Modeling of Twinning Stress

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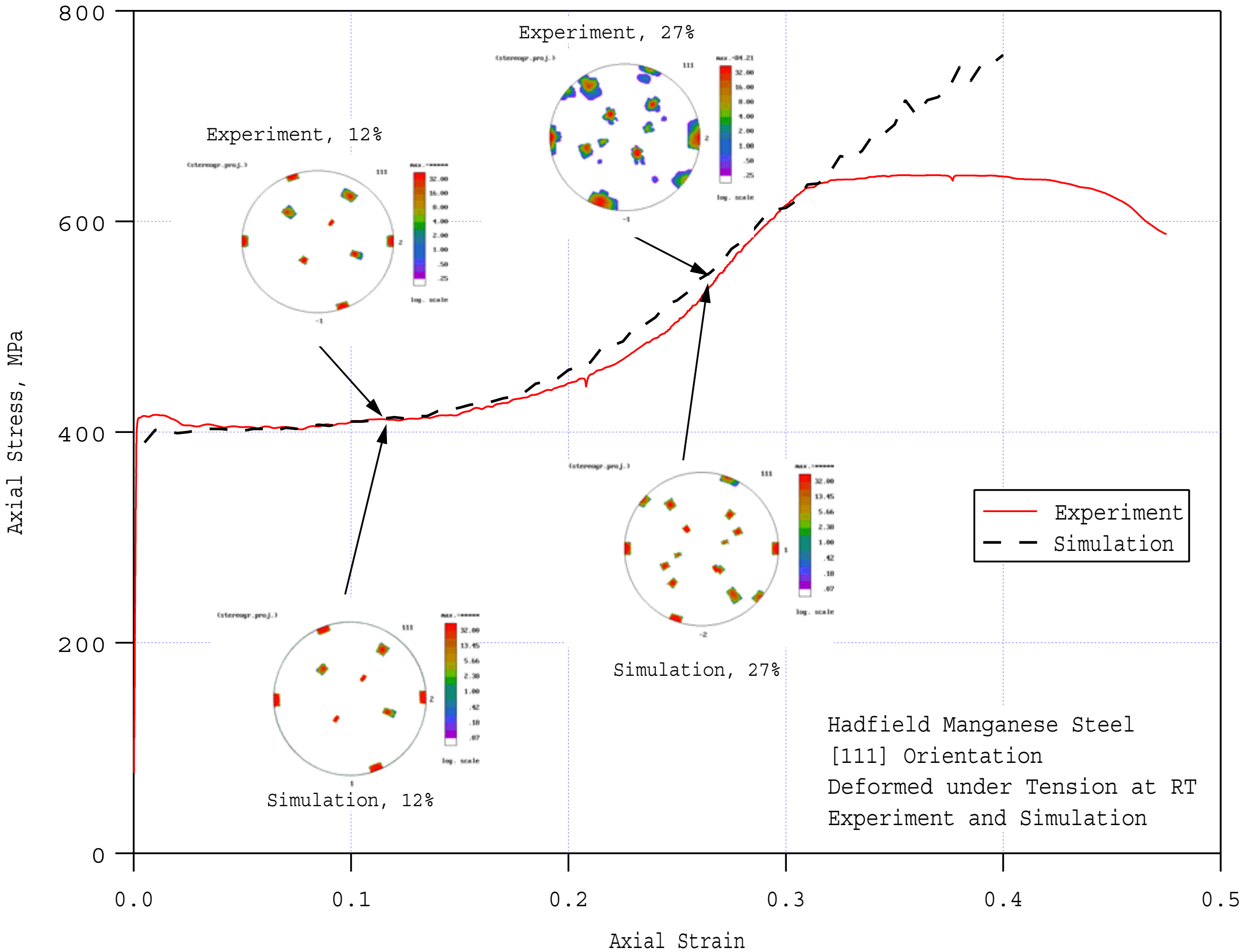
Presentation in honor of Prof. Alan Needleman, SES Meeting, August 14-16, 2006

Presentation Outline

- The need for a Twinning (nucleation) Stress Model
- Previous Twinning Models
- Fault Energies from DFT (Density Functional Theory)
- Twin Nucleus as 3-layers
- Energy Minimization (the Cu-Al example)
- Anti-twinning
- Conclusions

Hadfield Steel (fcc Fe-Mn-C steel)- [111] Orientation

twinning stress



I. Karaman, H. Sehitoglu,A. Beaudoin, Y.Chumlyakov, H.J.Maier, C. Tome, Acta Mat. 48 (2000) 2031-2047
I.Karaman, H. Sehitoglu,K.Gall, Y. Chumlyakov, H.J. Maier, Acta Mat. 48 (2000) 1345-1359

The twinning (nucleation) stress is currently obtained from experiments. A theory to obtain this quantity from first principles (for metals and alloys) is needed.

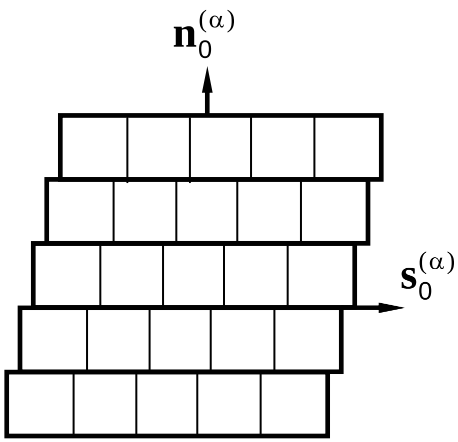
Twin Nucleation Stress

Nucleation Criteria used in Crystal Plasticity Models

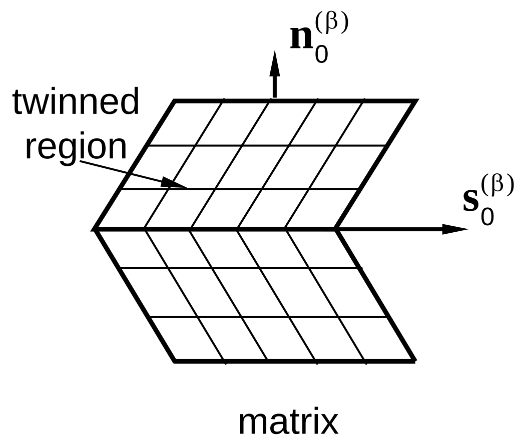
$$\frac{df^{(\beta)}}{dt} \geq 0 \qquad \text{if } \tau_{twin}^{(\beta)}\left(\Sigma, f^{(\beta)}\right) = \tau_{crit-twin}^{(\beta)}\left(f^{(\beta)}\right)$$

The twin volume fraction evolves when the resolved shear exceeds the twinning nucleation stress.

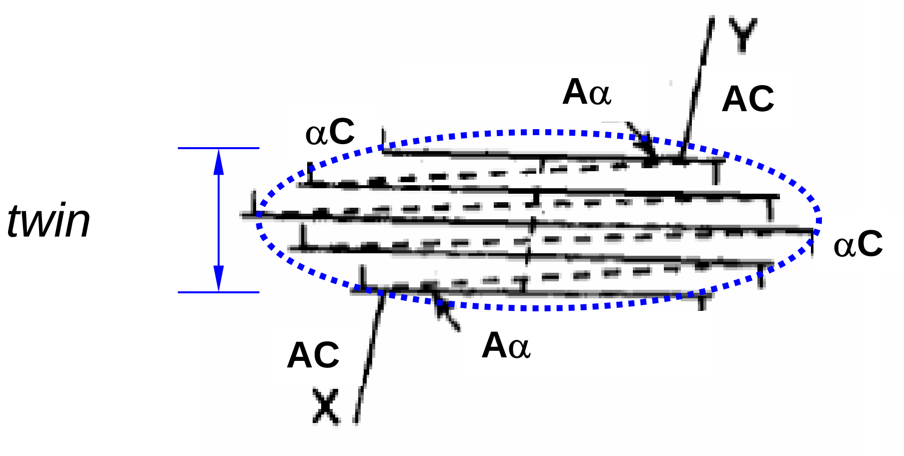
Deformation by slip



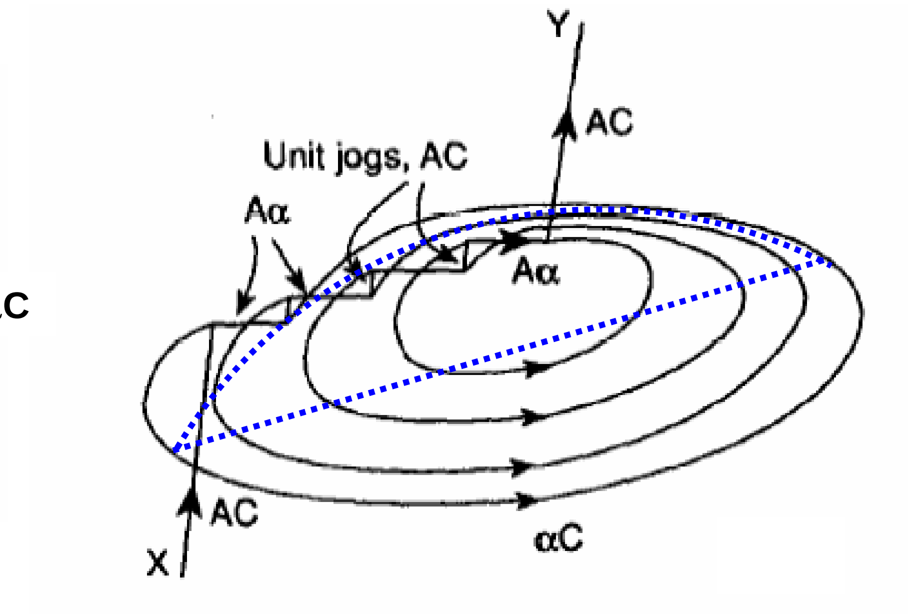
Deformation by twinning



Classical twin nucleation models for fcc alloys (contd.)



lenticular twin

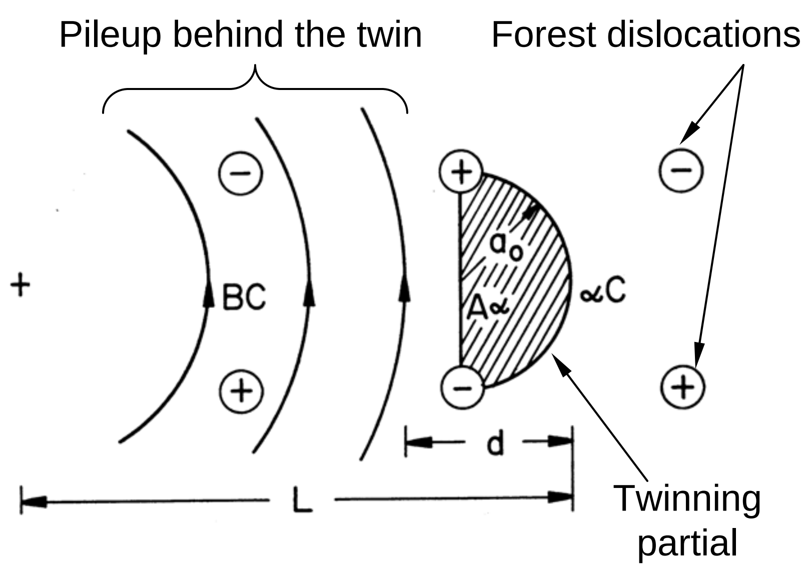


plano-convex twin

Pole mechanism for formation of a deformation twin

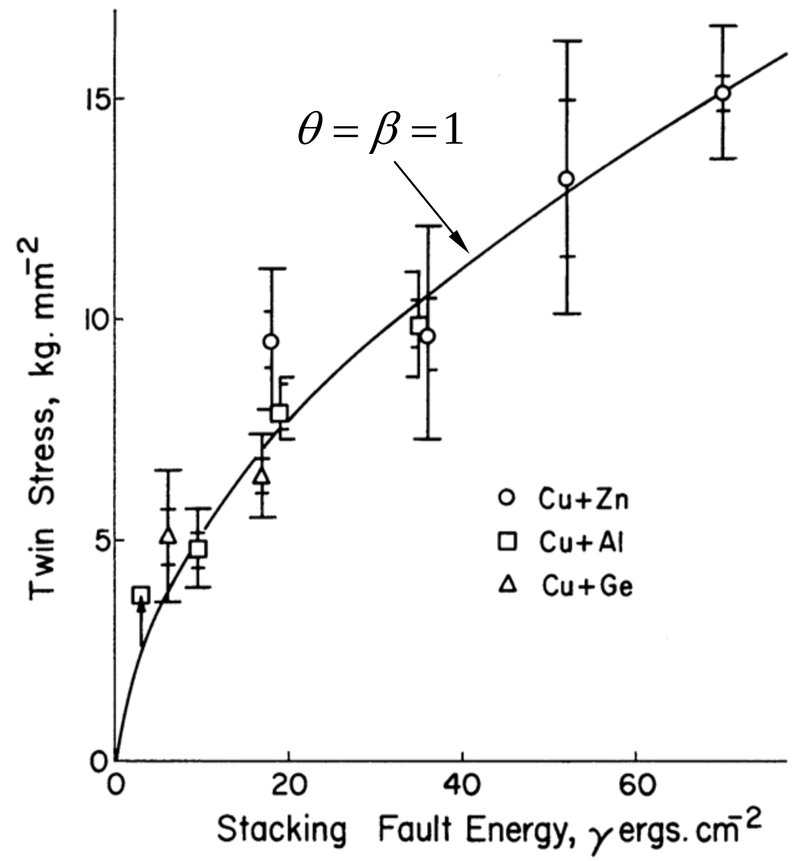
Venables, Deformation Twinning, Eds. Reed-Hill,Hirth and Rogers (1964)

Classical twin nucleation models (contd.)



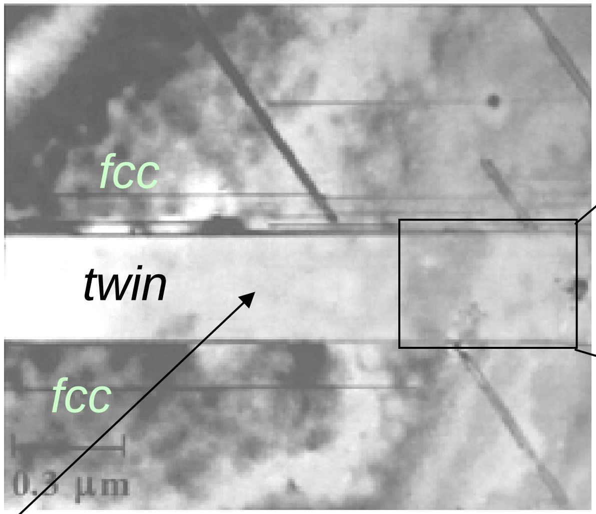
$$n\tau_{crit} = \frac{\gamma_{isf}}{b_p} + \frac{Gb}{2a_0}$$

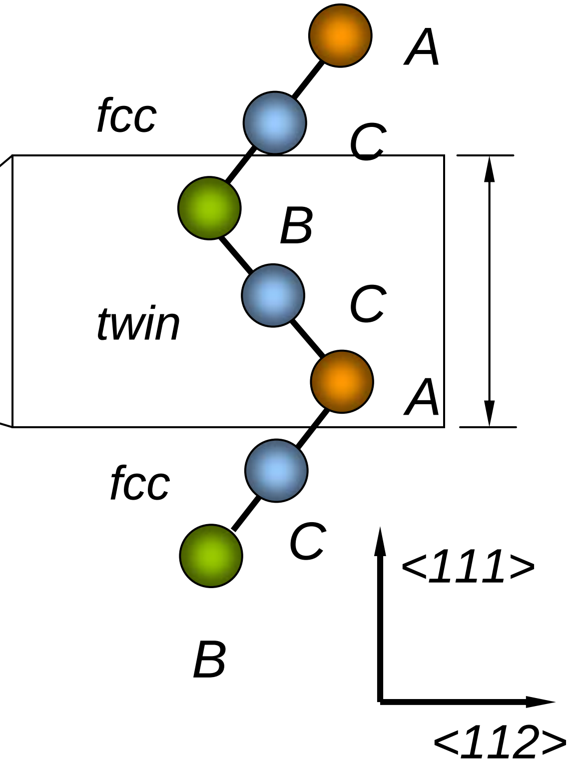
$$\left[\left(\frac{1-2\theta}{2\beta}\right) + K\theta^2\tau_{crit}\right]\tau_{crit} = \frac{\gamma_{isf}}{b_p}$$



Venables, Deformation Twinning, Eds. Reed-Hill,Hirth and Rogers (1964)

Lattice structure of deformation twins in fcc alloys

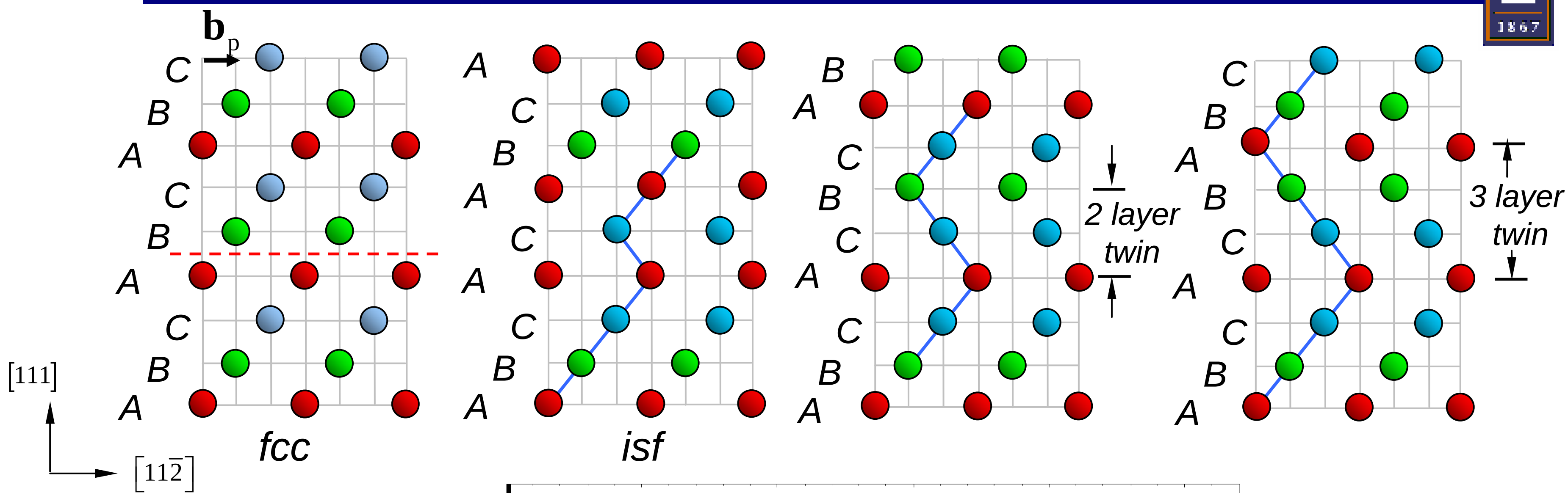


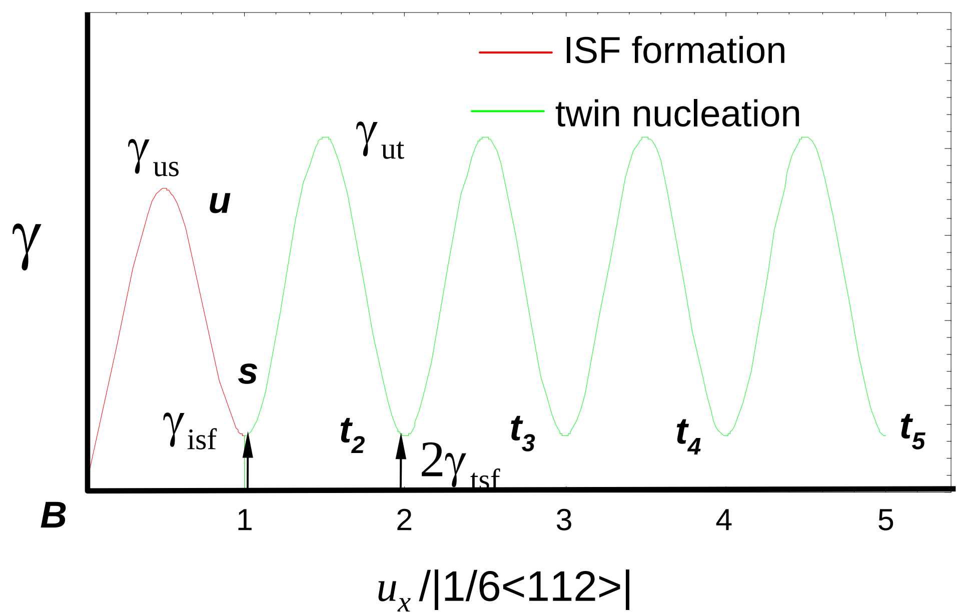


Deformation twin in Hadfield steel
[001] orientation 3% strain

I. Karaman, H. Sehitoglu, K. Gall, Y. I. Chumlyakov and H. J. Maier, Acta Mater.(2000).

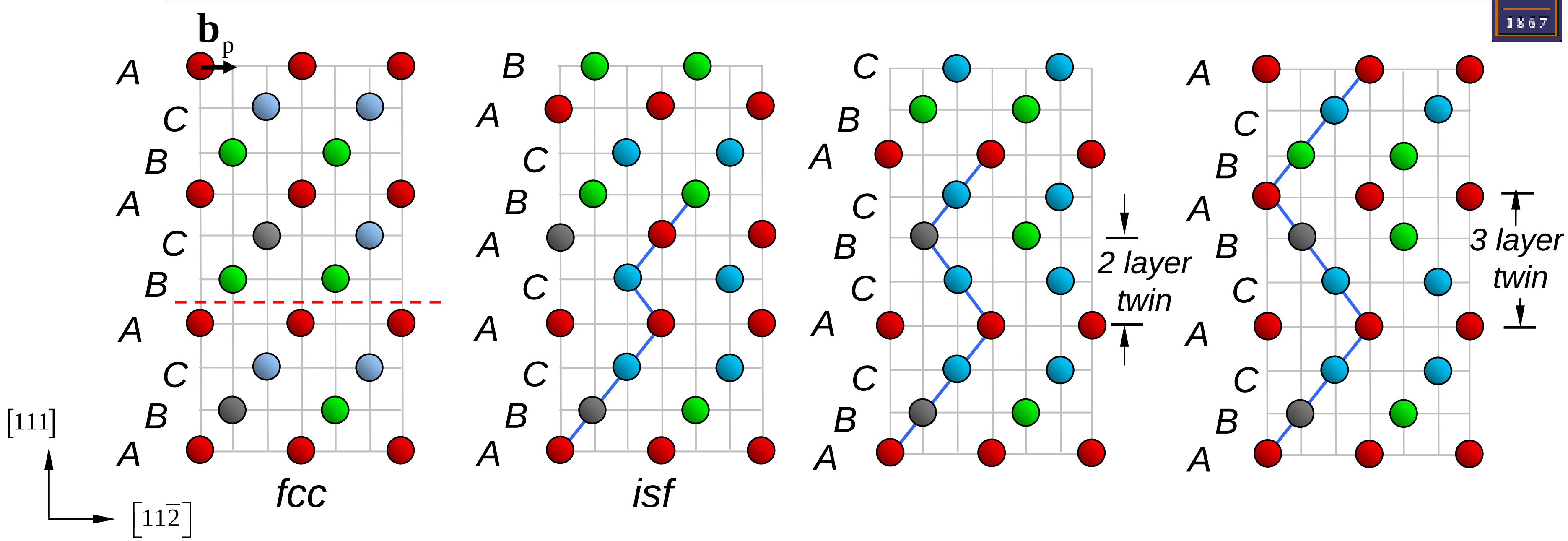
Generalized planar fault energy (GPFE) curve





Kibey, Liu, Curtis, Johnson, Sehitoglu Acta Mater. 54 (2006) 2991-3001

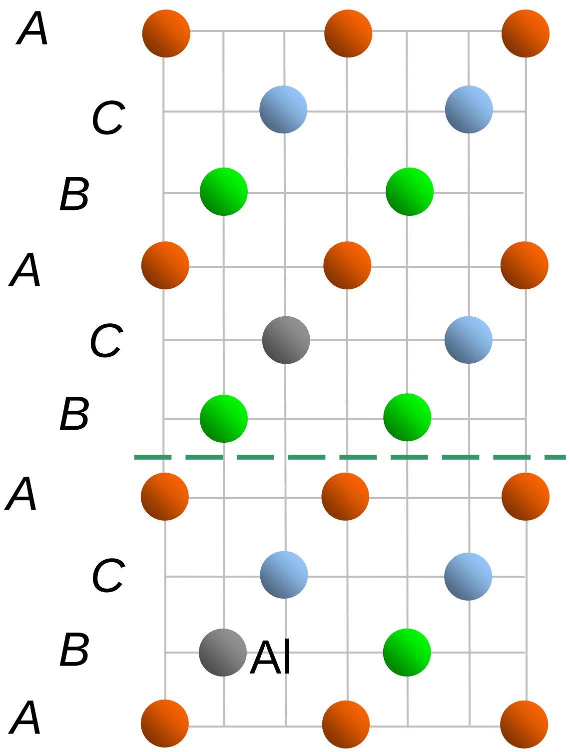
Formation of multi-layer twins in Cu-5.0%Al

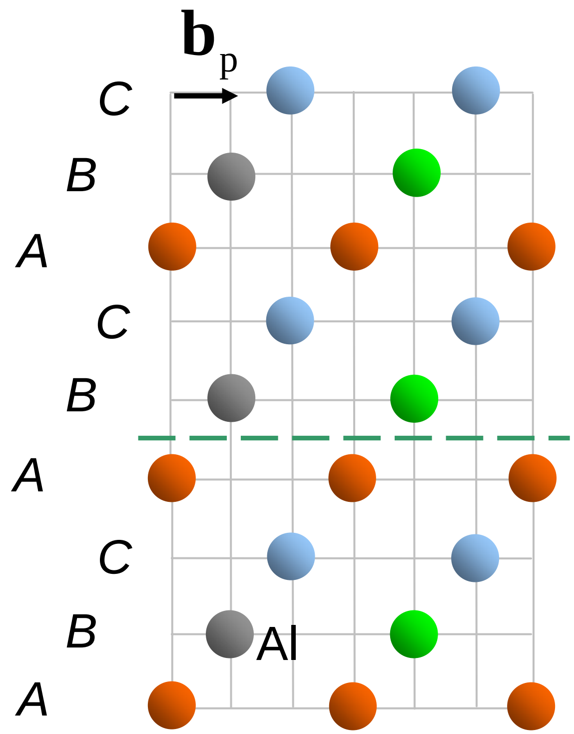


Twining in Cu-5.0at.%Al

Passage of 1/6<112> Shockley partials to produce 2 and 3 layer twins successively. The selected Al atom positions in the layers 2 and 6 within the 10 layer supercell permit a continuous shear to generate multiple twins with high symmetry.

Converged supercell sizes for Cu-xAl



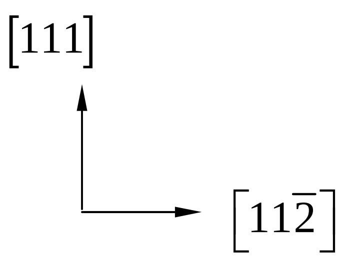


Cu-5.0at.%Al

10 layer supercell

Cu-8.3at.%Al

9 layer supercell



- VASP-PAW-GGA
- 8 x 8 x 4 k-point mesh with 273.2 eV energy cutoff.

VASP-PAW fault energies for Cu-xAl

	a_0(Å)	γ_{us}	γ_{isf}	γ_{ut}	$2\gamma_{tsf}$	δ_{us}^{ut}	T
Cu	3.64	181	41	200	40	19	1.05
	(3.61)[a]	180[b]	(45)[c]	210[b]	(48)[a]		
Cu-5.0at.%Al	3.65	170	20	179	32	9	1.09
	(3.6364)[d]	–	(20)[a]	–	(34)[a]		
Cu-8.3at.%Al	3.65	169	7	176	11	7	1.11
	(3.6466)[d]	–	(9)[a]	–	–		

all energies in mJ/m^2

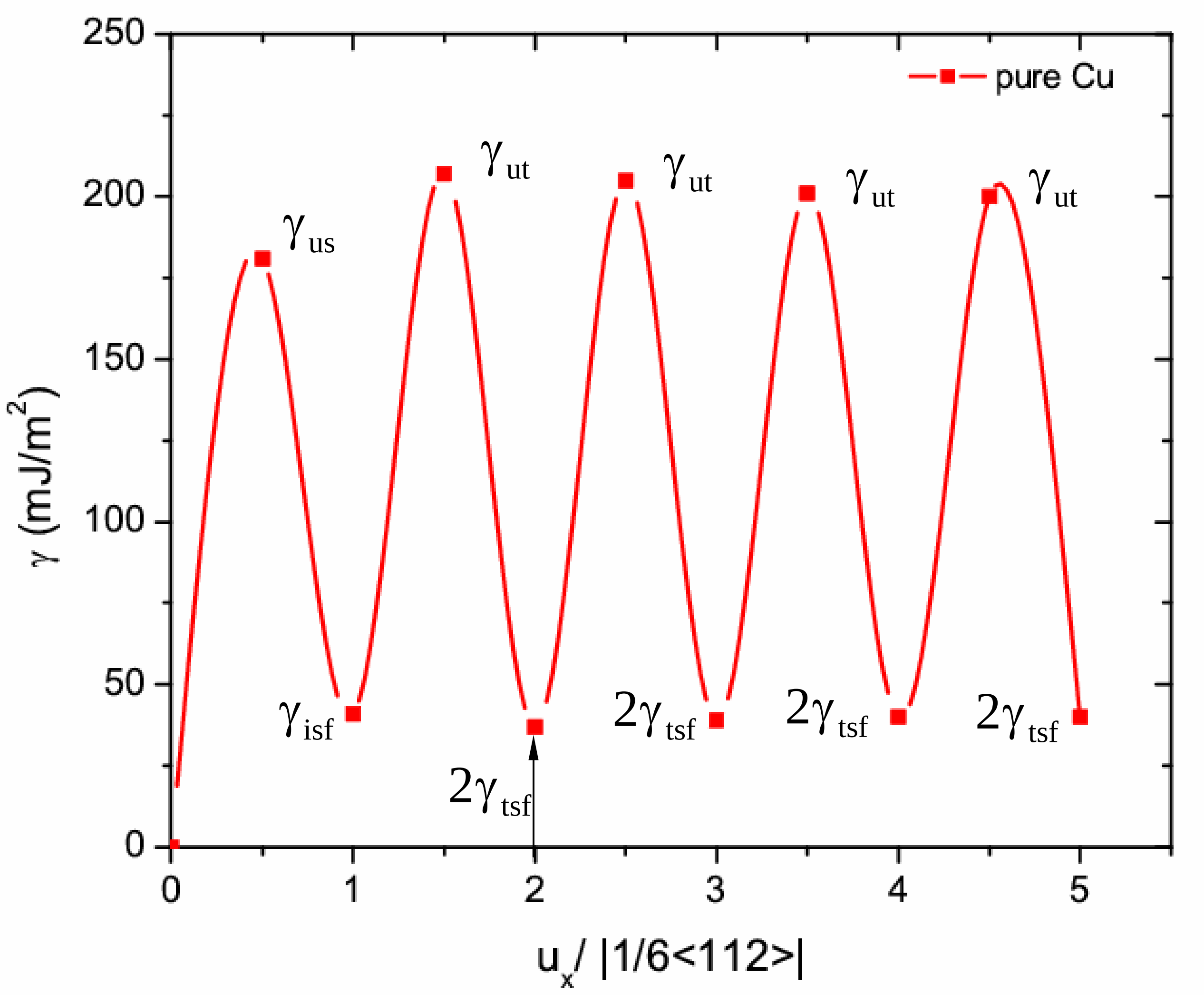
† *L. E. Murr, Interfacial Phenomena in Metals and Alloys (1975).*

‡ *S. Ogata, J. Li and S. Yip, Phys. Rev. B, **71**, 224102 (2005).*

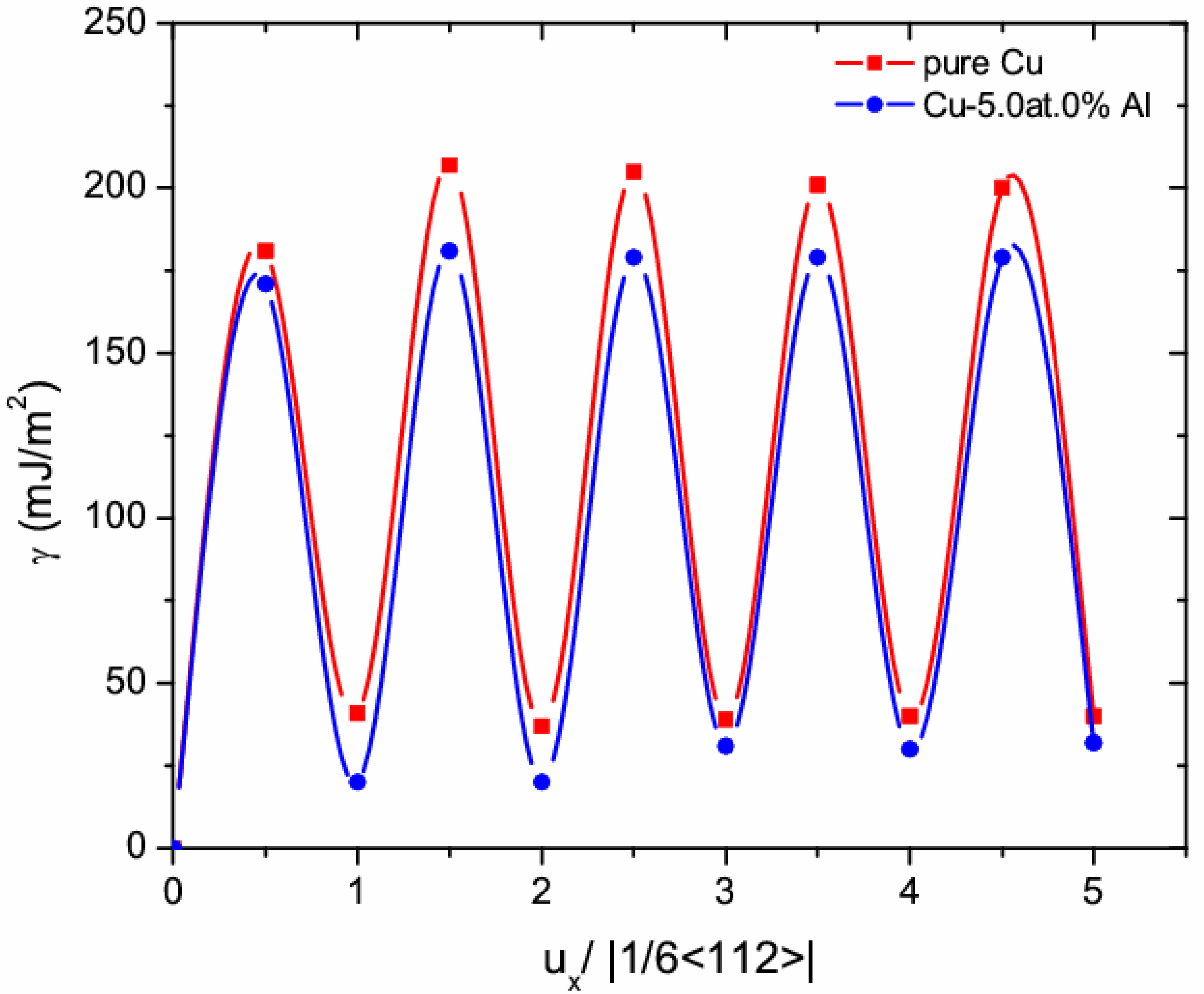
§ *C. B. Carter and I. L. Ray, Phil. Mag., **35**, 189 (1977).*

§§ *W. B. Pearson in: G. V. Raynor (Ed.), A Handbook of Lattice Spacings and Structures of Metals and Alloys (1958).*

GPFE curve for pure Cu

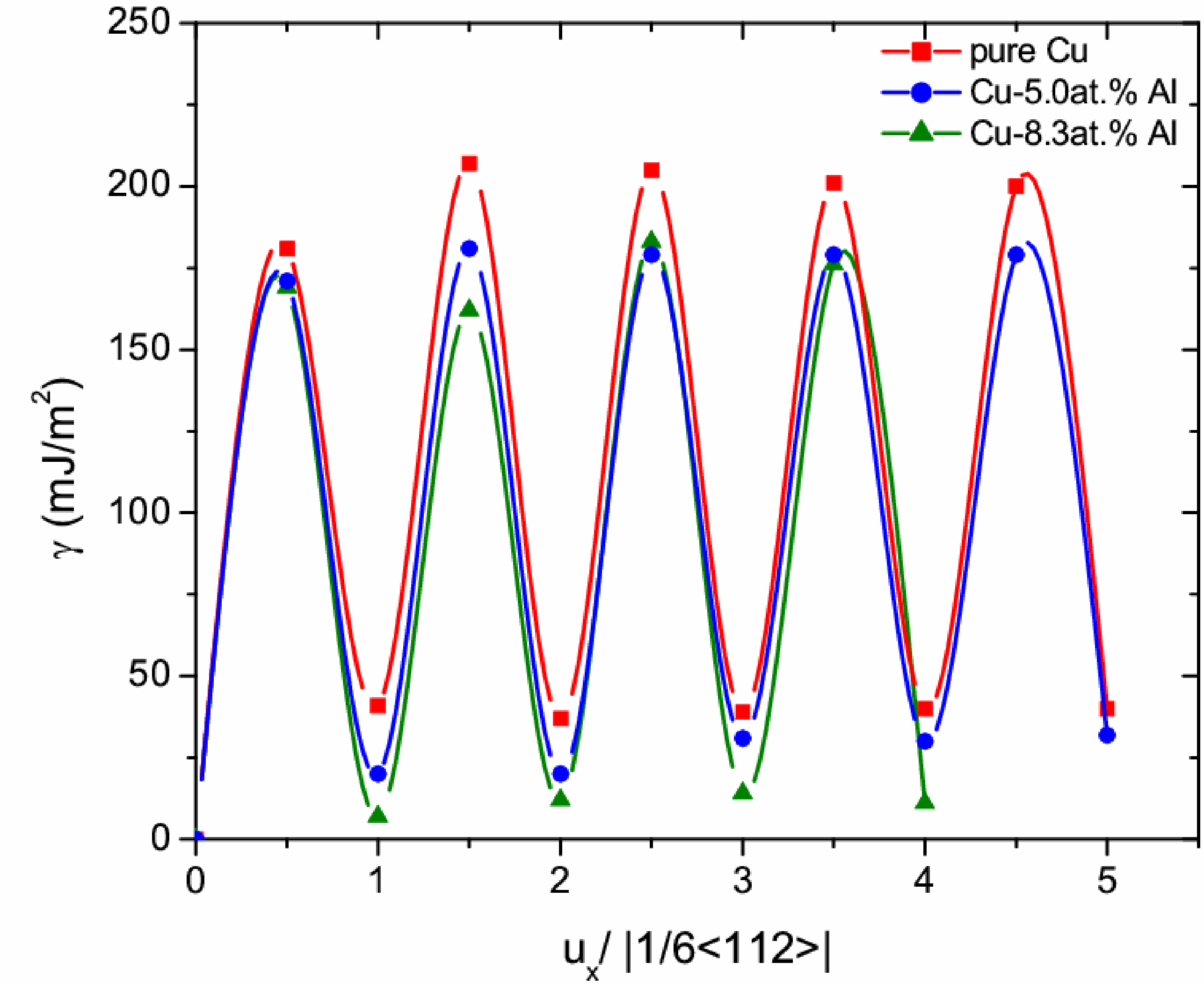


GPFE curves for Cu-xAl alloys



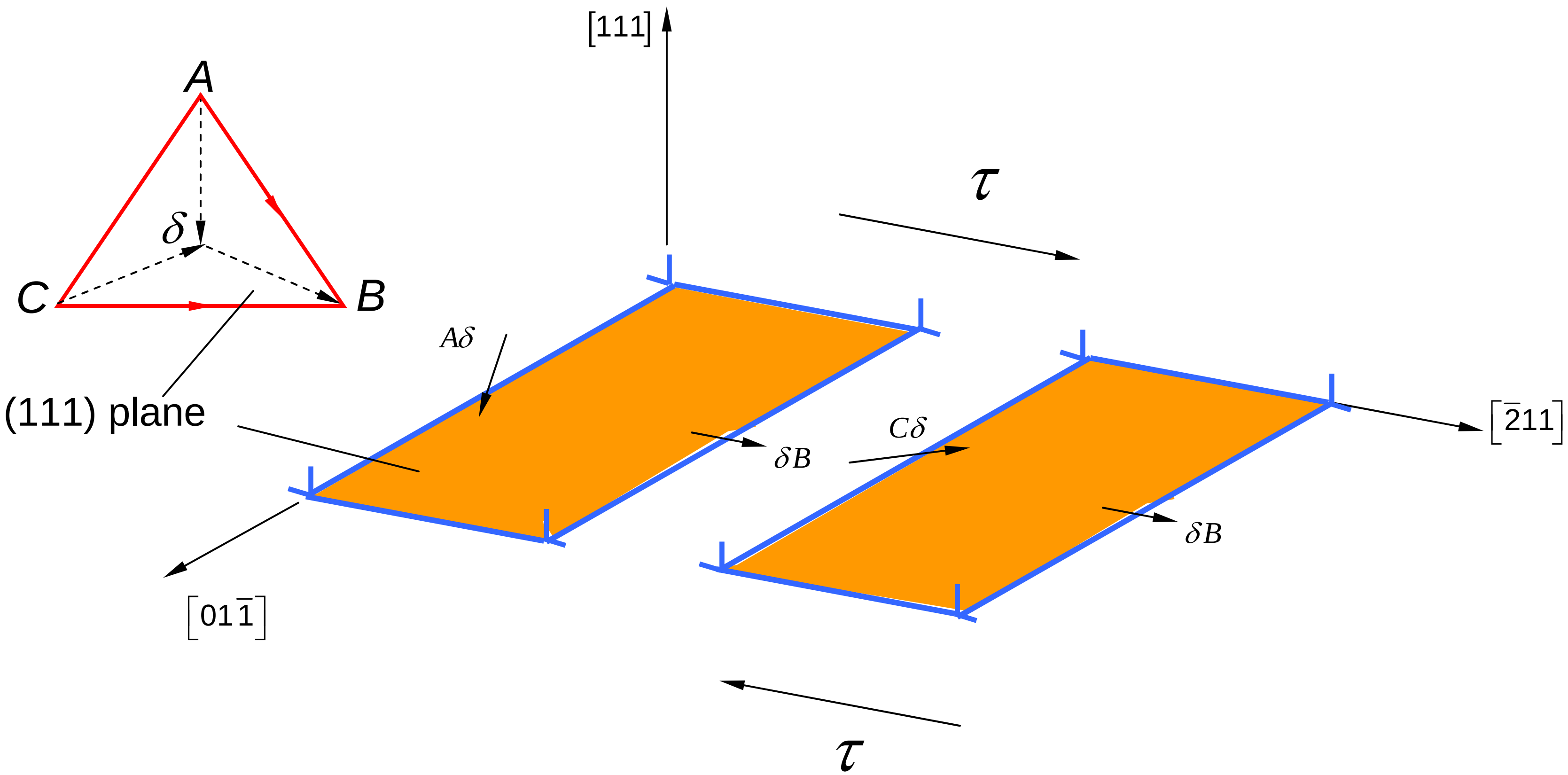
S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitolgu, submitted to Appl. Phys. Lett. (2006)

GPFE curves for Cu-xAl alloys (contd.)



S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, submitted to Appl. Phys. Lett. (2006)

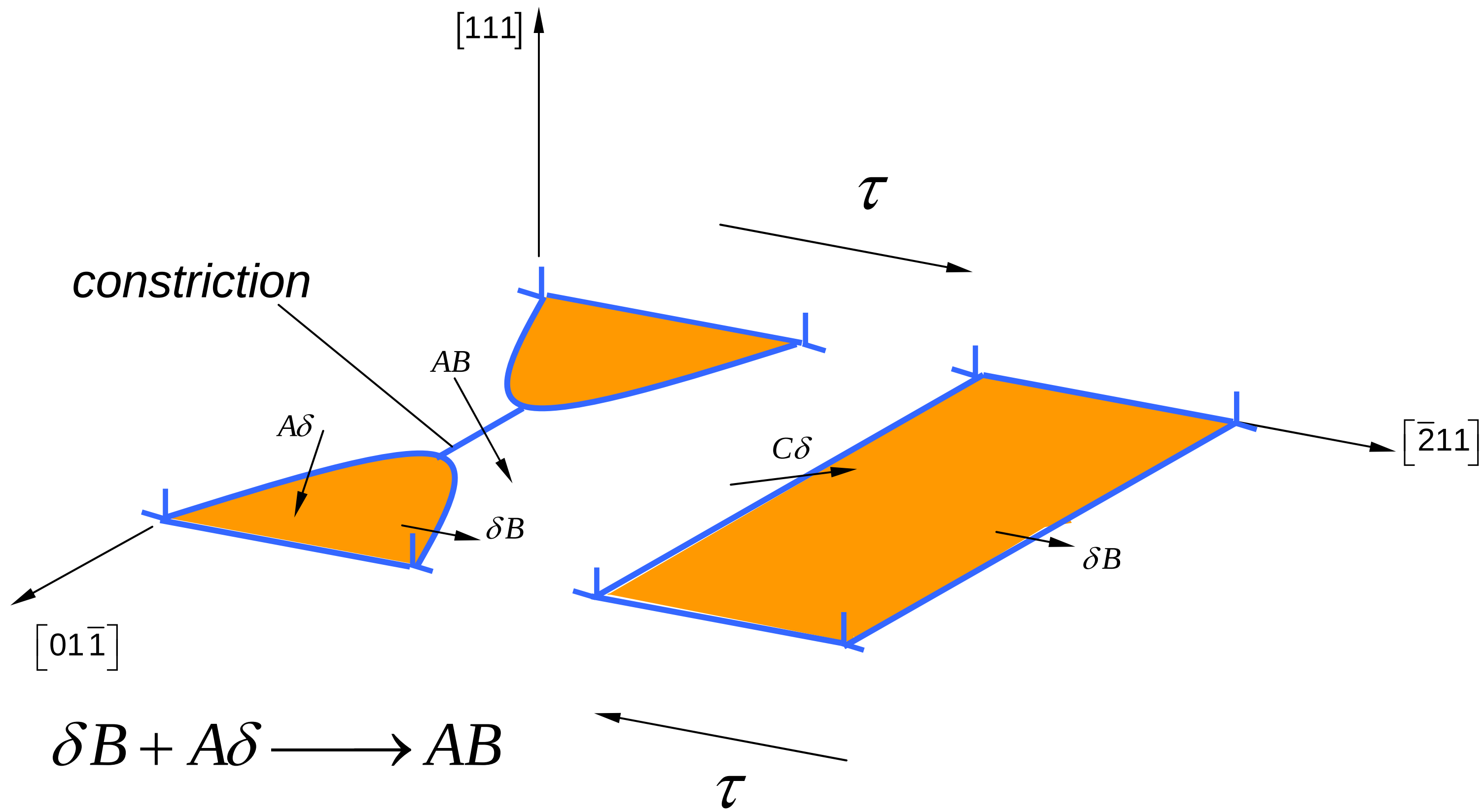
Formation of the Twin Nucleus



Intrinsic SFs on {111} plane interact to form a twin nucleus

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

Formation of constriction *AB*

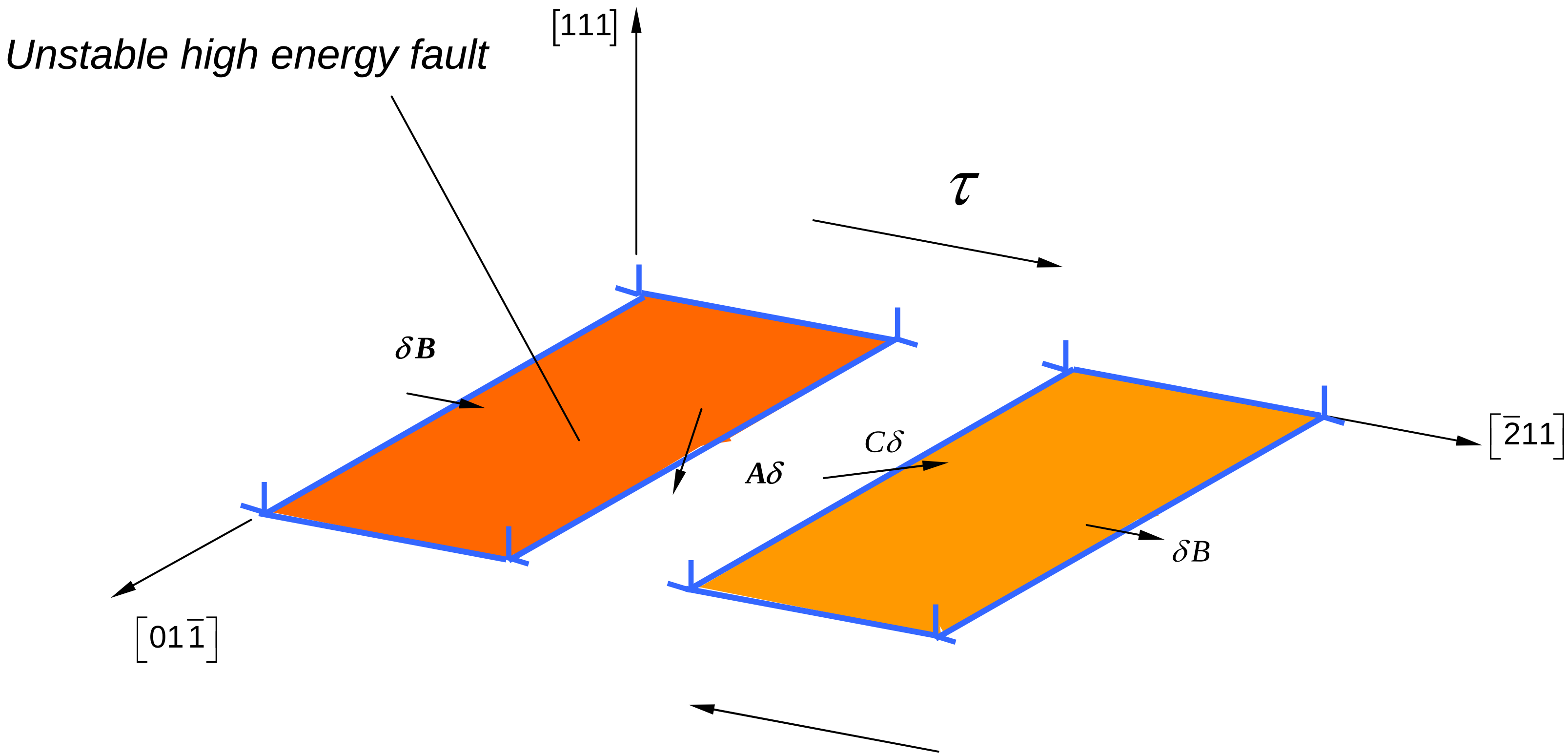


$$\delta B + A\delta \longrightarrow AB$$

leading trailing

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

AB dissociates into an unstable, high energy fault



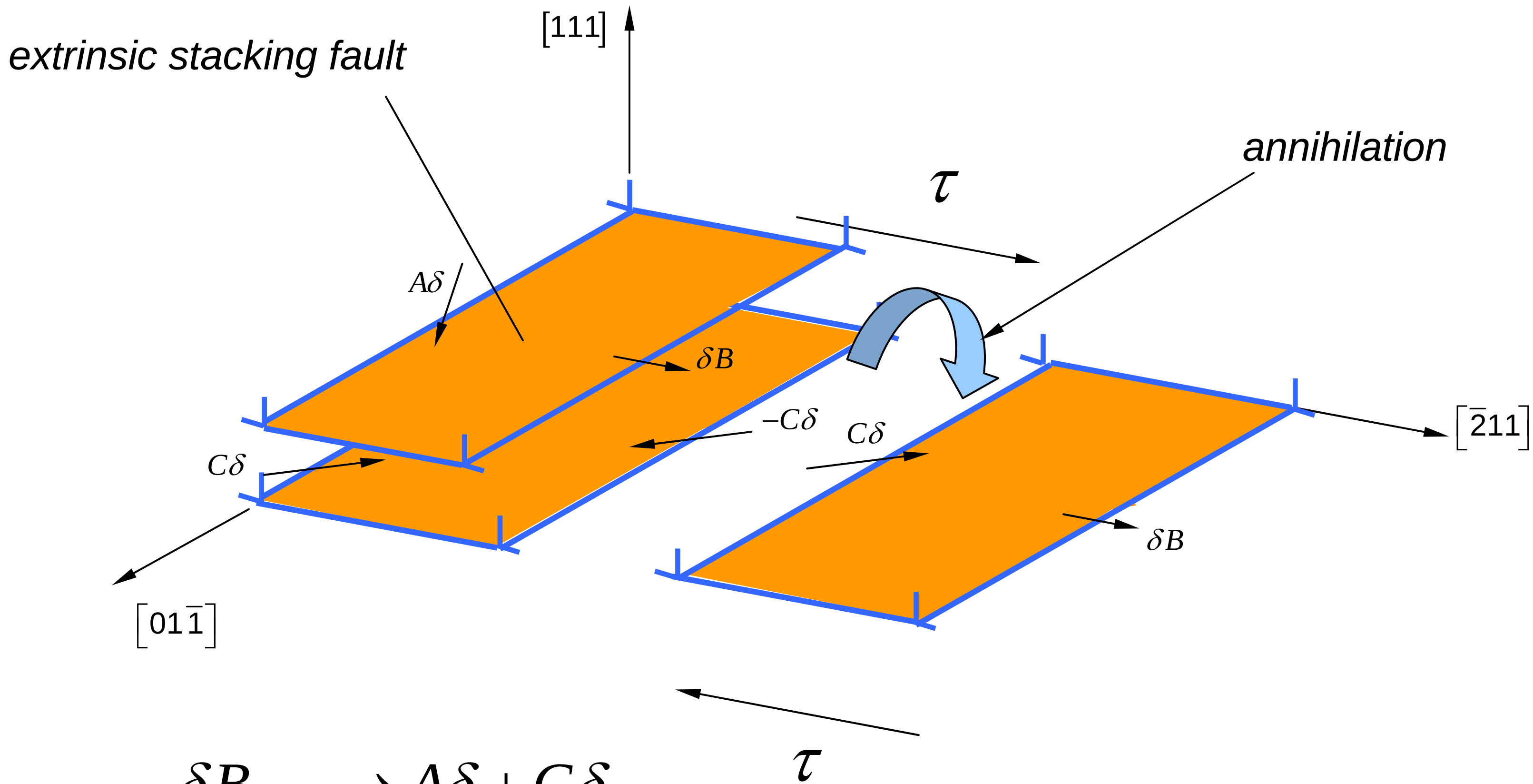
$$AB \longrightarrow A\delta + \delta B$$

leading *trailing*

The above sequence of leading and trailing partials is inconsistent with Thompson's rule and forms a high energy unstable fault, which will dissociate into an extrinsic stacking fault.

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

High energy fault dissociates into a stable extrinsic SF

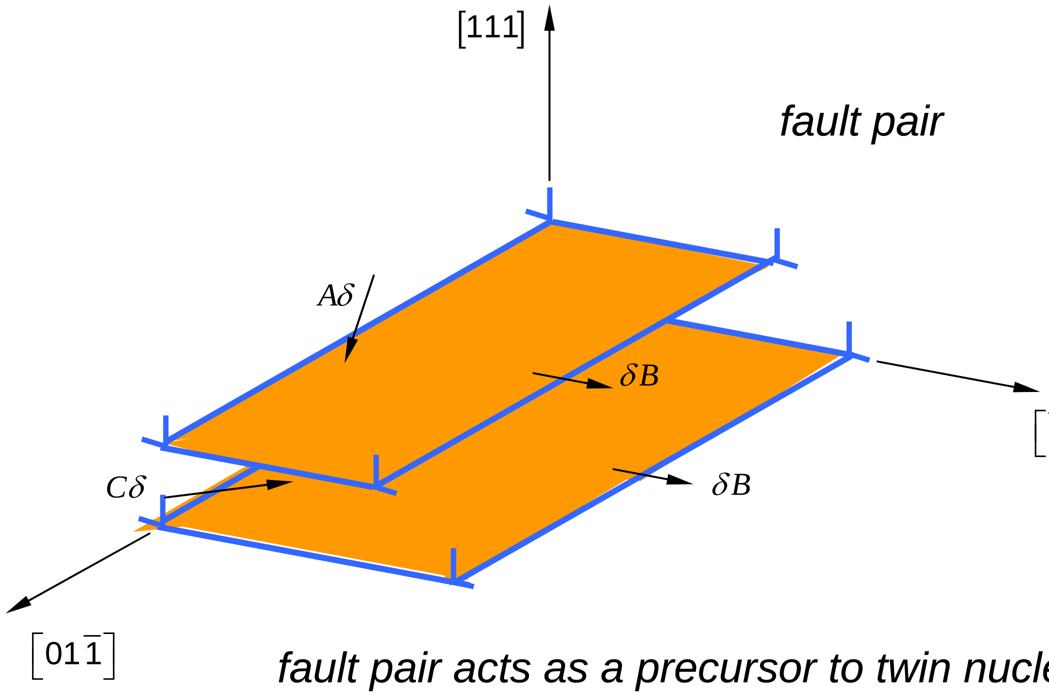


$$\delta B \longrightarrow A\delta + C\delta$$

$$A\delta \longrightarrow \delta B + \delta C$$

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

Fault pair formation after annihilation

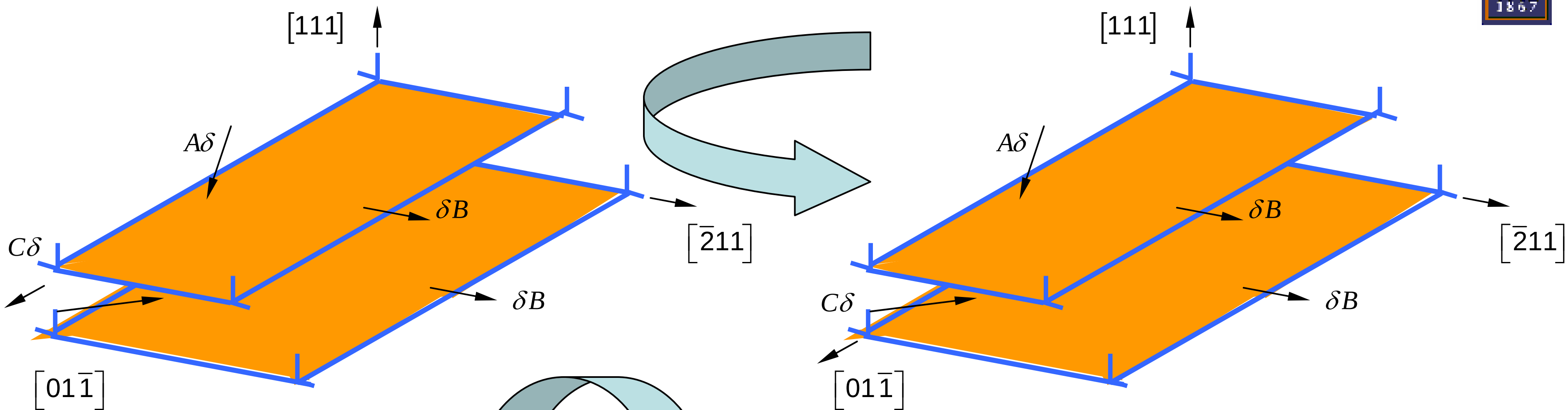


fault pair acts as a precursor to twin nucleation

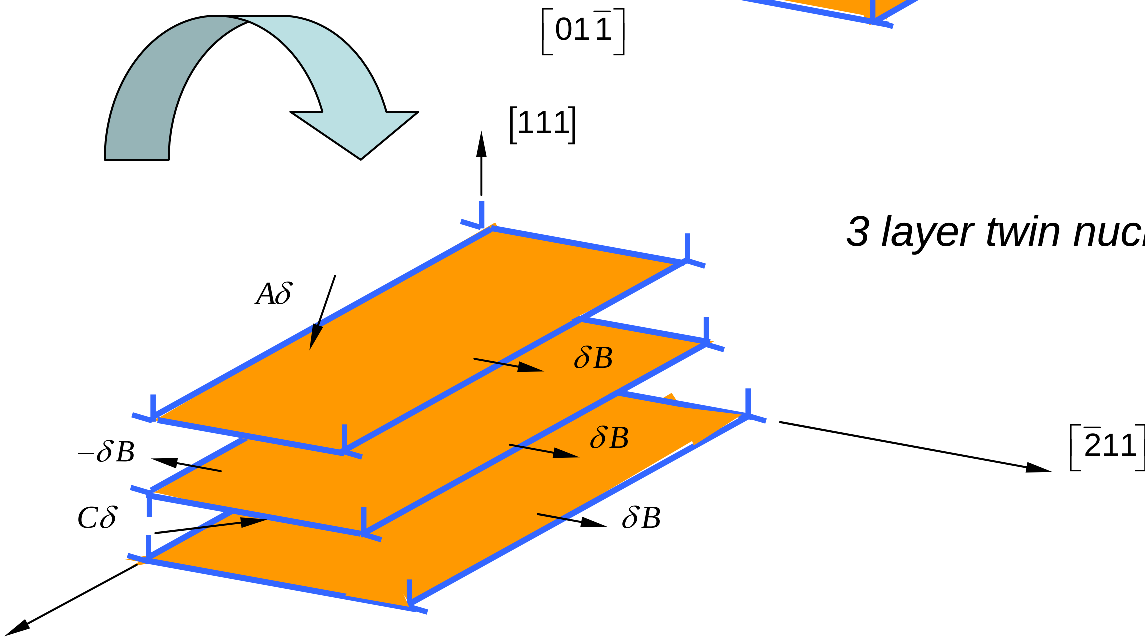
According to Mahajan and Chin (1973), two identical fault pairs interact to produce a 3 layer twin nucleus.

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

Fault pairs interact to form a 3 layer twin nucleus



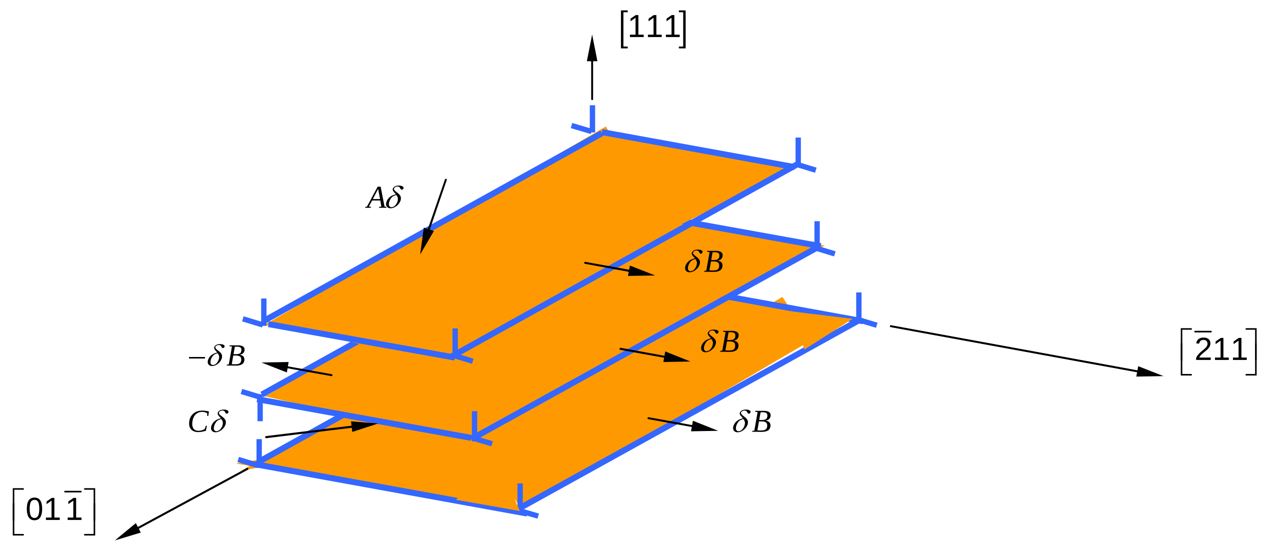
Fault pairs interact to give



3 layer twin nucleus

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

Proposed twin nucleus



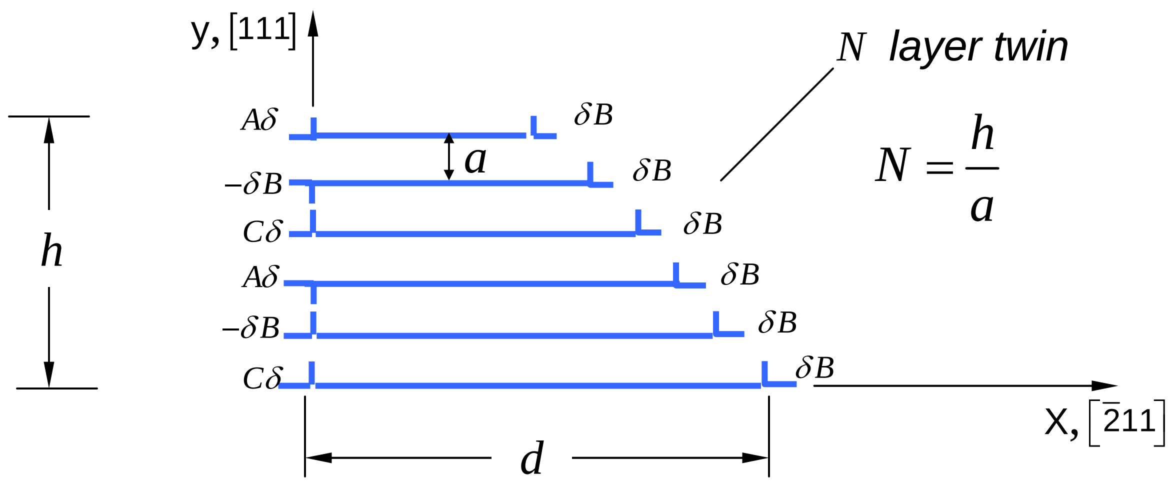
Mahajan and Chin (1973) have also proposed a 3 layer twin as the nucleus for twinning.

Our GPFE convergence trends are in agreement with above proposition.

Mahajan and Chin, Acta Metallurgica, vol. 21 (1973) 1353-1363.

Growth of a twin from the nucleus

•*These 3 layer nuclei grow into each other to form a finite sized twin.*



We can determine the aspect ratio that will minimize the total energy of the twin. Because the twin thickness is small with respect to its width, Friedel (1964) treats the dislocations as co-planar.

Total energy of the twin nucleus

To determine non-ideal twinning stress required to nucleate a twin, minimize the total energy of the 3-layer twin nucleus.

Total energy of the twin nucleus:

$$E_{total} = E_{edge} + E_{screw} + E_{\gamma\text{-}twin} - E_{\gamma\text{-}SF} - W_{\tau}$$

- E_{edge}: energy contribution of edge components
- E_{screw}: energy contribution of screw components
- $E_{\gamma\text{-}twin}$: energy required to pass successive twinning partials
- $E_{\gamma\text{-}SF}$: energy required to create ISF
- W_{τ}: work done by resolved shear stress

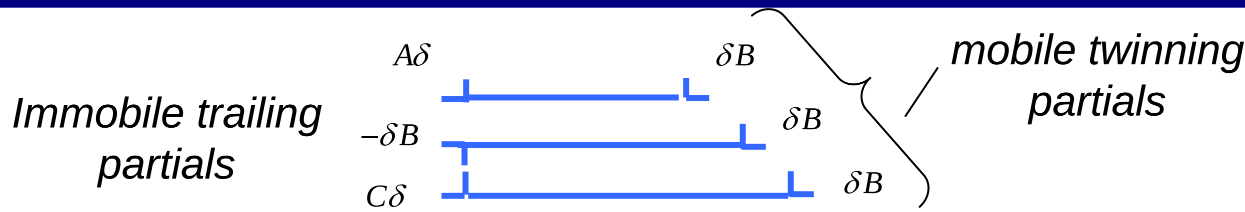
A closed form expression for total energy can be written with following assumptions:

- *Assuming a thin twin and treating the edge components as a single pileup*

$$E_{edge} = \frac{Gb_e^{\,2}d}{4\pi(1-\upsilon)}\left[N^2\left\{ln\left(\frac{d}{N}\right)+\frac{1}{2}\right\} - N\,ln\left(\frac{d}{r_0}\right) - \frac{1}{6}ln(N)\right]$$

Chou and Li in 'Mathematical Theory of Dislocations', ed: T. Mura, ASME (NY) 1969, p. 116

Total energy of the twin nucleus (contd.)



- *Since only $A\delta$ and $C\delta$ are mixed dislocations, the screw components can be treated as a finite sized vertical wall:*

$$E_{screw} = \frac{Gb_s^{\,2}}{9\pi} dN^2 \left[ln\left(\frac{d}{N}\right) - \frac{1}{2} \right]$$

[*J.C.M. Li, Acta Metall., vol. 8 (1960) p 563-574*]

- *The energy required to pass successive twinning partials is given by:*

$$E_{\gamma\text{-}twin} = (N-1)\, d \int_0^d \gamma_{twin}\, dx$$

- *The energy required for formation of the intrinsic SF and for cross-slip:*

$$E_{\gamma\text{-}SF} = d \int_0^d \gamma_{SF}\, dx$$

Total energy of the twin nucleus (contd.)

- *Work done by resolved shear stress in displacing twinning partials :*

$$W_\tau = N\tau d^2 b_{twin}$$

Total energy of the twin:

$$E_{total} = E_{edge} + E_{screw} + E_{\gamma\text{-}twin} - E_{\gamma\text{-}SF} - W_\tau$$

$$E_{total} = \frac{Gb_e^2 d}{4\pi(1-\upsilon)}\left[N^2\left\{ln\left(\frac{d}{N}\right)+\frac{1}{2}\right\} - N\,ln\left(\frac{d}{r_0}\right) - \frac{1}{6}ln(N)\right]$$

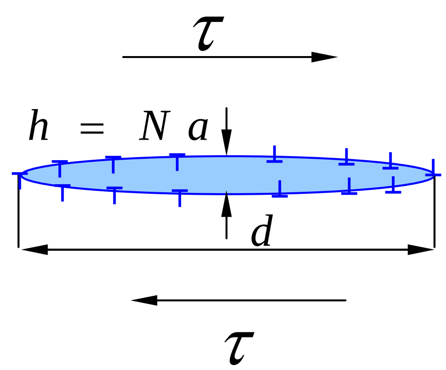
$$+\frac{Gb_s^2}{9\pi}dN^2\left[ln\left(\frac{d}{N}\right)-\frac{1}{2}\right]$$

$$+(N-1)d\int_0^d \gamma_{twin}\,dx - d\int_0^d \gamma_{SF}\,dx - N\tau d^2 b_{twin}$$

Critical twin size and twinning stress can be determined by minimizing E_{total} *relative to* d *and* N*.*

Twinning stress equation

Relation between twin size and twinning stress based on present analysis:



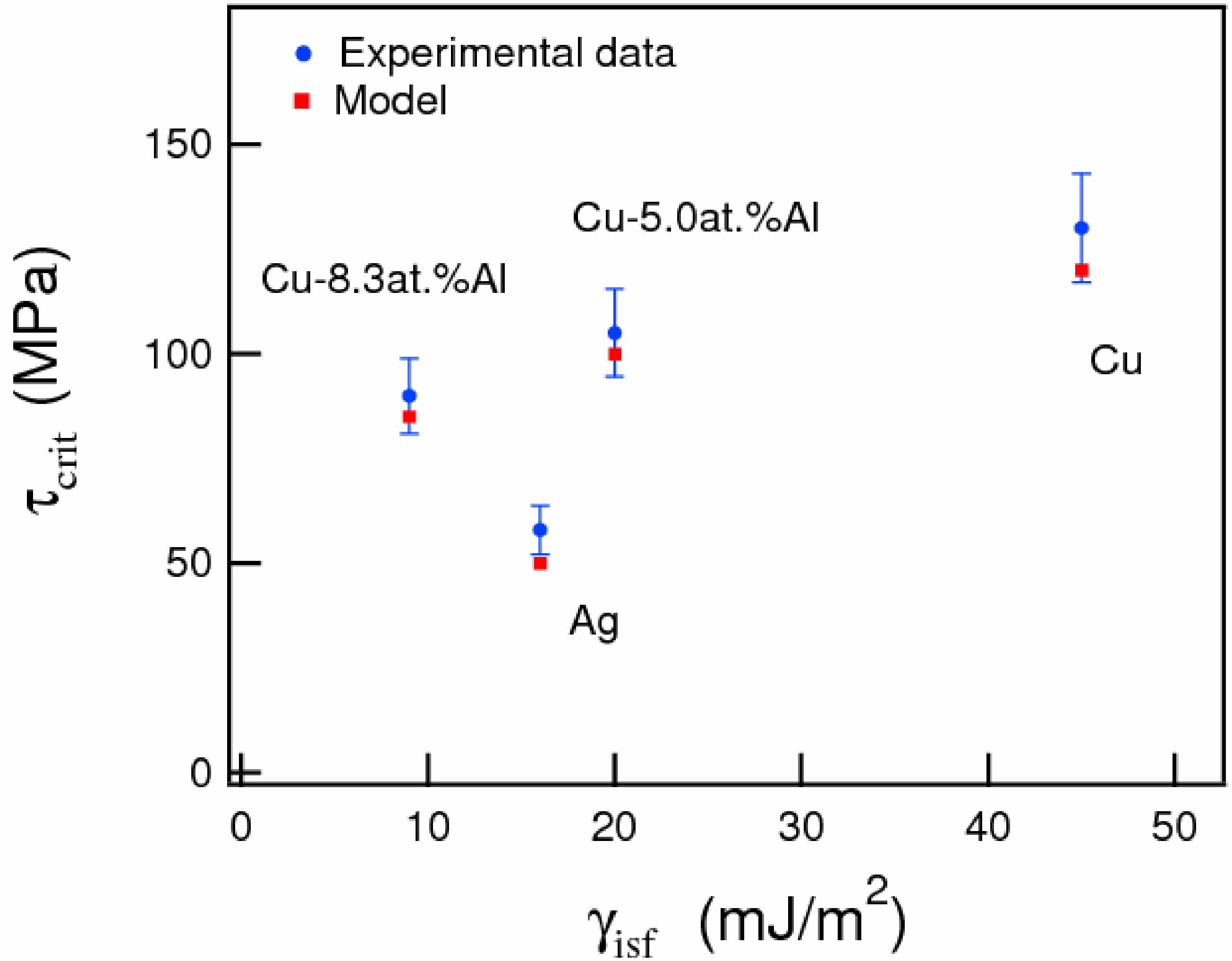
$$\tau_{crit} = \frac{GN}{\pi}\left[\frac{b_e^{\,2}}{(1-\upsilon)} + b_s^{\,2}\right] + \frac{2}{3N}\left(\frac{3N}{4}-1\right)\left[\gamma_{ut} + \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\frac{1}{b_{twin}}$$

$$+\frac{1}{6b_{twin}}\left[\gamma_{ut} - \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right)\right]$$

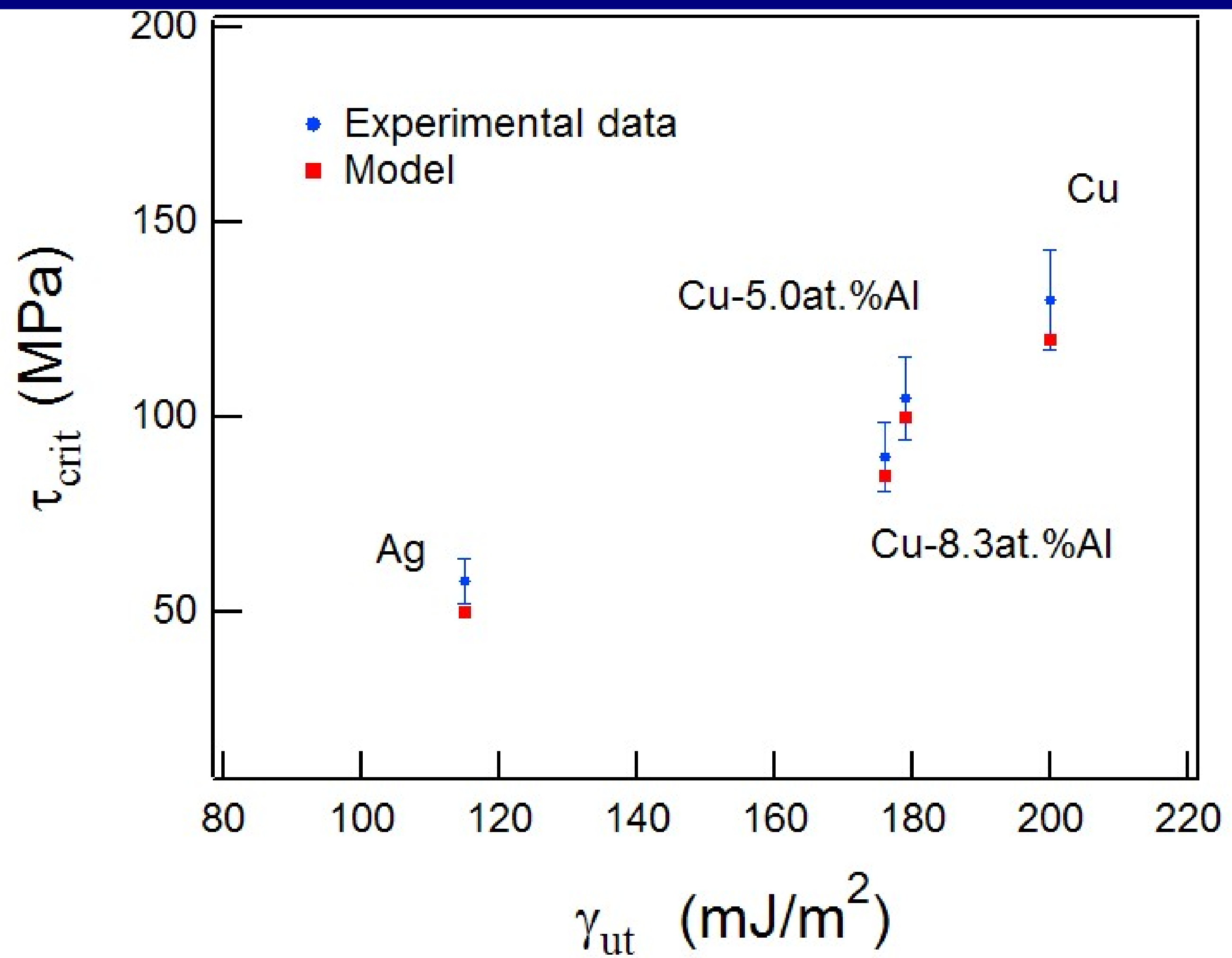
$$-\frac{(N-1)}{3N}\frac{1}{b_{twin}}\left[\gamma_{ut} - \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right) + \frac{d}{\sqrt{d^2+w^2}}\right]$$

$$-\frac{2}{3N}\left(\frac{\gamma_{us}+\gamma_{isf}}{b_{twin}}\right) + \frac{1}{3N}\left(\frac{\gamma_{us}-\gamma_{isf}}{b_{twin}}\right)\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right) + \frac{d}{\sqrt{d^2+w^2}}\right]$$

Predicted twinning stress for fcc alloys



Twinning stress vs. unstable twin SFE barrier



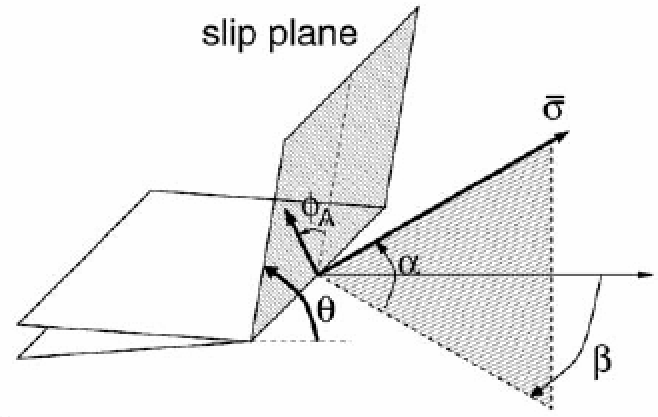
Narita and Takamura in 'Dislocations in Solids' ed: Nabarro vol. 9 (1992) p. 135-189.; Szczerba, Mater. Sci. Engg. A234-236 (1997) p 1057.; Szczerba, Phil. Mag. vol. 84 (2004) p. 481.

Twinnability of fcc alloys

Twinning tendency T_t :

$$T_t = \frac{K^{\text{trailing partial}}}{K^{\text{twinning partial}}} = \lambda_{\text{crit}} \sqrt{\frac{\gamma_{\text{us}}}{\gamma_{\text{ut}}}}$$

orientation dependent parameter



Twinnability T is the orientation average of twinning tendency over all possible orientations.

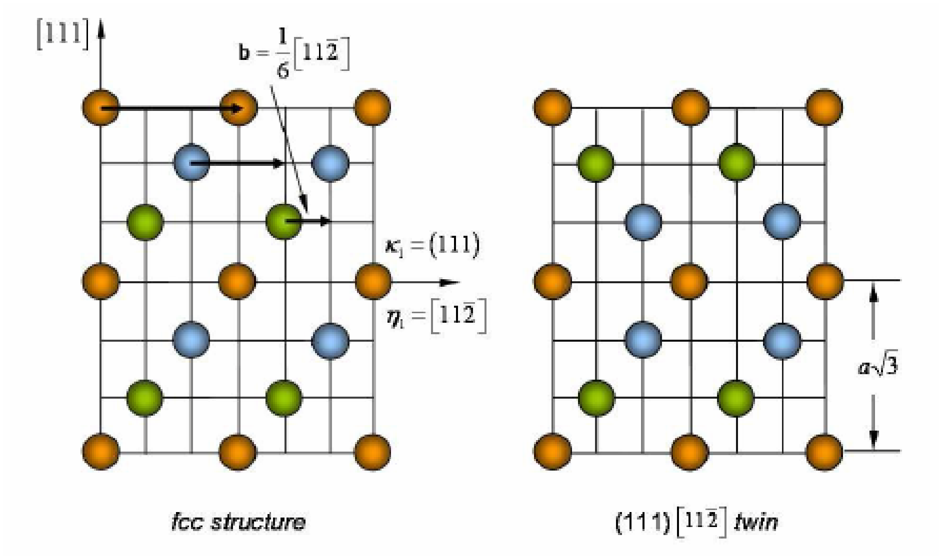
$$T = \frac{1}{\Omega}\int (T_t)_{\min} \mathrm{d}\alpha \mathrm{d}\beta \mathrm{d}\theta \mathrm{d}\phi_A, \text{ where, } (T_t)_{\min} = \lambda_{\min}\sqrt{\frac{\gamma_{\text{us}}}{\gamma_{\text{ut}}}}$$

Bernstein and Tadmor (2004) have given an approximate form for twinnability as

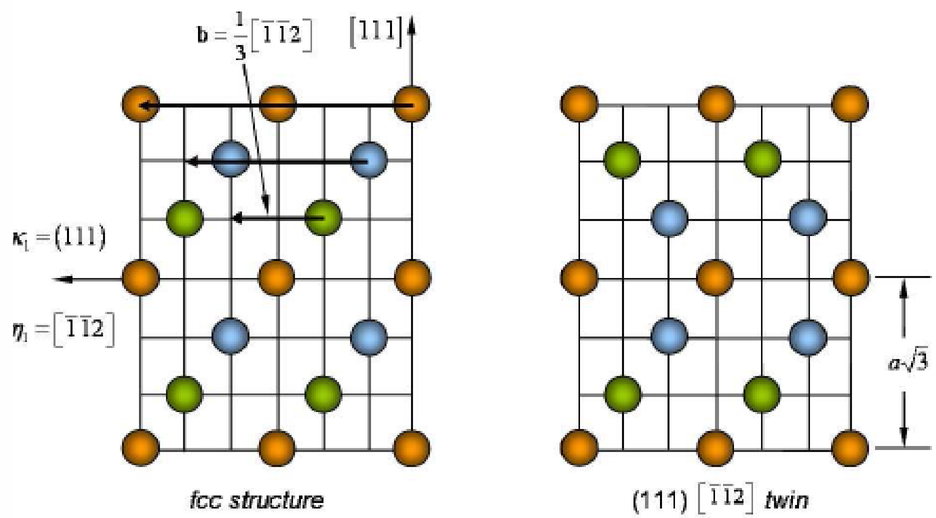
$$T = \left[1.136 - 0.151\frac{\gamma_{\text{isf}}}{\gamma_{\text{us}}}\right]\sqrt{\frac{\gamma_{\text{us}}}{\gamma_{\text{ut}}}}$$

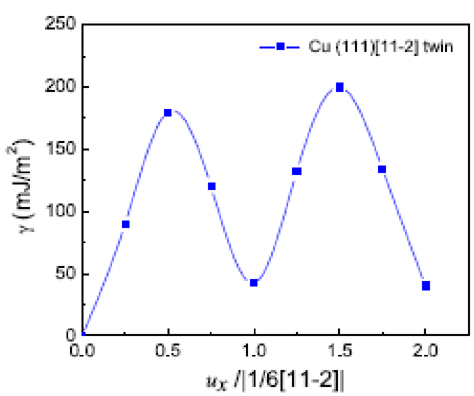
Directionality in twinning

Energetically favorable and observed

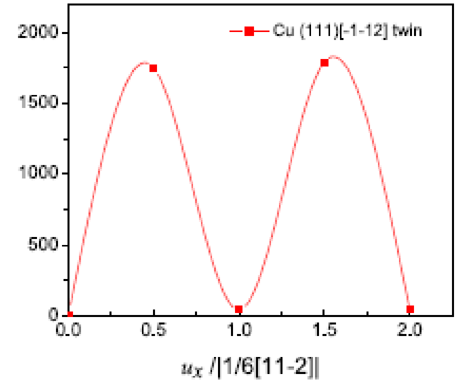


Energetically unfavorable and not observed





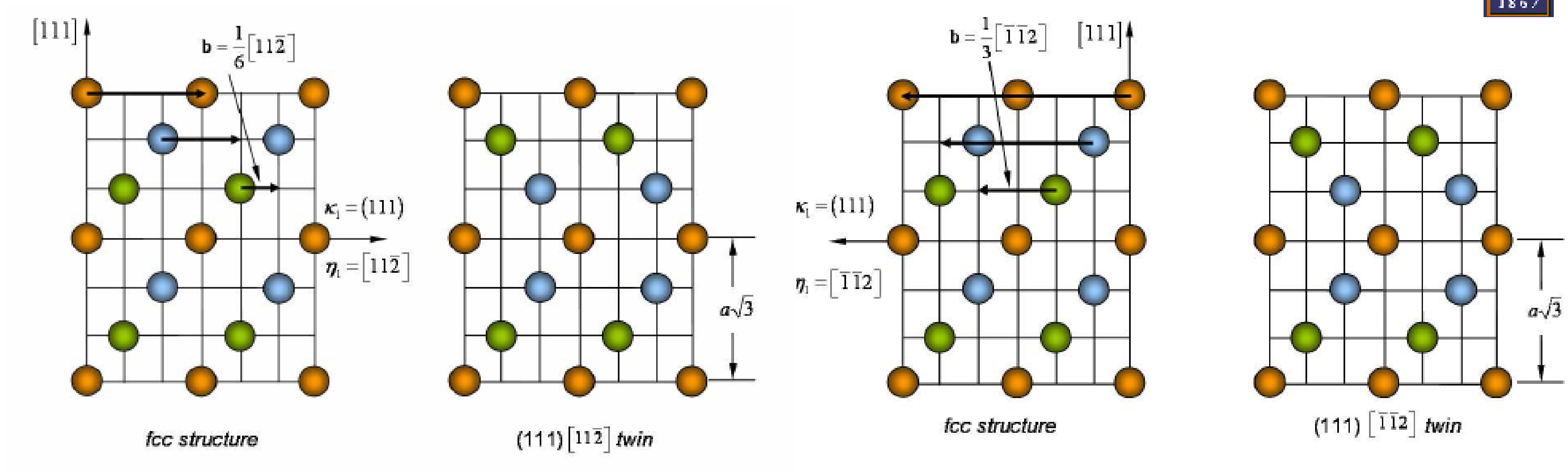
T =1.02

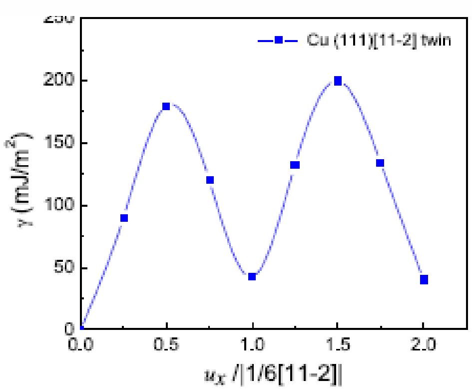


T =1.12

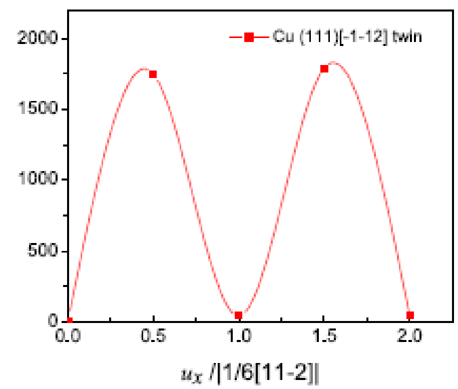
$$T = \left[1.136 - 0.151\frac{\gamma_{\text{isf}}}{\gamma_{\text{us}}}\right]\sqrt{\frac{\gamma_{\text{us}}}{\gamma_{\text{ut}}}}$$

Comparison of predicted twinning stress





τ_{crit} =120 MPa



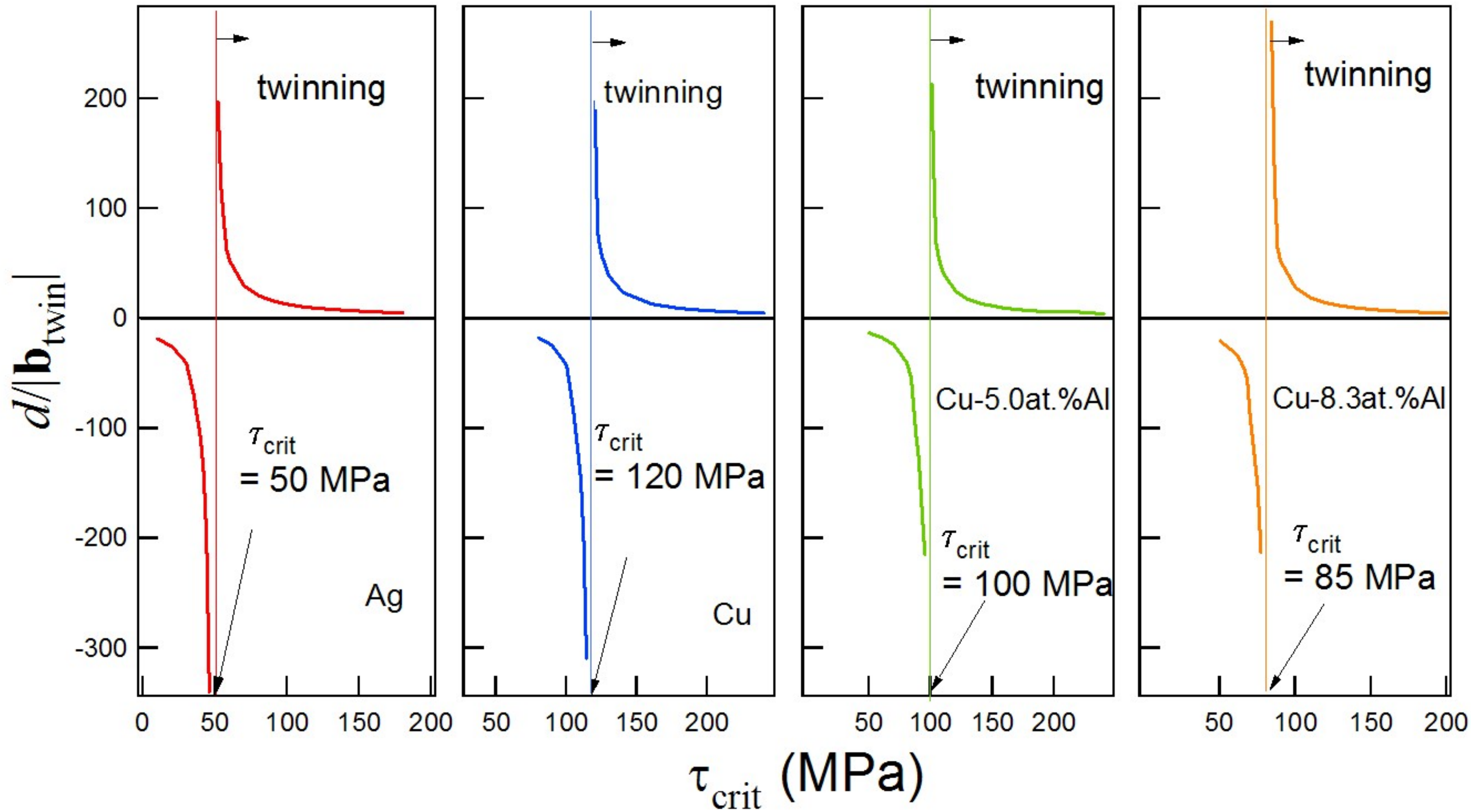
τ_{crit}=867 MPa

Present model for twinning stress predicts the twinning directionality correctly, while the twinnability criterion does not.

Conclusions

- *Our twinning model predicts that in fcc alloys, a 3 layer twin is the twin nucleus, and the twinning stress was computed by minimizing the total energy of the 3 layer twin nucleus.*
- *The model predicts that twinning stress depends on the unstable SFE and unstable twin SFE barriers, in addition to intrinsic SFE.*
- *The model rules out twinning in the anti-twinning direction.*

Backup slide for twinning stress



Twinning stress vs. unstable SFE barrier