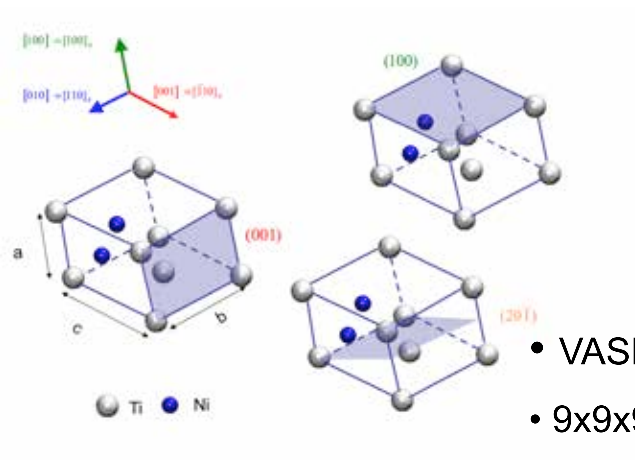
Atoms	*Shear plane*	*Shear direction*	*Shear magnitude s*	*Shuffle (Å)*	*Shuffle direction*
Ti	(1 1 $\bar{1}$)	[0 1 1]	0.28040	-	-
Ni	(1 1 $\bar{1}$)	[0 1 1]	0.28040	0.6385	[2 0 5] and [$\bar{2}$ 0 5]

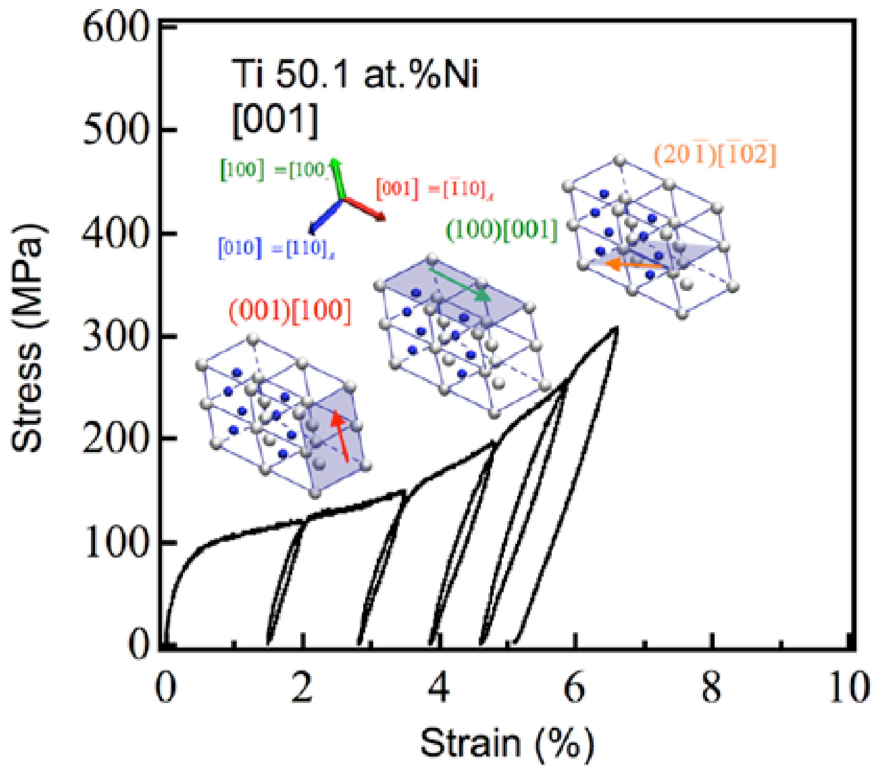


Ezaz -Sehitoglu., APL, 2011

Outline

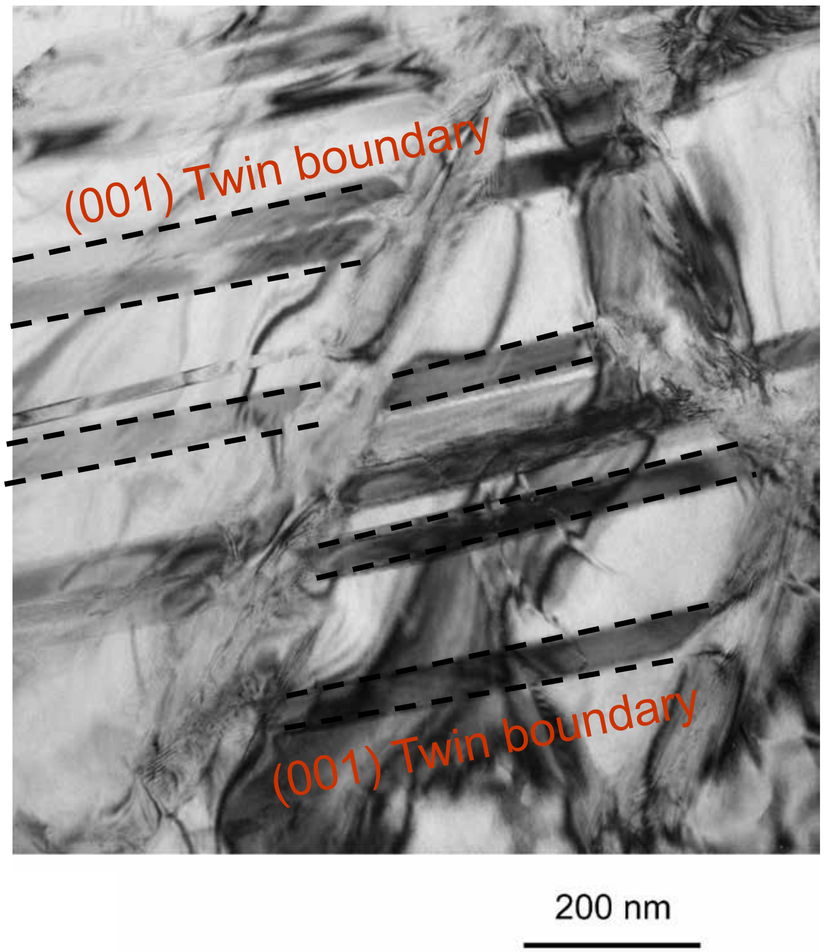
- Detwinning mechanism of Type II-1 tw in Martensitic NiTi
- Compound twinning in Martensite (001), (100) and (20$\bar{1}$)
- Twinning in Austenite, (112) and (114)

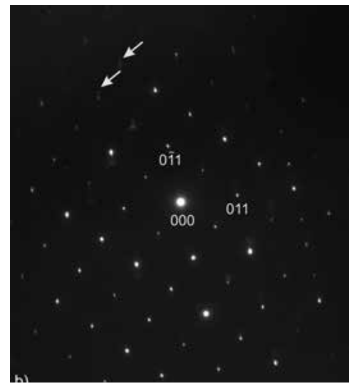


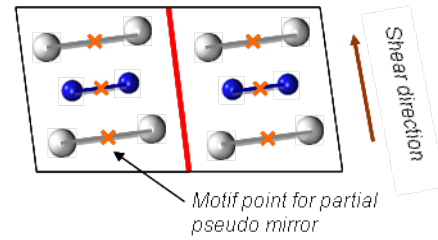


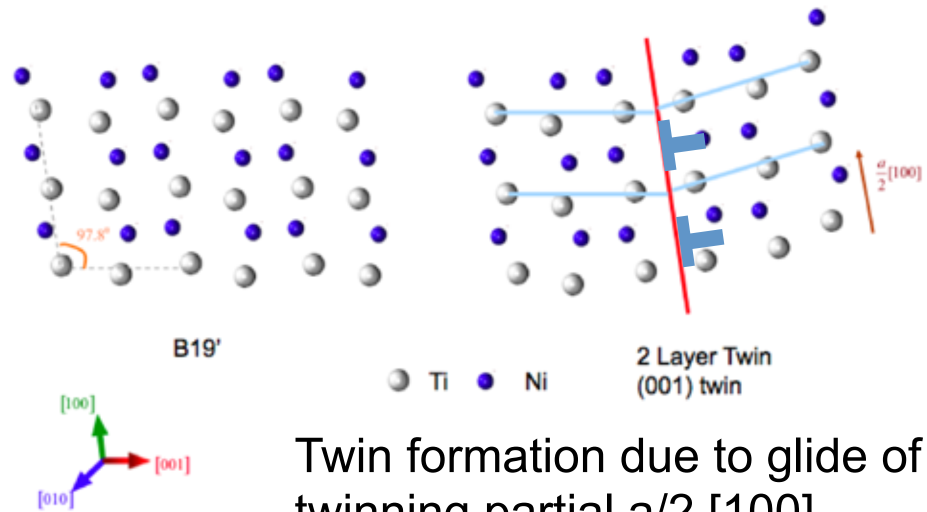
- VASP-PAW-GGA
- 9x9x9 k-point mesh with 273.2 eV energy cutoff.
- Convergence assessed with increasing L

(001) Compound Twin



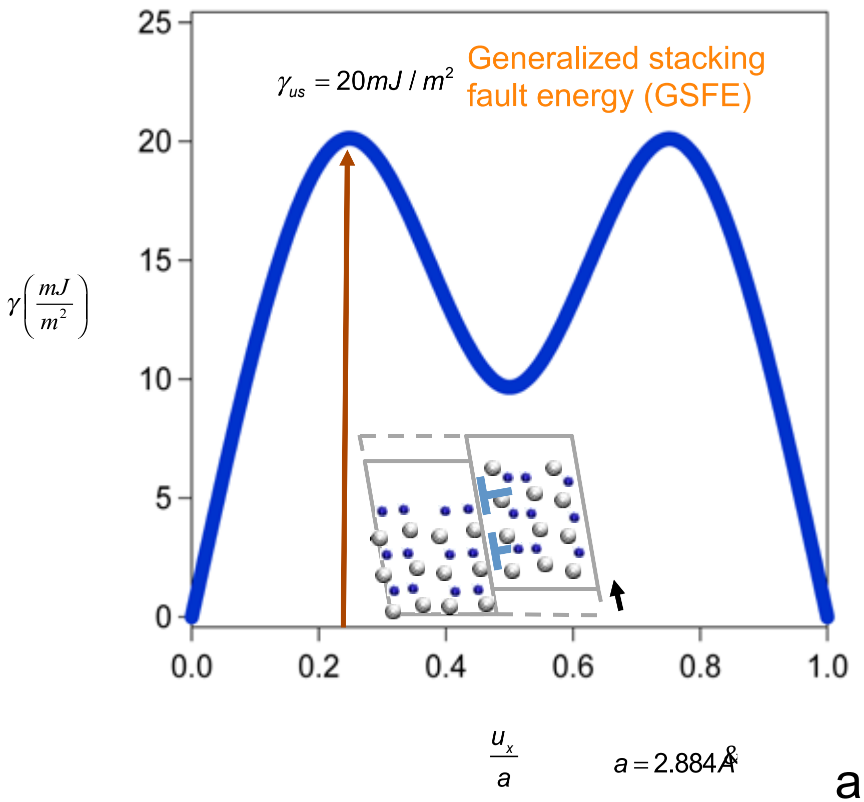


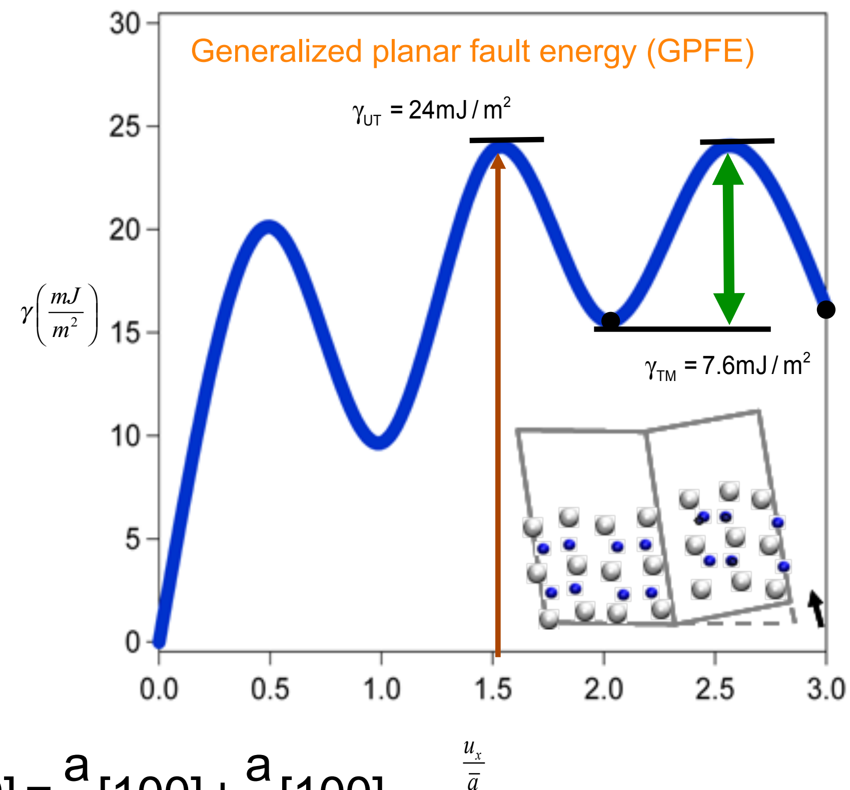




Twin formation due to glide of twinning partial a/2 [100]

(001) Compound Twin-GSFE and GPFE

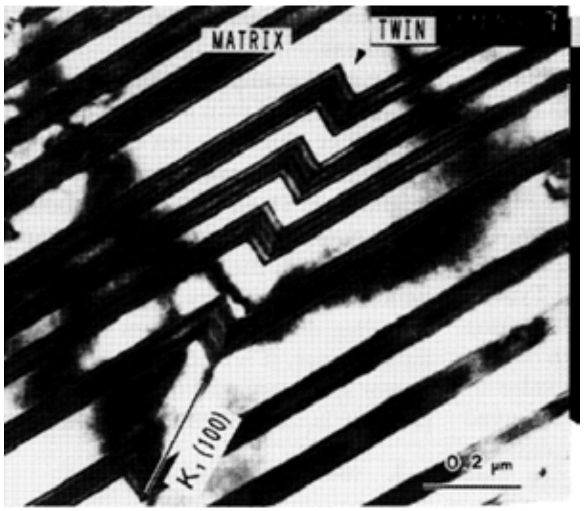




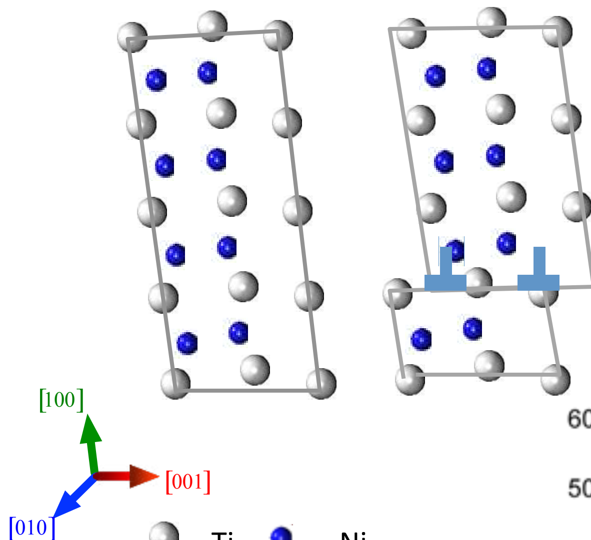
$$a[100] = \frac{a}{2}[100] + \frac{a}{2}[100]$$

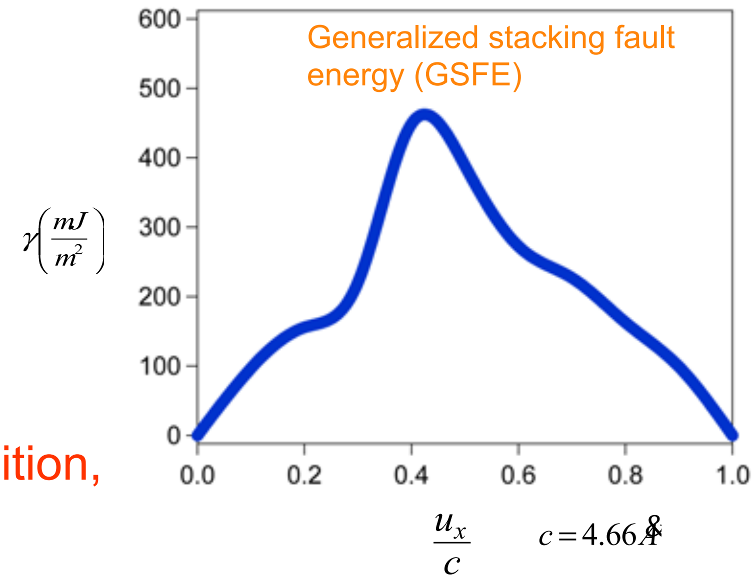
Ezaz, Sehitoglu, Acta. Mat, 2011

(100) Compound Twin



Onda et al., 33,354,1992, JIM, Mats. Trans.

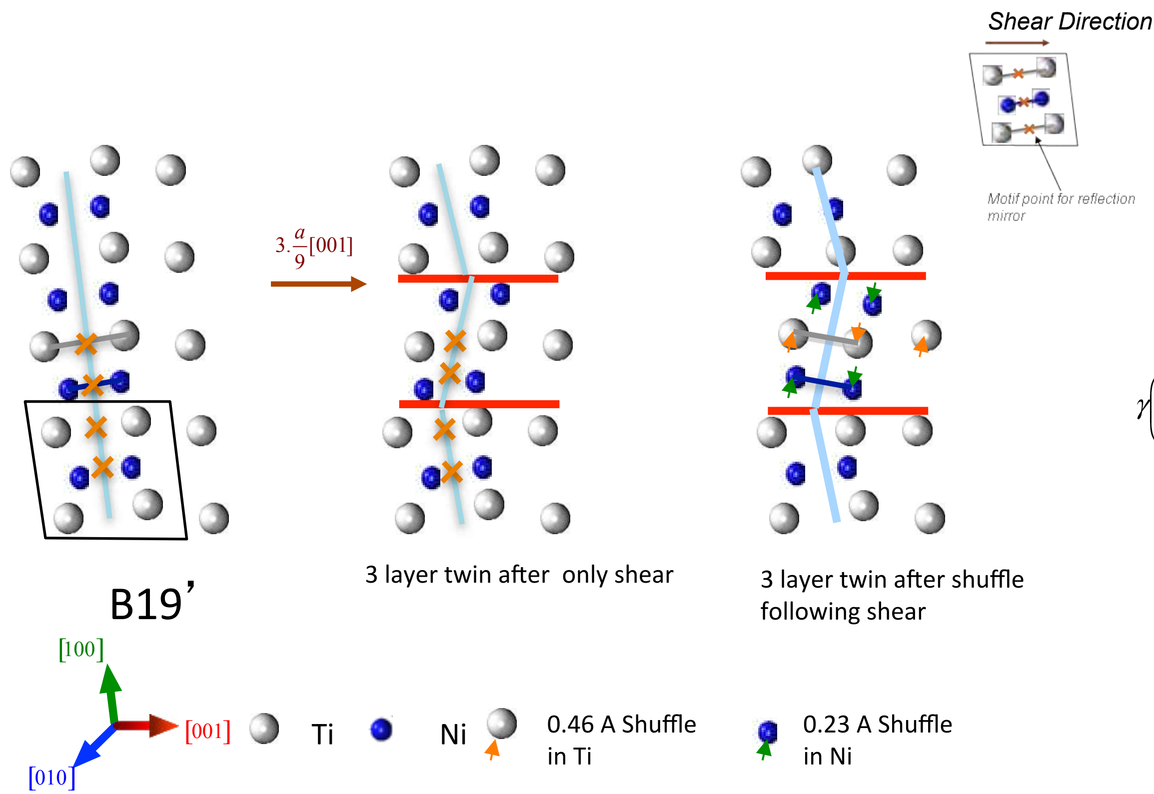


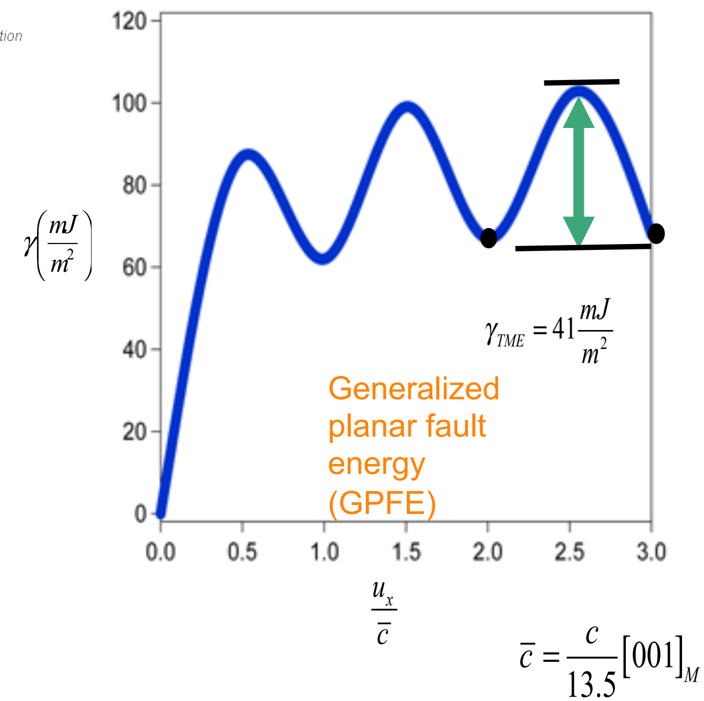


No Metastable Position,

Barrier too high

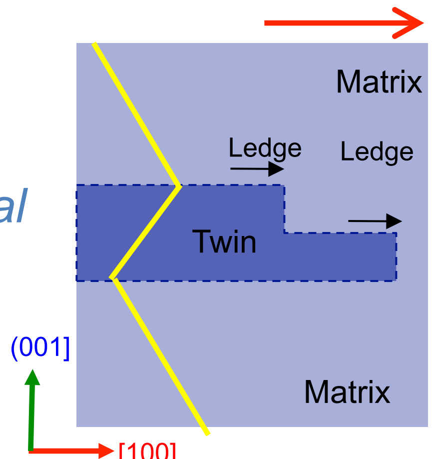
Energy Barrier of (100) Twin



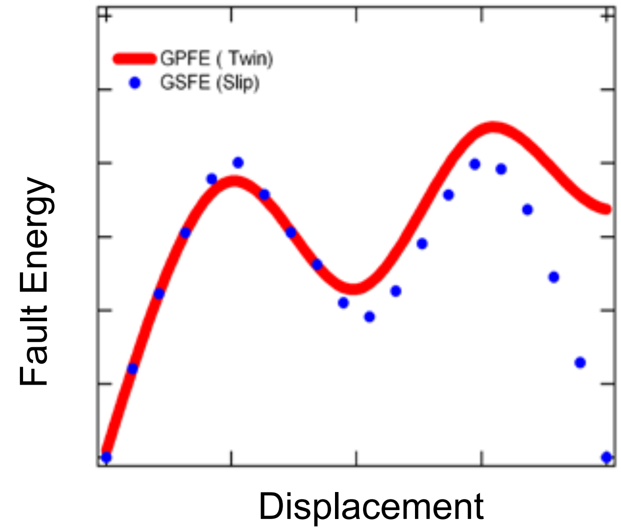


Two different Twin growth mechanism

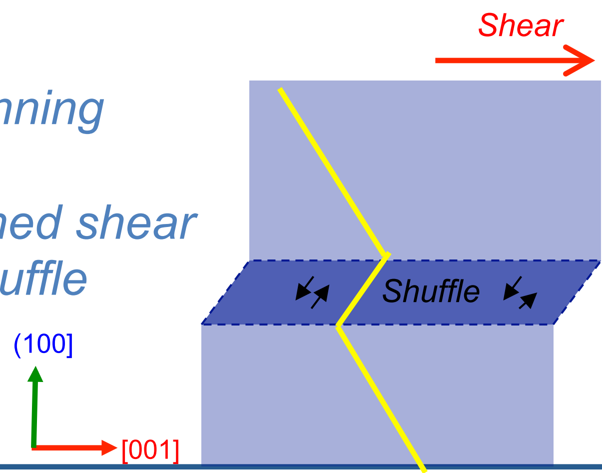
Aided by twinning partial

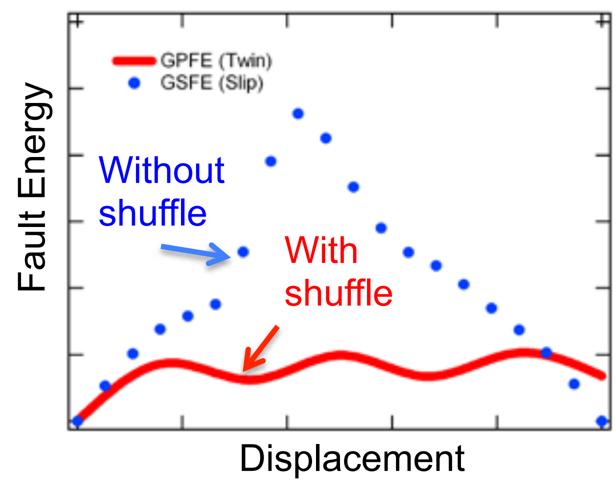


$$a[100] \rightarrow \frac{a}{2}[100] + \frac{a}{2}[100]$$

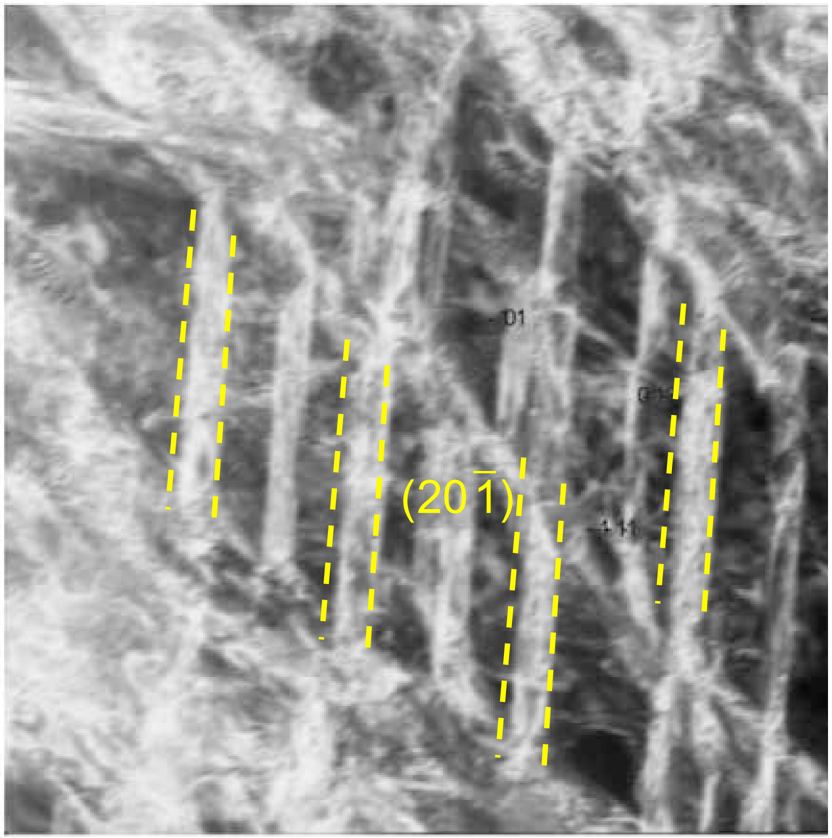


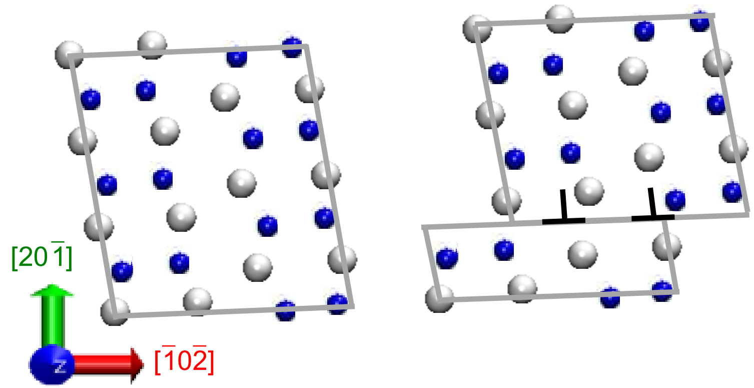
No twinning partial, combined shear and shuffle

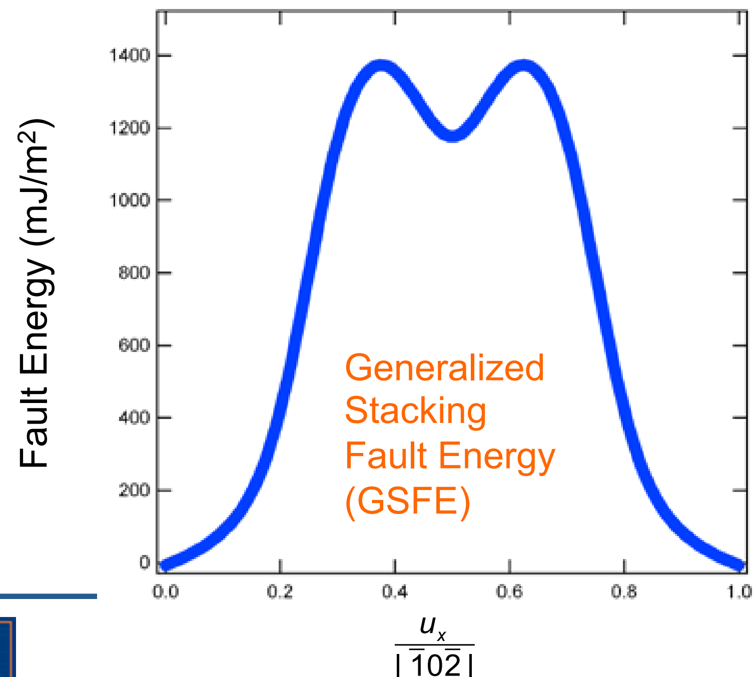




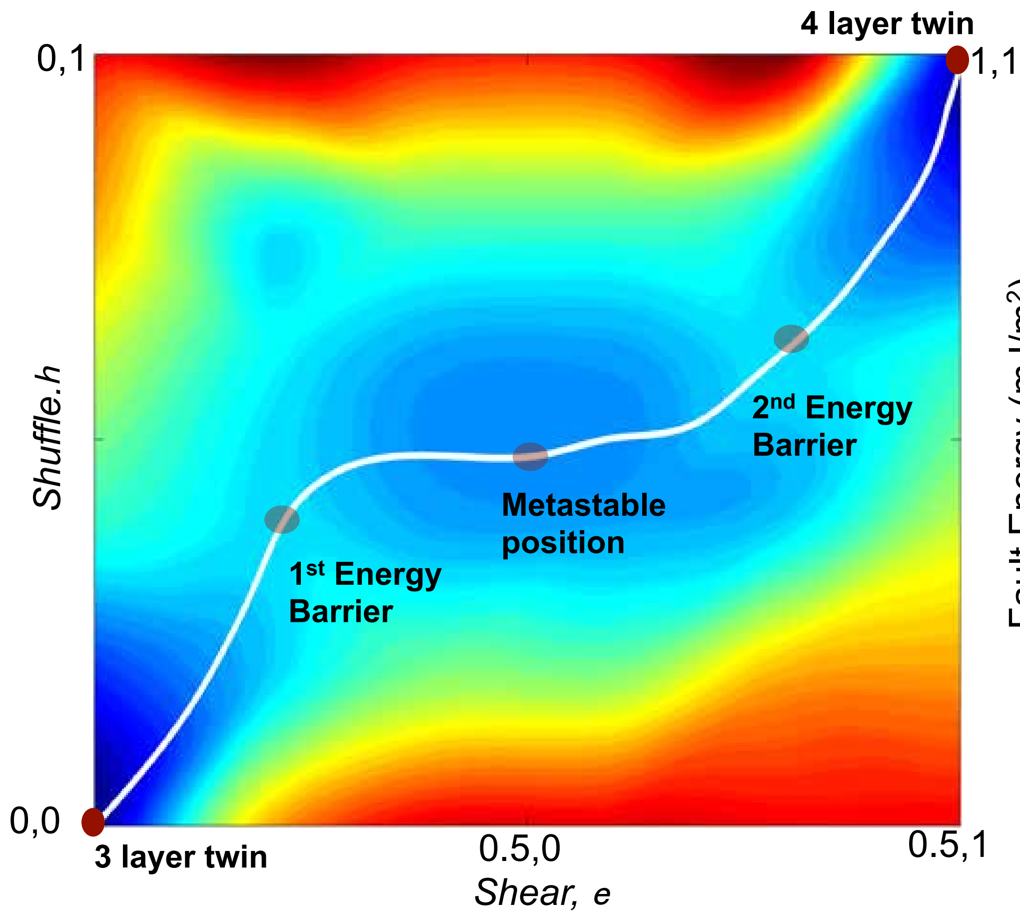
$(20\bar{1})$ Compound Twin

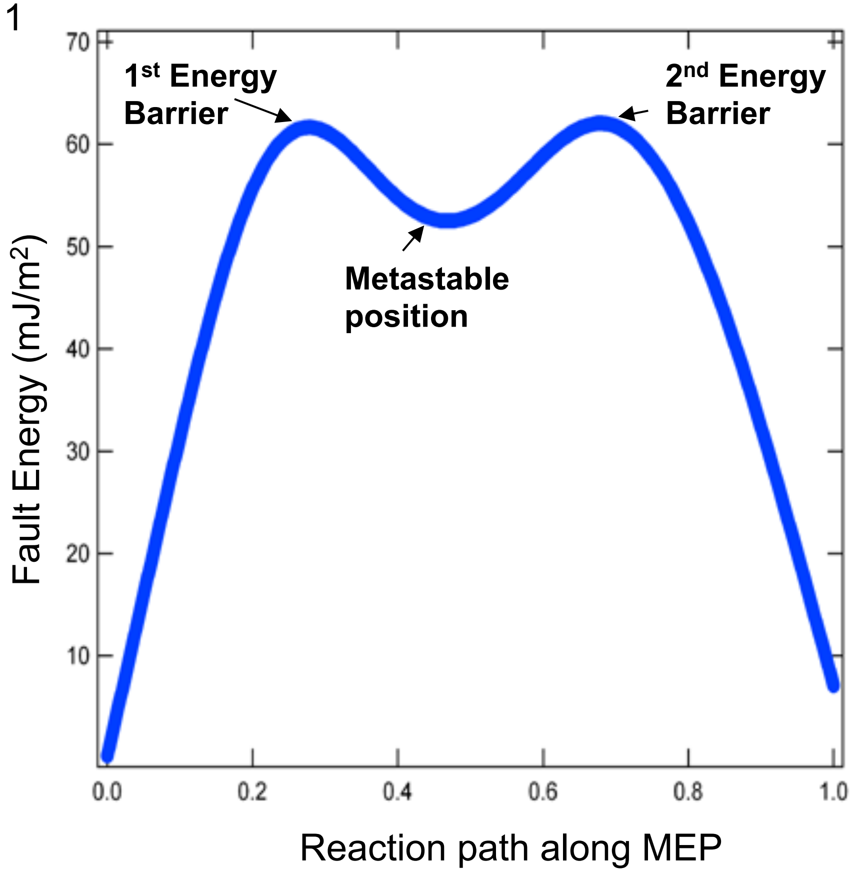






Energy Barrier of $(20\bar{1})$ Twin





Gives the exact coupling of Shear and shuffle

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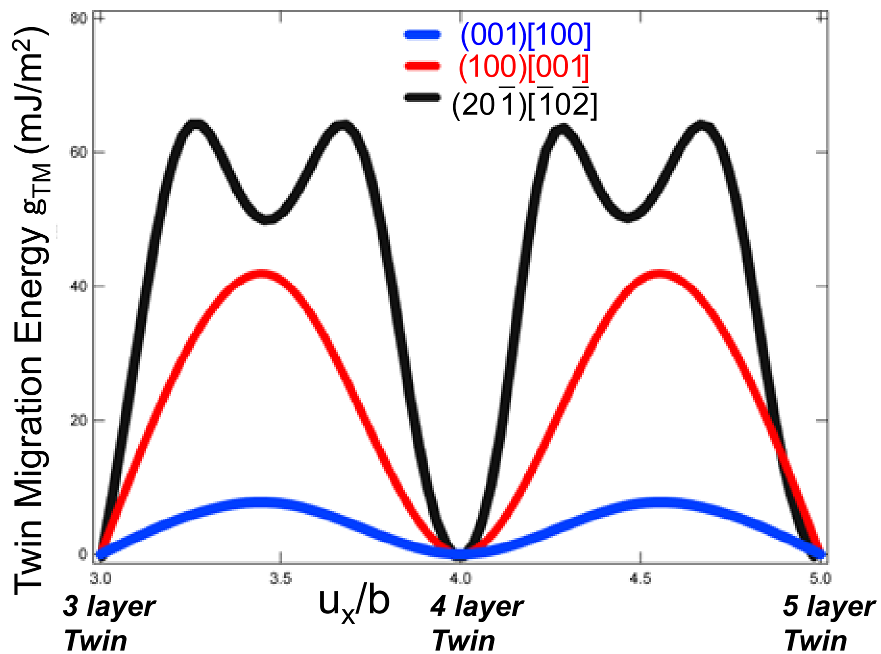
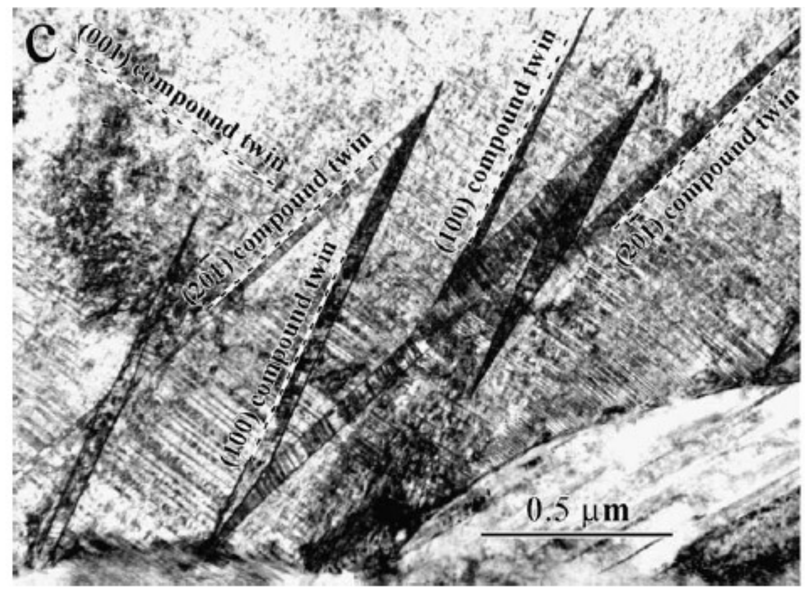
Computationally extensive!

(001), (100), $(20\bar{1})$ Compound Twins





Ishida et al., 2005

Twin growth stress is proportional to the twin migration energy

K_1	η_1	$(\tau_{shear})_{ideal} = \left.\frac{\delta\gamma}{\delta u_x}\right\|_{max}$ (MPa)	$\left(\tau_{TMideal} = \pi\{\gamma_{TM}/\bar{b}_{twin}\}\right)$ (MPa)
(001)	[100]	277	165
(100)	[001]	4530	1790
$(20\bar{1})$	$[\bar{1}0\bar{2}]$	107060	3900

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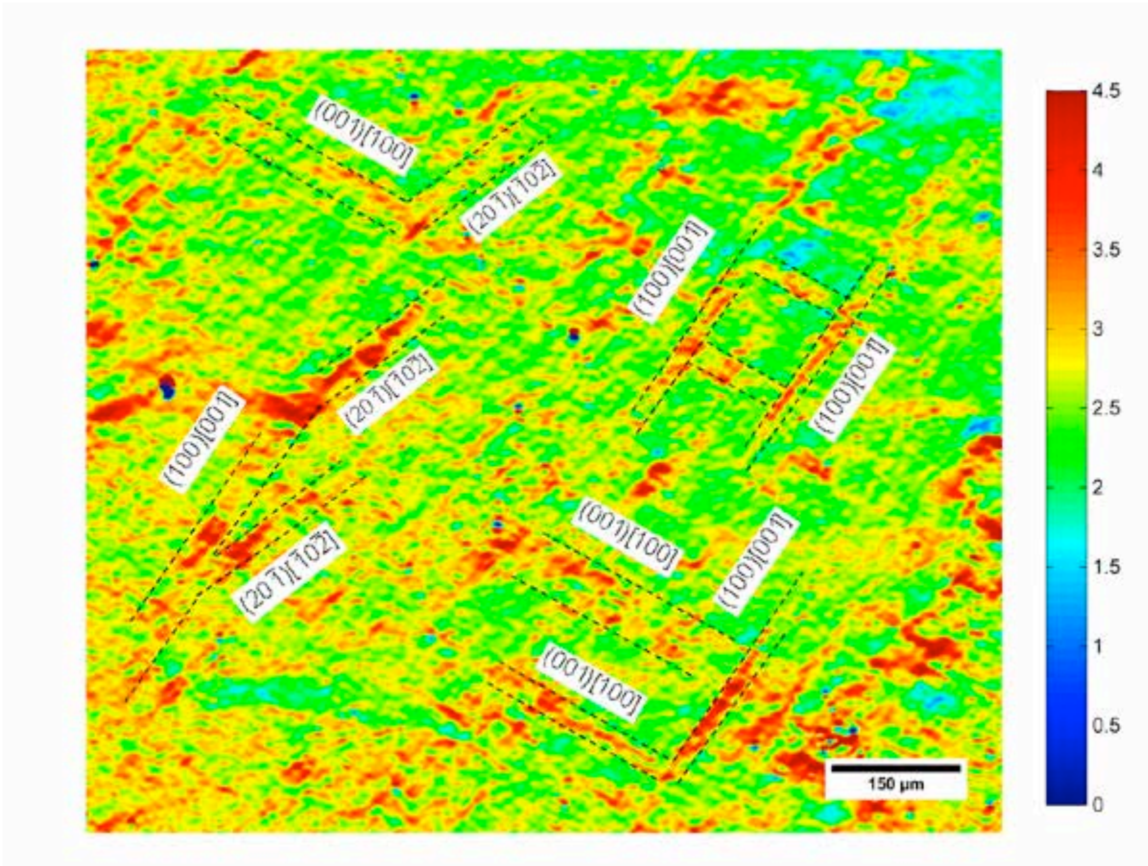
Digital Image Correlation Results displaying Multiple Twin Modes During Deformation of Martensite

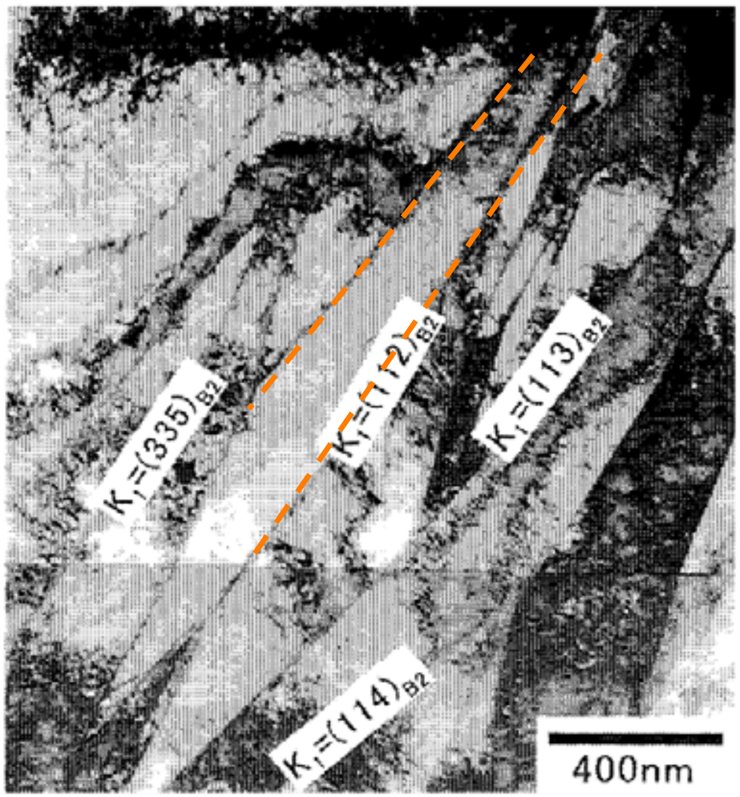


Outline

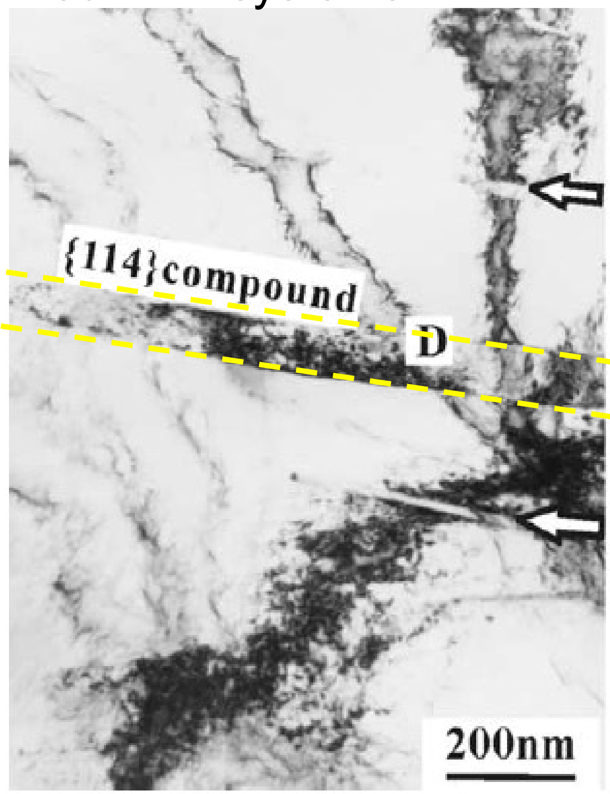
- Introduction to NiTi
  - Applications
  - Shape Memory Behavior
- Detwinning mechanism of Type II twin in Martensitic NiTi
- Compound twinning in Martensite (001), (100) and $(20\bar{1})$
- Twinning in Austenite, (112) and (114)

(112) and (114) Twin in Austenite

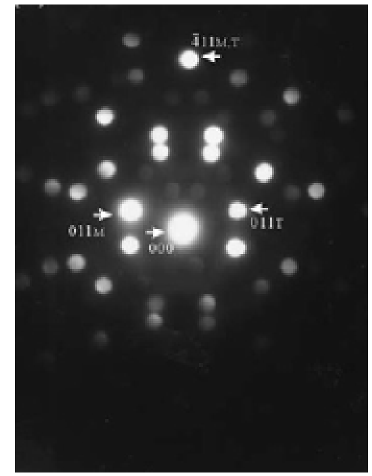
(112) And (114) are the mostly observed twin systems



(112) Twin

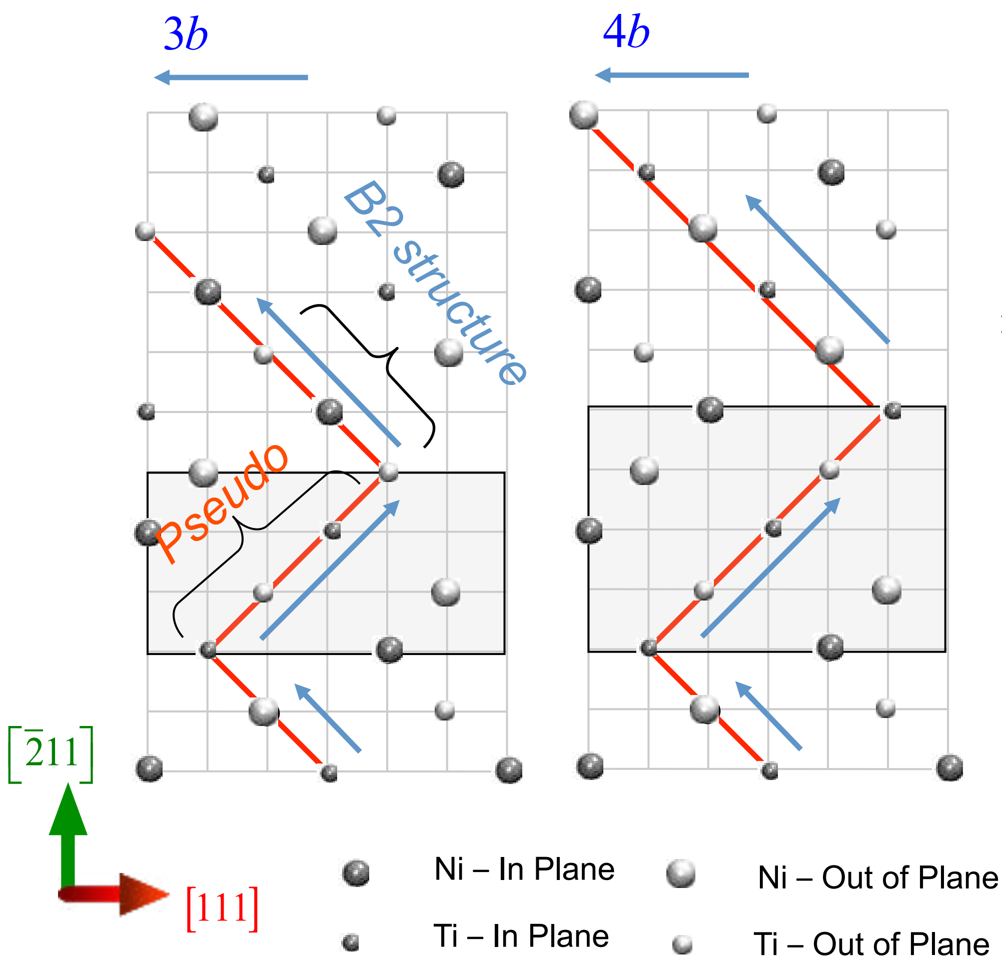


(114) Twin

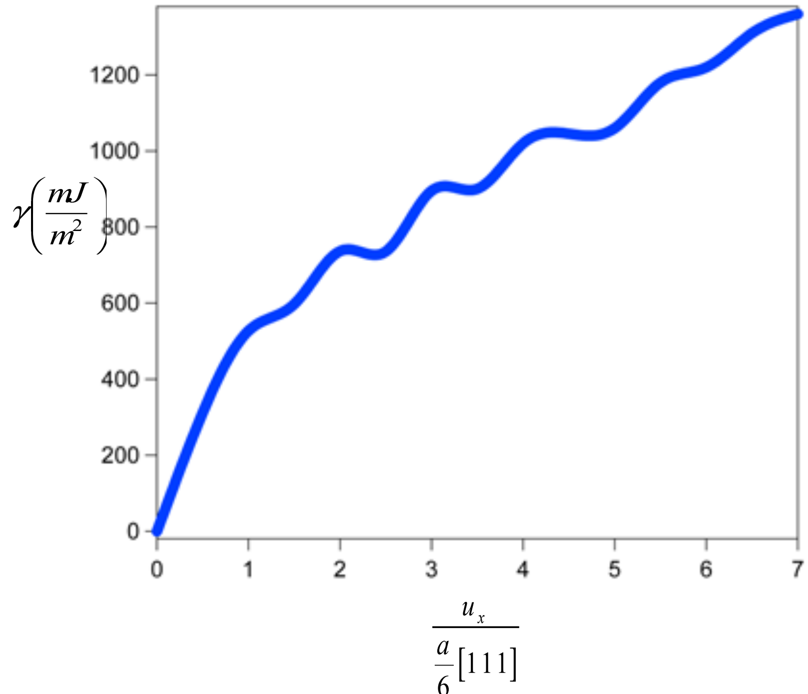


Nishida et al., 2003

(112) Pseudotwinning in B2 NiTi



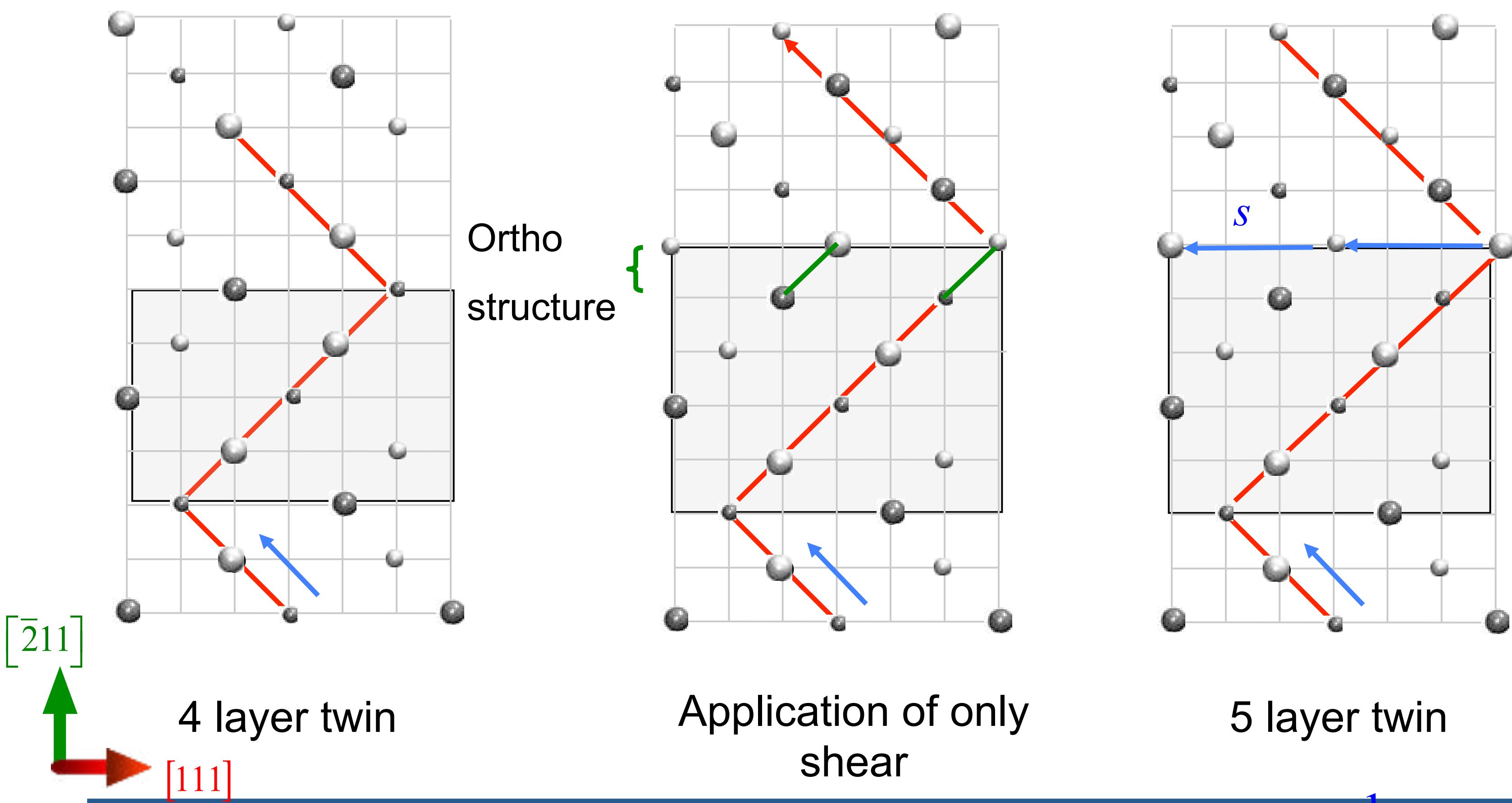
No metastable position, and labeled as 'impossible'.



Shear Magnitude $s = \frac{1}{\sqrt{2}}$

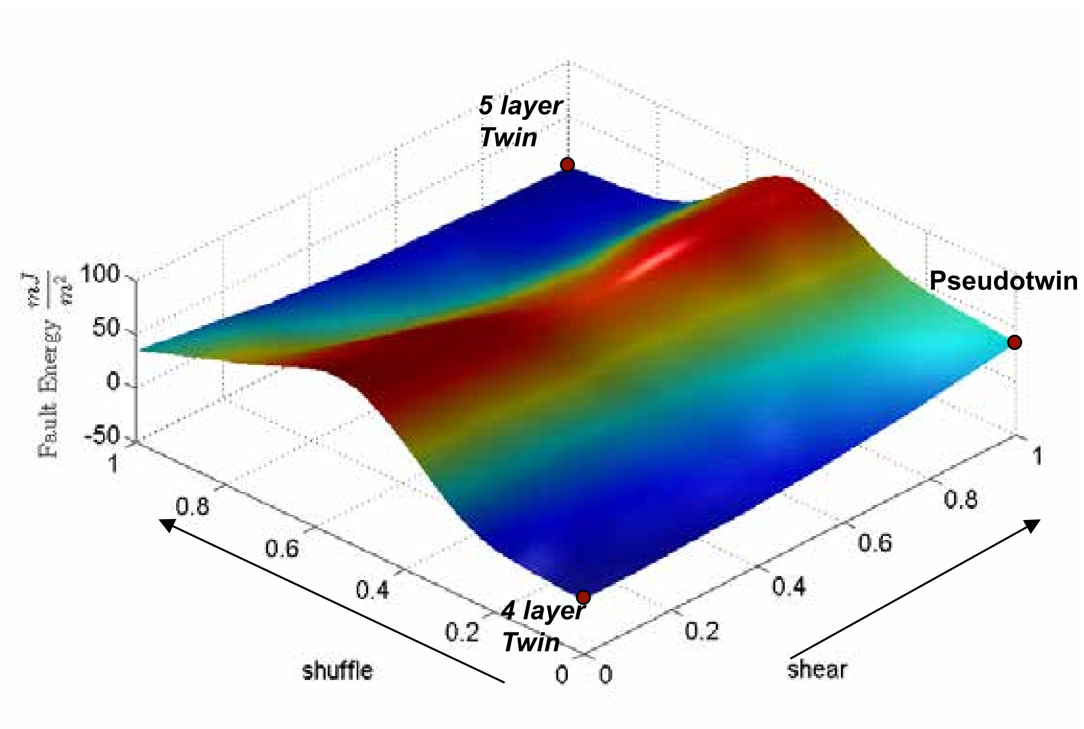
Shear Direction $b = a/6[111]$

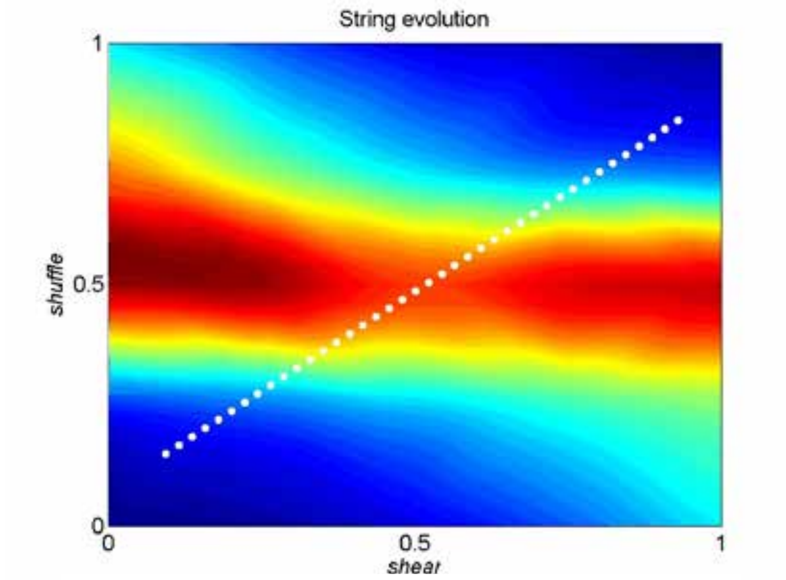
Coupled shear and shuffle mechanism during (112) twin growth

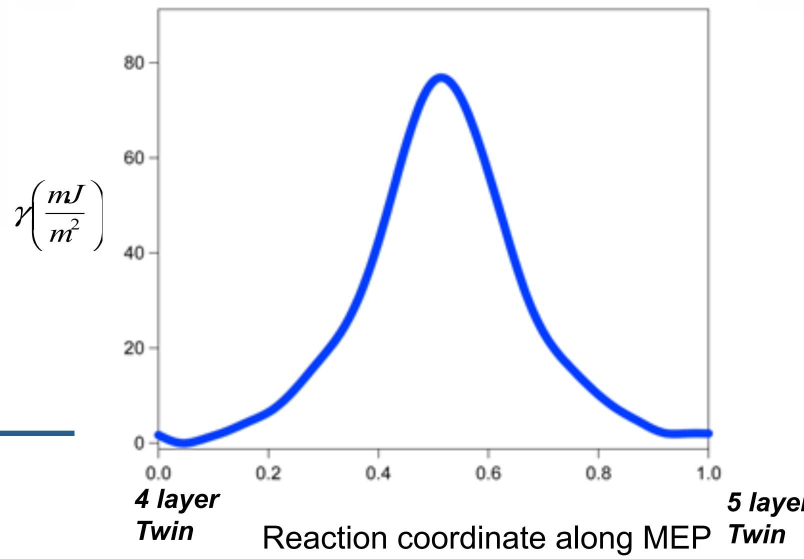


$$b = \frac{a}{6}[111] \quad s = \frac{1}{\sqrt{2}}$$

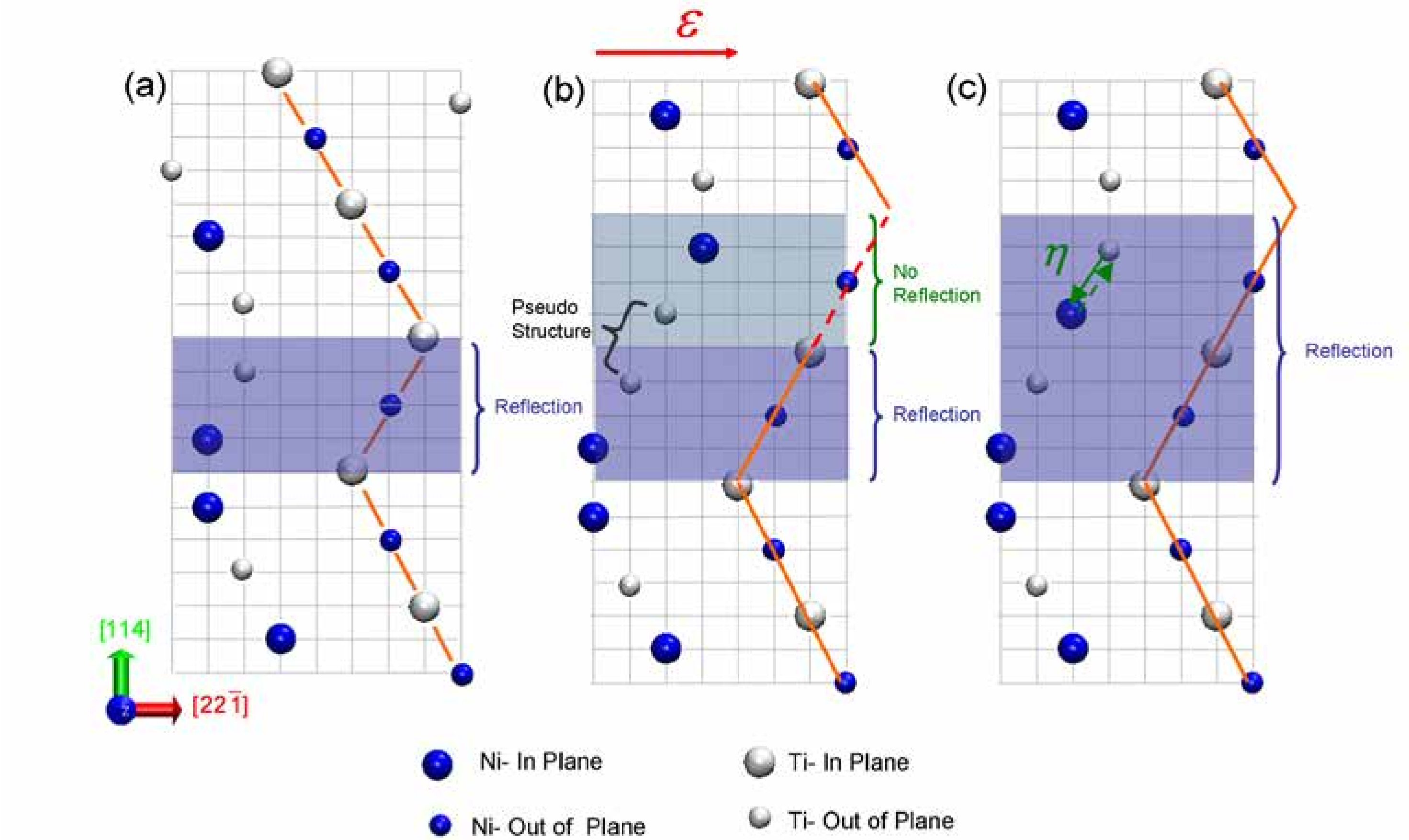
PES and MEP of (112) Twin



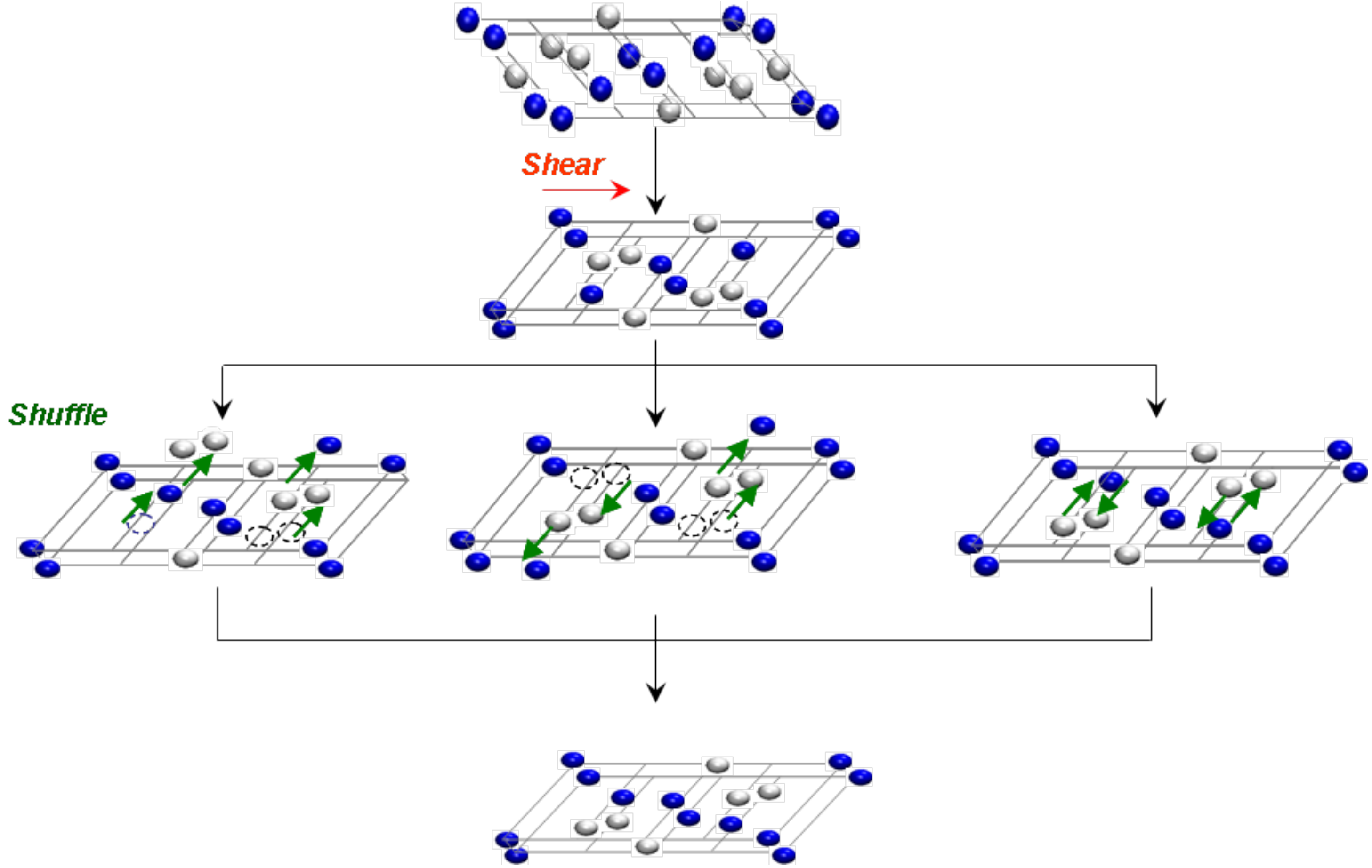




(114) Deformation Twin (B2)- The 'elusive' one

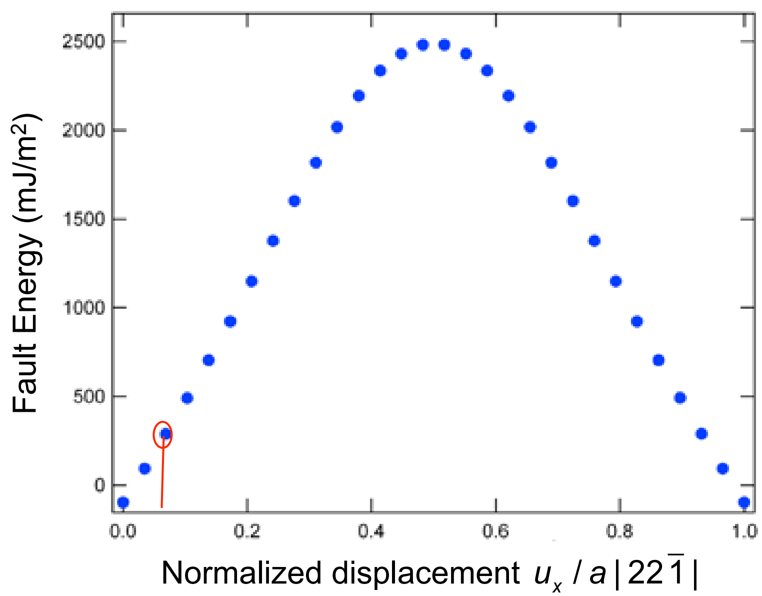


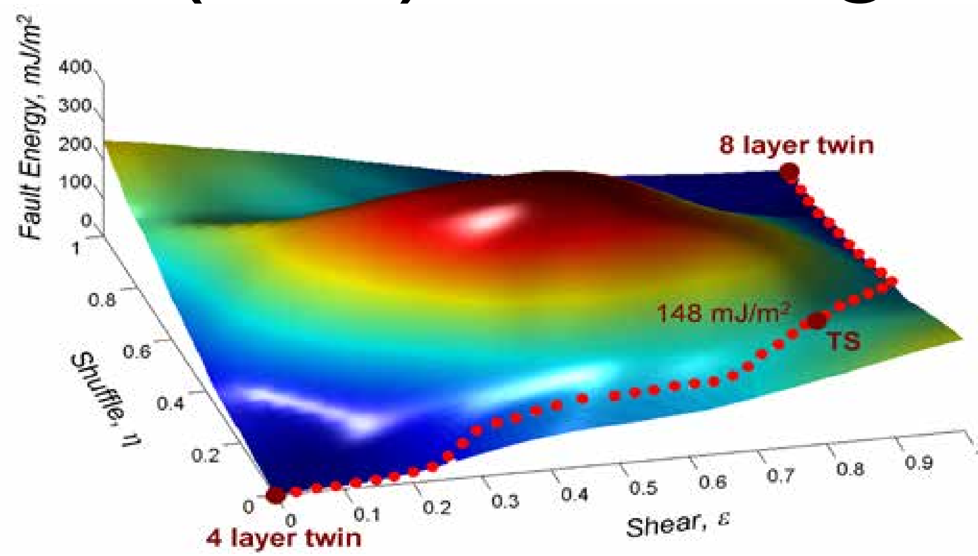
Different Shuffle Possibilities



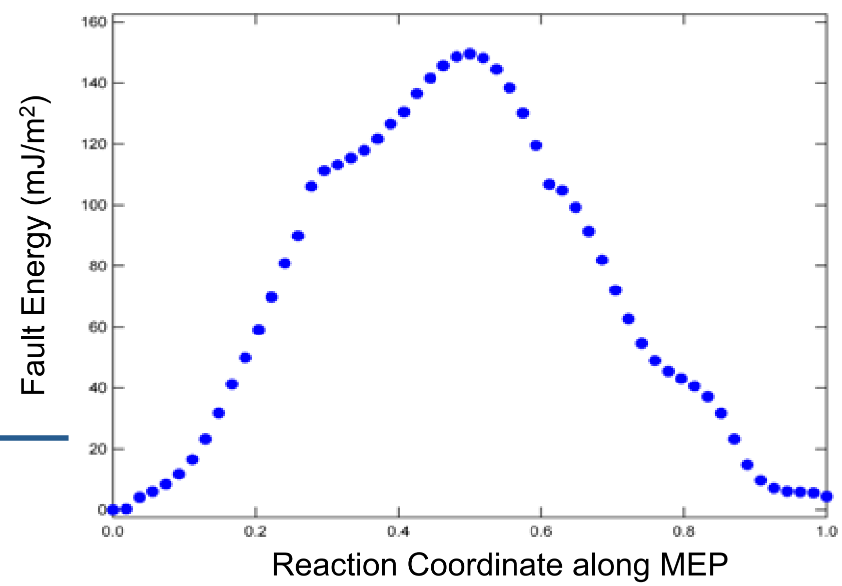
(114)$[22\bar{1}]$ Coupled shear-unidirectional shuffle (mJ/m^2)	(114)$[22\bar{1}]$ Coupled shear- bidirectional shuffle with perfect reflective boundary (mJ/m^2)	(114)$[22\bar{1}]$ coupled shear-bi directional shuffle with sharp boundary (mJ/m^2)	(114)$[22\bar{1}]$ Slip No reflection (mJ/m^2)
1210	610	148	2520

PES and MEP in (114) twinning

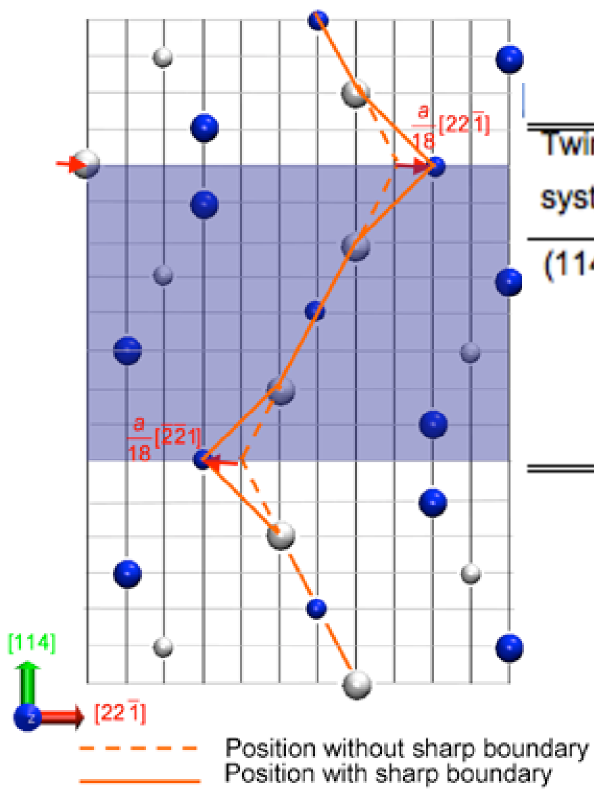




- No Energy well at $b = a/18[22\bar{1}]$
- Twinning combines shear and shuffle.
- Barrier energy of 148 mJ/m^2



Sharp Boundaries Further Lower the Energy Barriers



Twin shear system	Shear magnitude	Shuffle plane	Shuffle magnitude	Transition state	Boundary shift
(114)[22$\bar{1}$]	$1/\sqrt{2}$	(110)	$a/2<001>$	Normalized shear, ε =0.82† Normalized shuffle, η =0.22‡	$a/18[22\bar{1}]$ and $a/18[\bar{2}\bar{2}1]$

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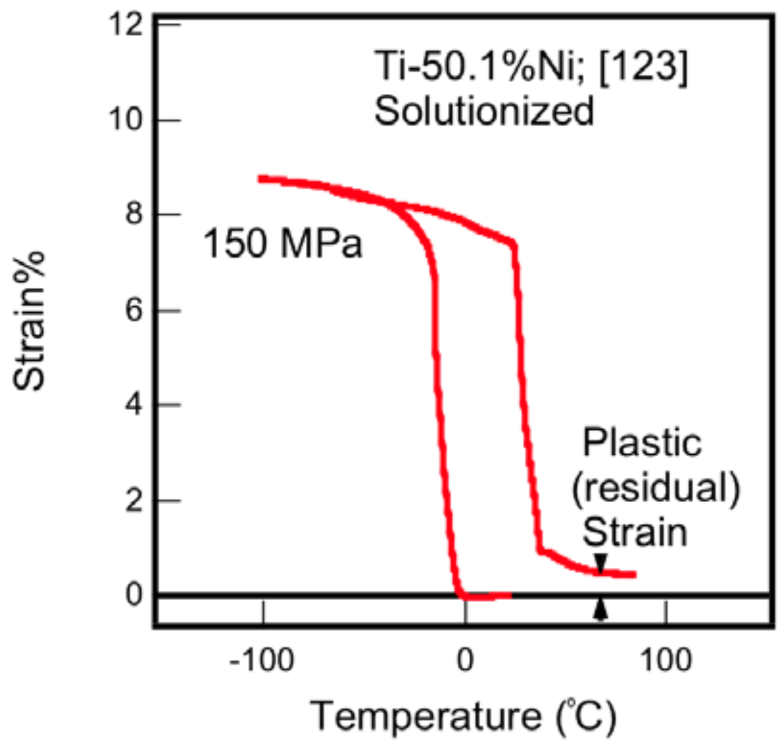
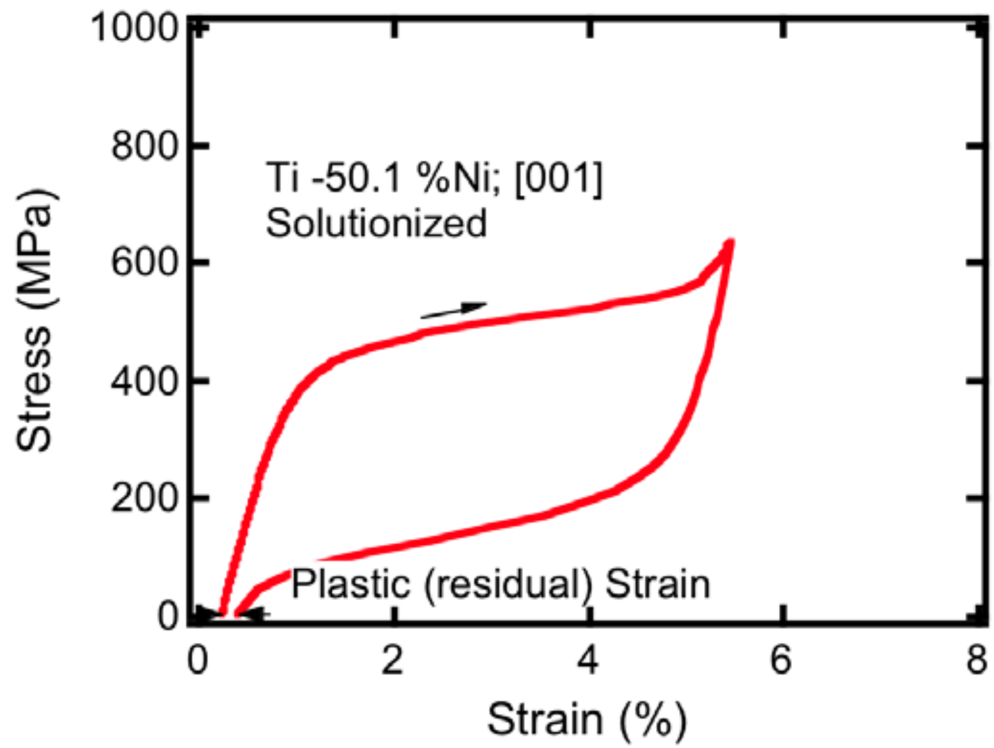
- Slip in B2 NiTi

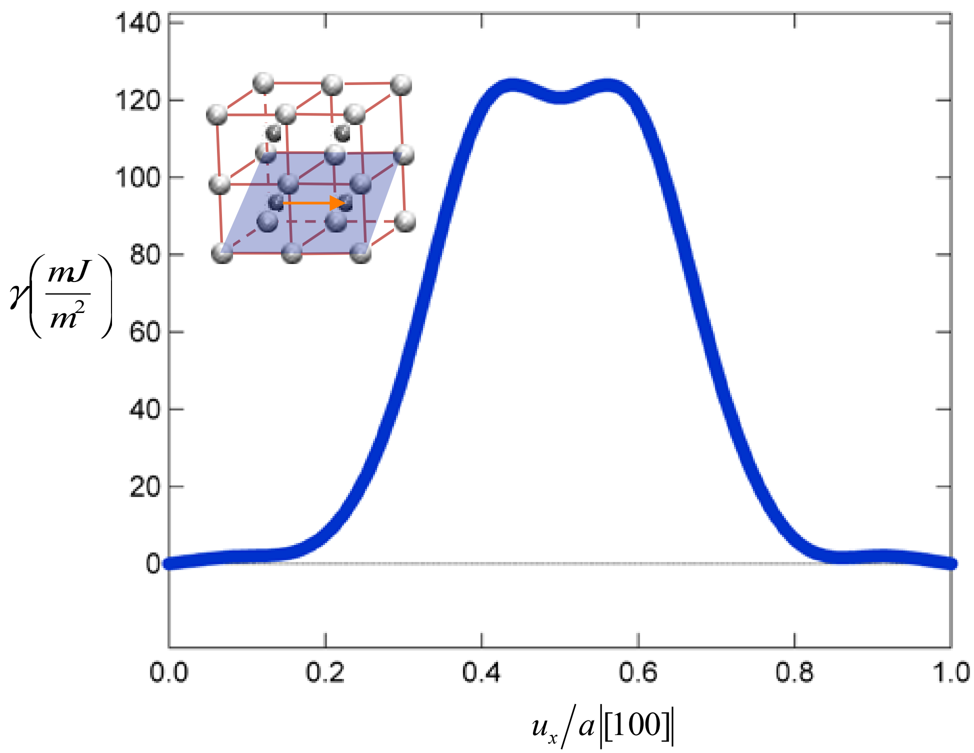
Consequence of Slip in Shape Memory





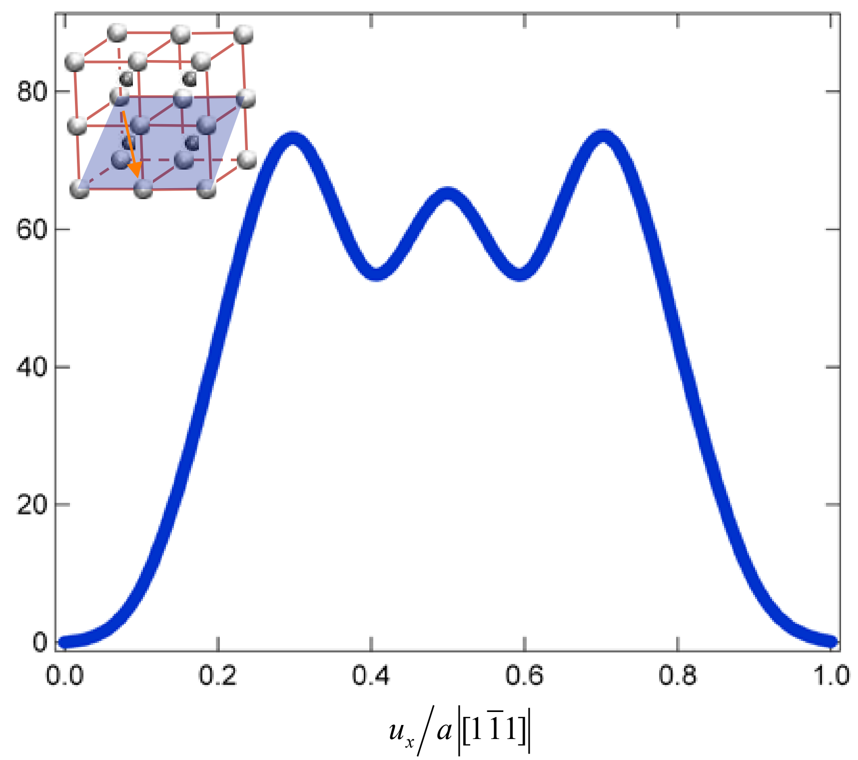
Slip Systems in B2 NiTi

(011)[100]

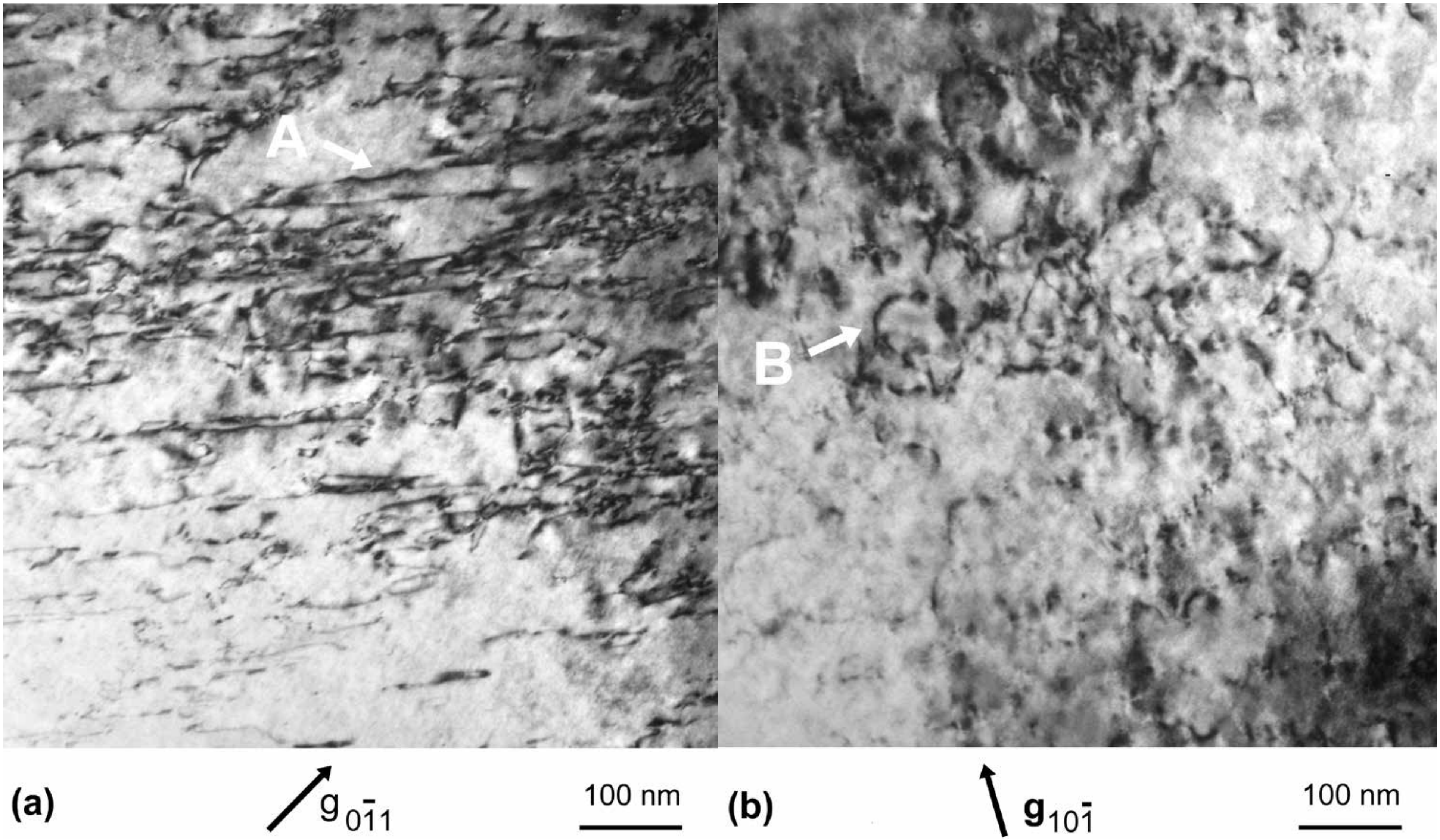


Most observed slip system in B2 NiTi, Chumlyakov, 2004, Norfleet et al., 2010, Delville et al. , 2010

(011)[1$\bar{1}$1]



Not presented in early work, lower barrier energy in (1-11) direction



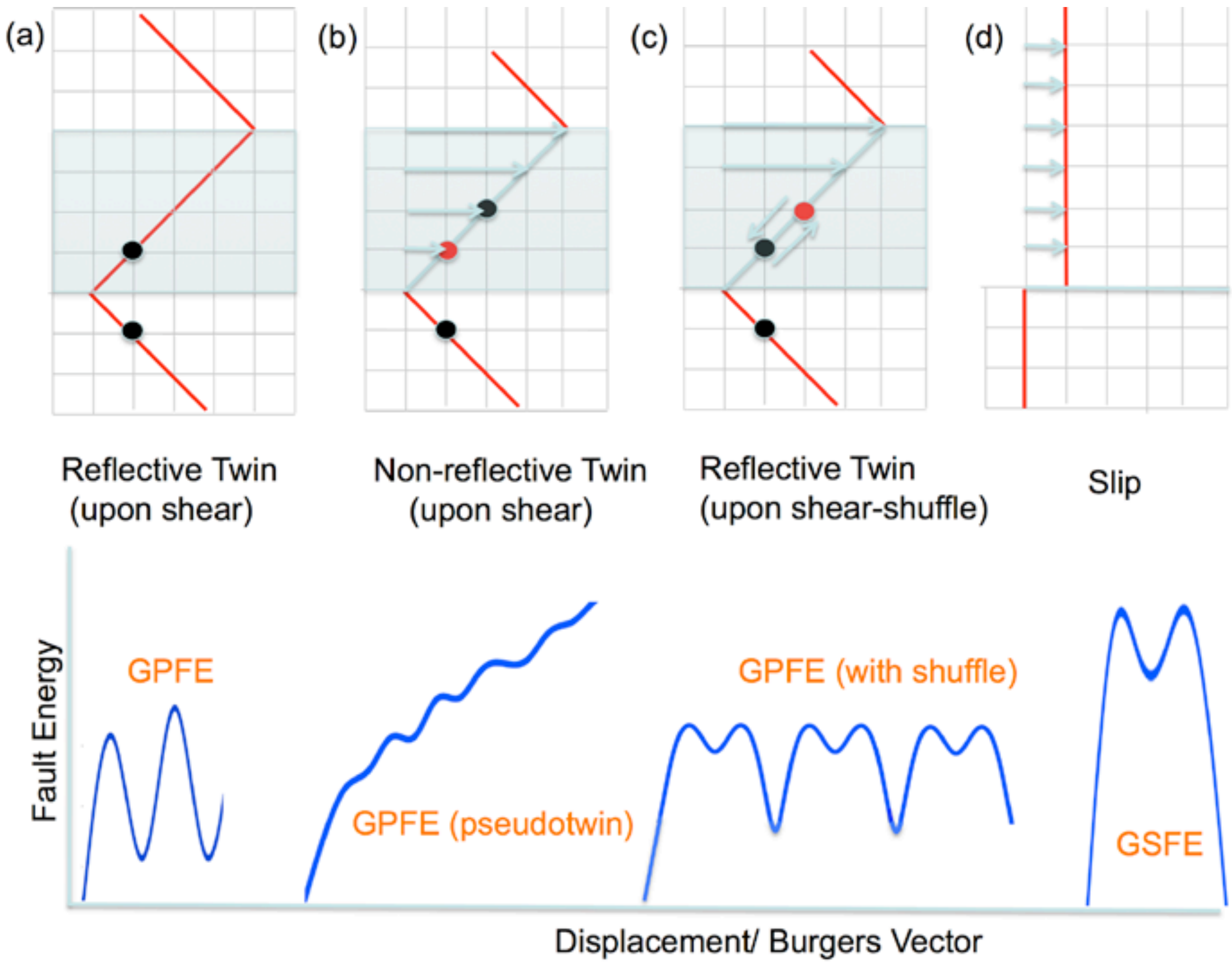
(011)[100]

(011)[1 $\bar{1}$ 1]

Summary of Slip Systems

Slip Plane	Slip Direction	$(\tau_{shear})_{ideal} = \left.\frac{\delta\gamma}{\delta u_x}\right\|_{\max}$ (MPa)
(011)	[100]	1034
(011)	$[1\bar{1}1]$	726
$(\bar{2}11)$	[111]	7430
(100)	[010]	9320

Summary



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Conclusions

- Twinning is favored over slip in the case B19' martensite (a key reason why shape memory works).
- Shuffles play a significant role in Type II-1, (100), $(20\bar{1})$ twinning in martensite.
- (112) and (114) twinning in B2 NiTi has to overcome much lower barrier with shear and shuffle with comparable
- $[1\bar{1}1](011)$ slip has been shown to be significant in B2 NiTi along with [100](011) slip both with experiments and simulations.

Thank You