Experiments and Simulations in Plasticity- From Atoms to Continuum

Huseyin Sehitoglu
Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign

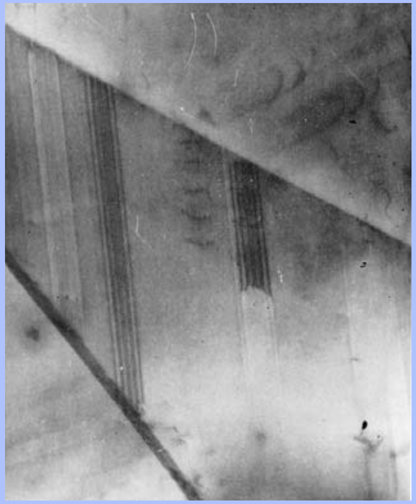
Symposium in Honor of David McDowell, St.Thomas, January 7, 2009

Collaborators: S. Kibey, D. Johnson, J.B.Liu, C. Efstathiou, M.Sangid

Funding: NSF-DMR Metals Program

Overview of the Presentation

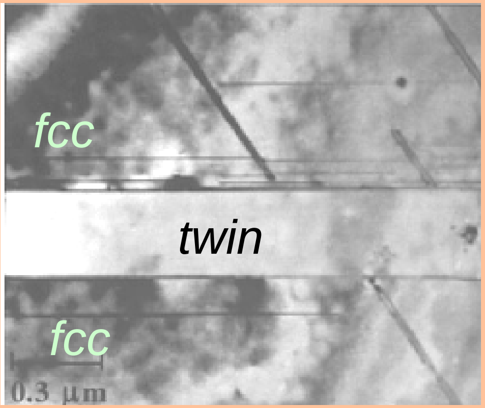
Stacking faults



Whelan et al., Proc. Roy. Soc. London (1957).

face centered cubic (fcc) metals and alloys

Deformation twins



Karaman-Sehitoglu et al., Acta Mater (2000).

Sehitoglu et al. Acta Mat., APL, (2006-2008)

face centered cubic (fcc) metals and alloys

Outline

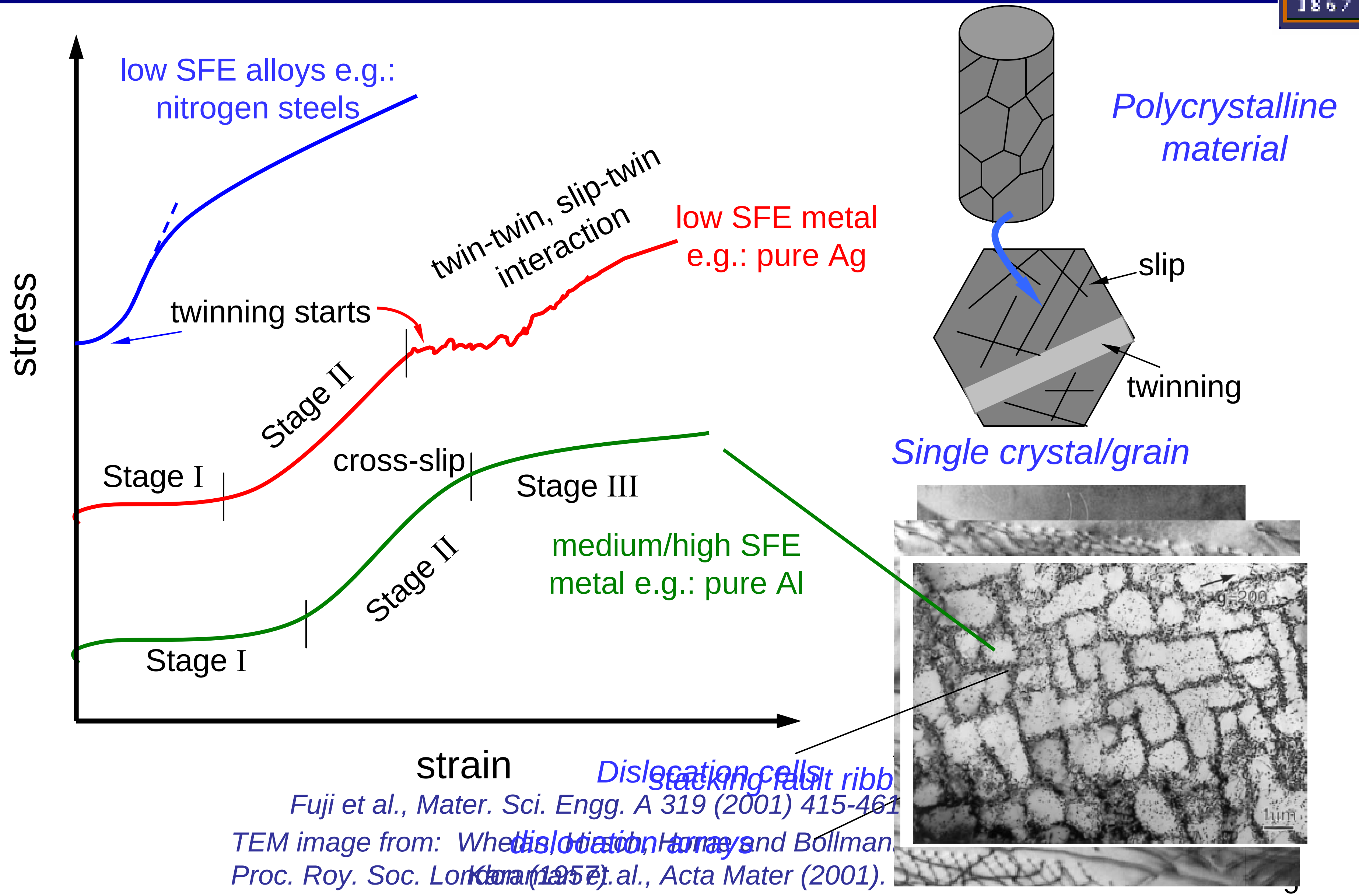
- Stacking faults in fcc materials.
  - Energy landscape/pathway (GSFE) – atomic level.

- Deformation twinning in fcc metals.
  - Energy landscape/pathway (GPFE).
  - Mesoscale twinning stress model

- Material Design (Cu-Al, Hadfield Steel with Nitrogen)

- Summary

Plastic flow in fcc materials: slip and cross-slip



Dislocation cells

stacking fault ribb

Fuji et al., Mater. Sci. Engg. A 319 (2001) 415-461

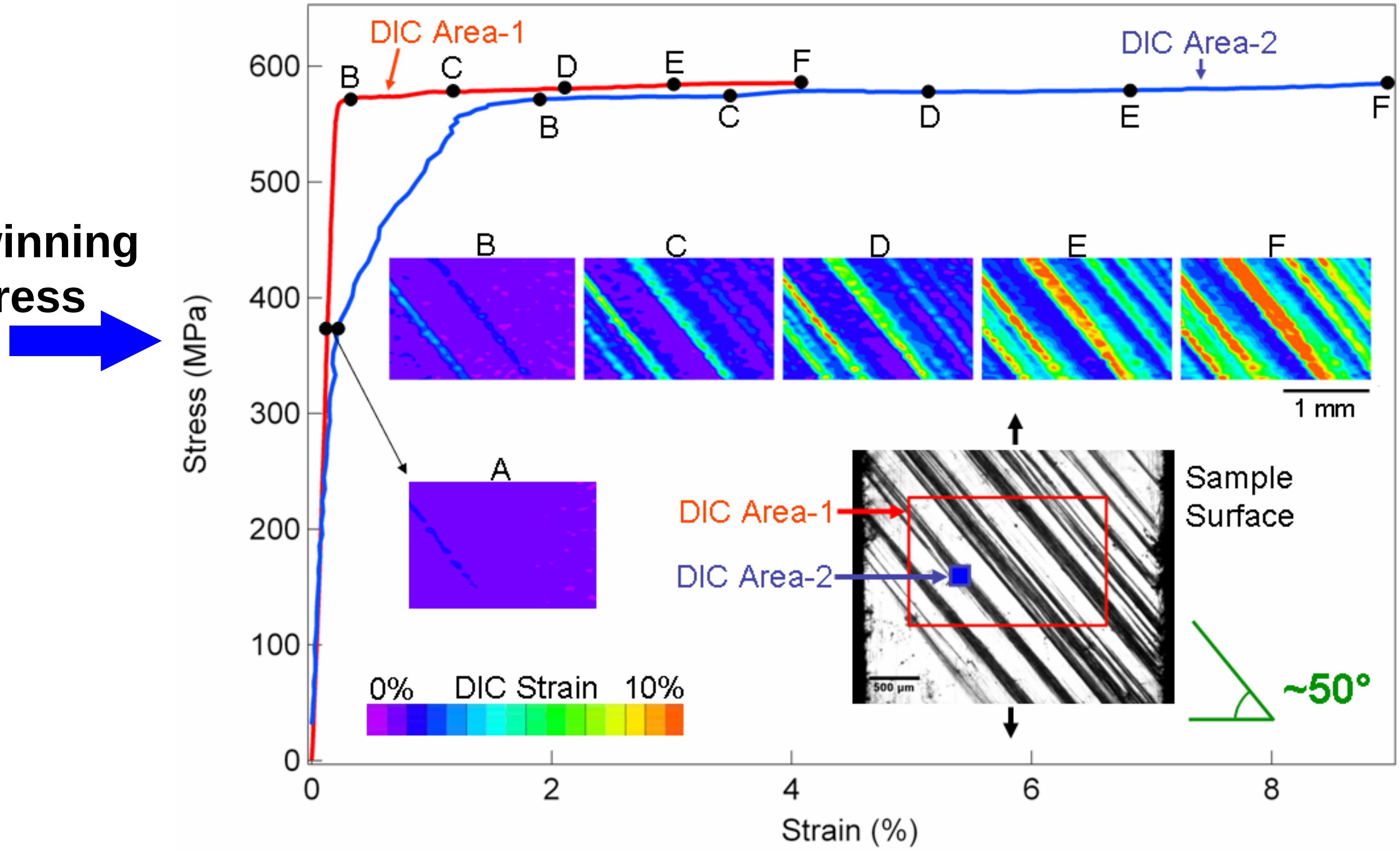
TEM image from: Whelan, Hirsch, Horne and Bollman. Proc. Roy. Soc. London (1957).

dislocation arrays

Karaman et al., Acta Mater (2001).

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

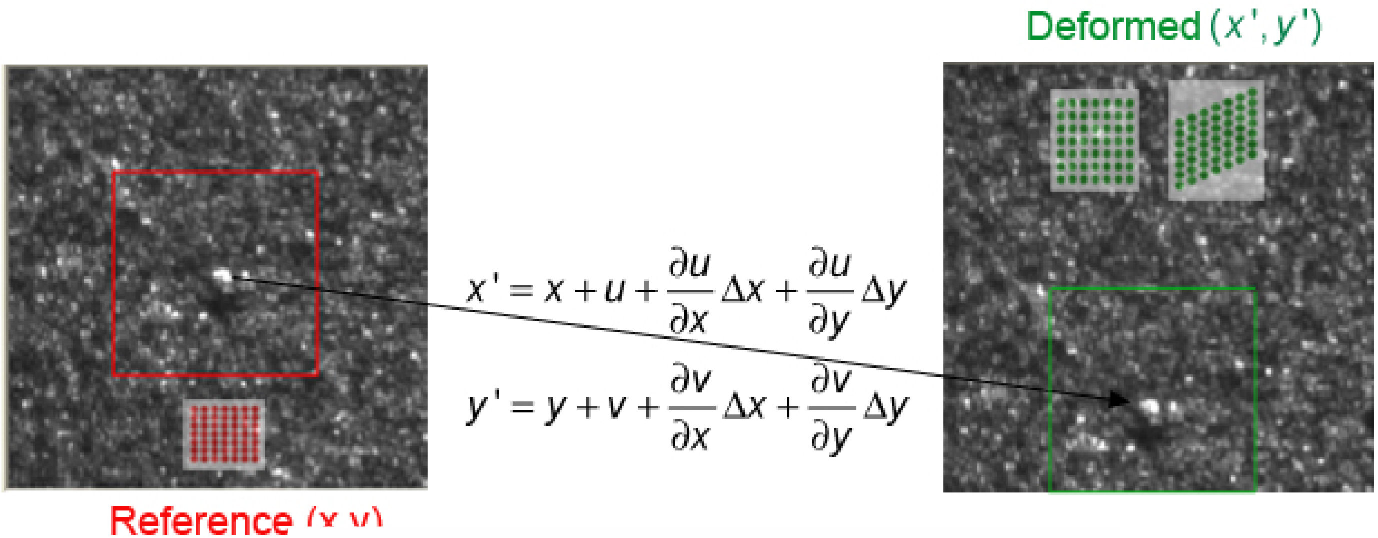
twinning stress



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
C. Efstathiou, H. Sehitoglu (2008), Unpublished work

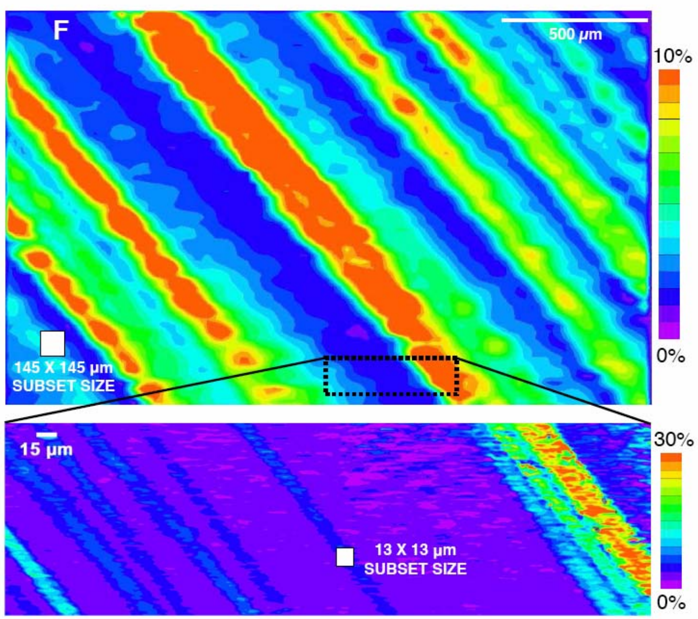
The twinning (nucleation) stress is currently obtained from experiments. A theory to obtain this quantity from first principles (for metals and alloys) is needed.

The main principle of the DIC (Digital Image Correlation) technique is shown. Small square regions illustrate a subset. Displacement gradients are noted in the figure.



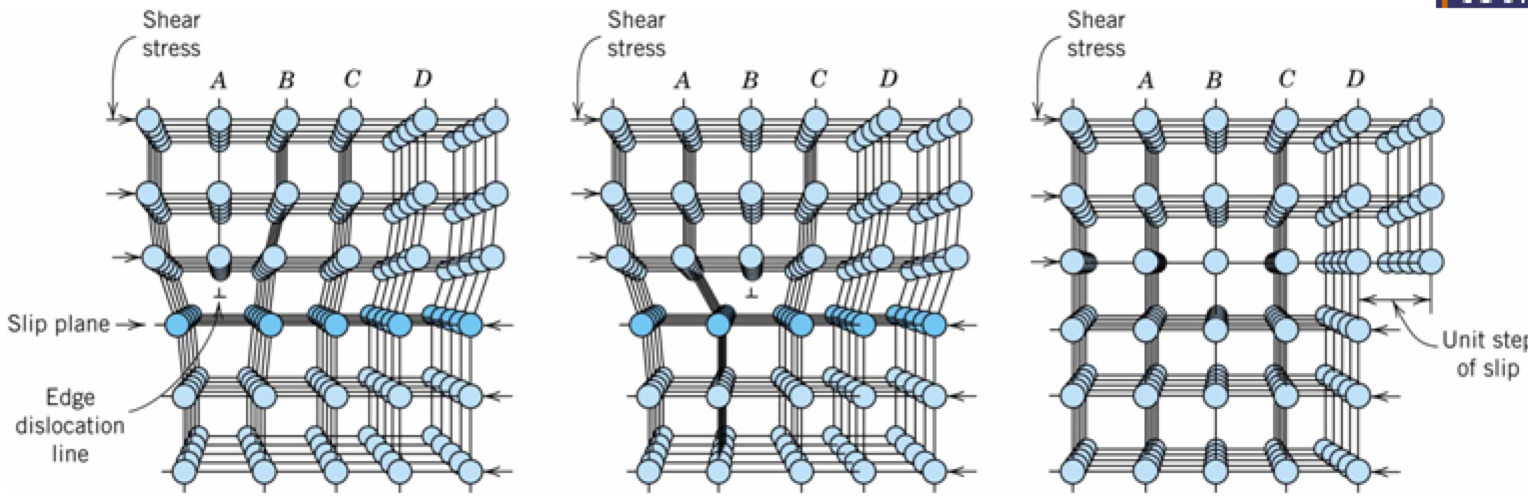
$$x' = x + u + \frac{\partial u}{\partial x}\Delta x + \frac{\partial u}{\partial y}\Delta y$$

$$y' = y + v + \frac{\partial v}{\partial x}\Delta x + \frac{\partial v}{\partial y}\Delta y$$



Plastic deformation due to slip

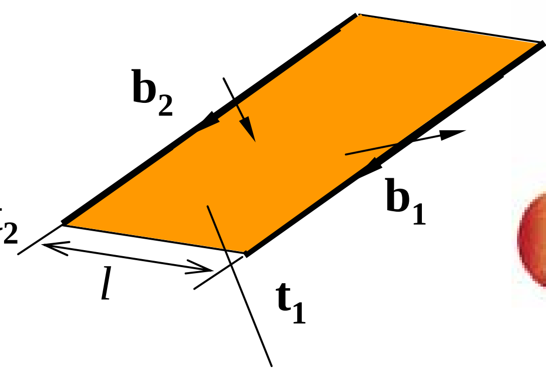
Slip due to a perfect dislocation



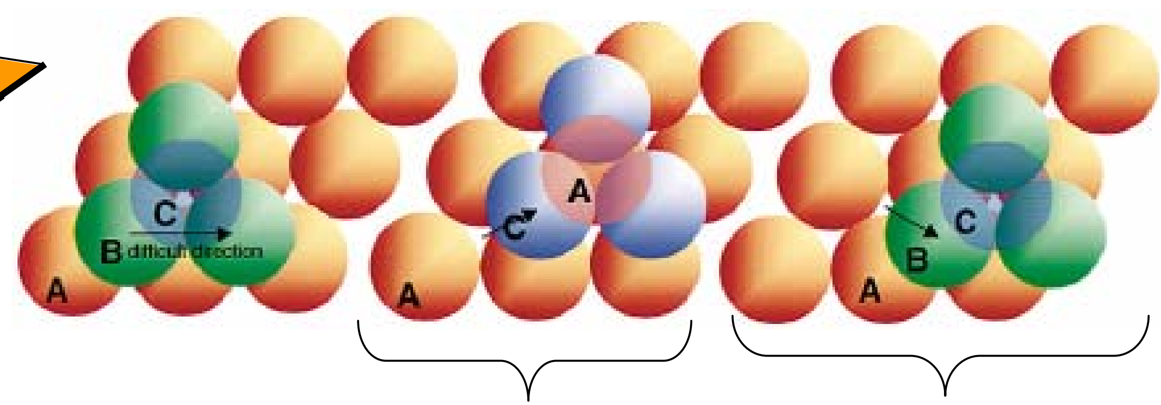
Callister (2000)

A perfect dislocation may split into partial dislocations…

extended dislocation



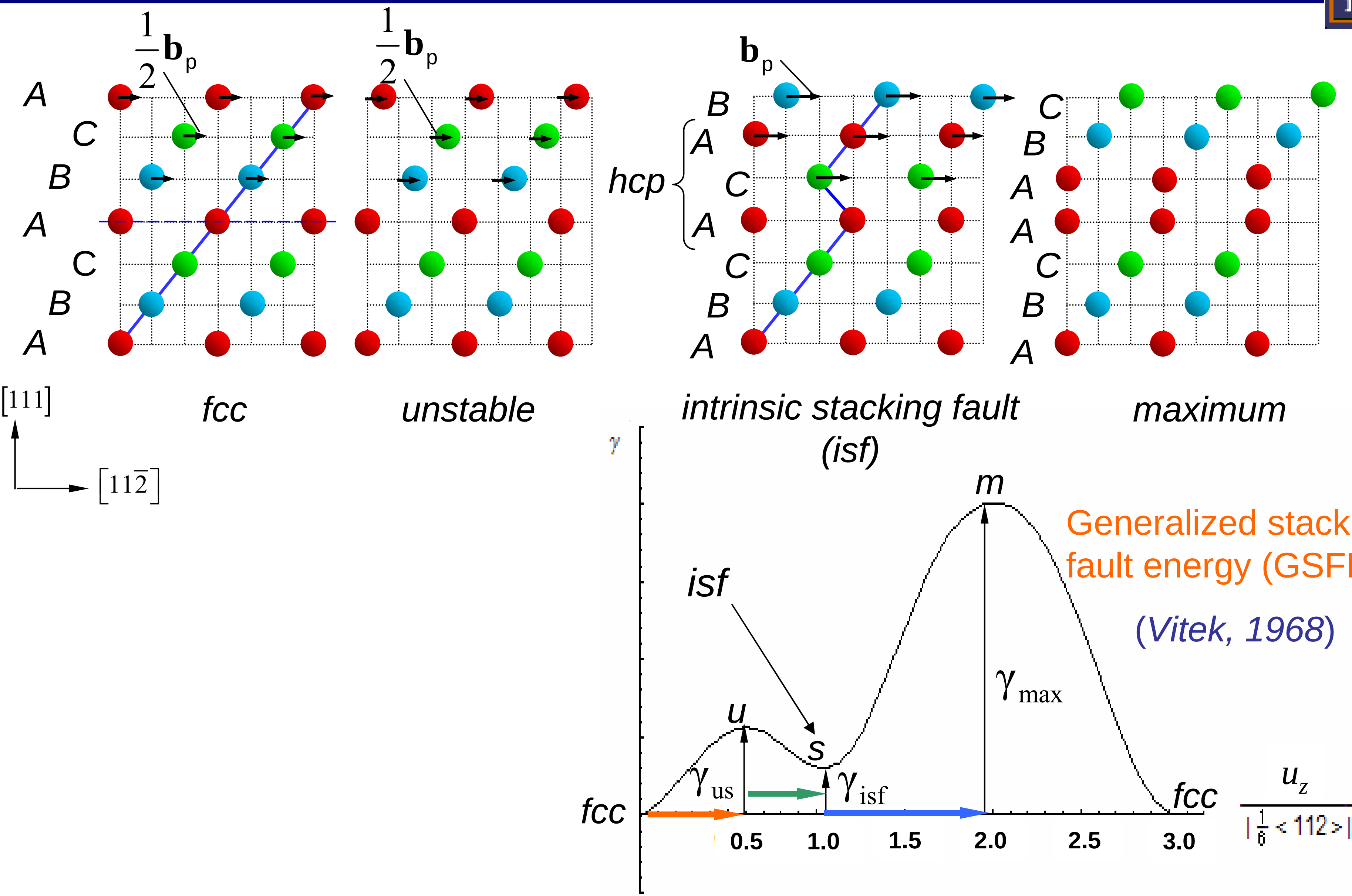
Intrinsic stacking fault



Intrinsic stacking fault *slipped state*

Lee et al., Acta Mater (2001)

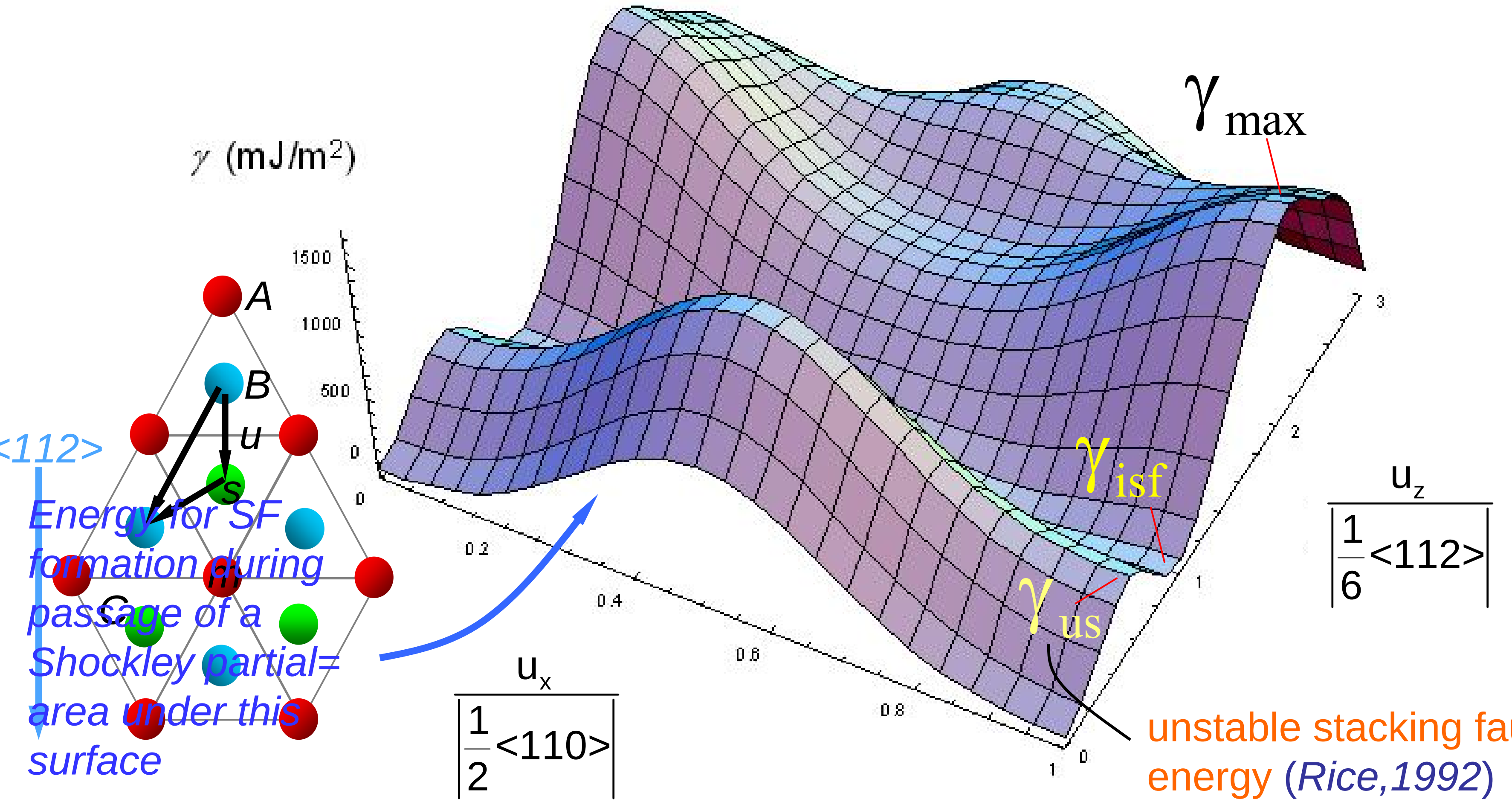
Energy pathway for a stacking fault



Generalized stacking fault energy (GSFE)

(*Vitek, 1968*)

Energy landscape for a stacking fault (γ-surface)

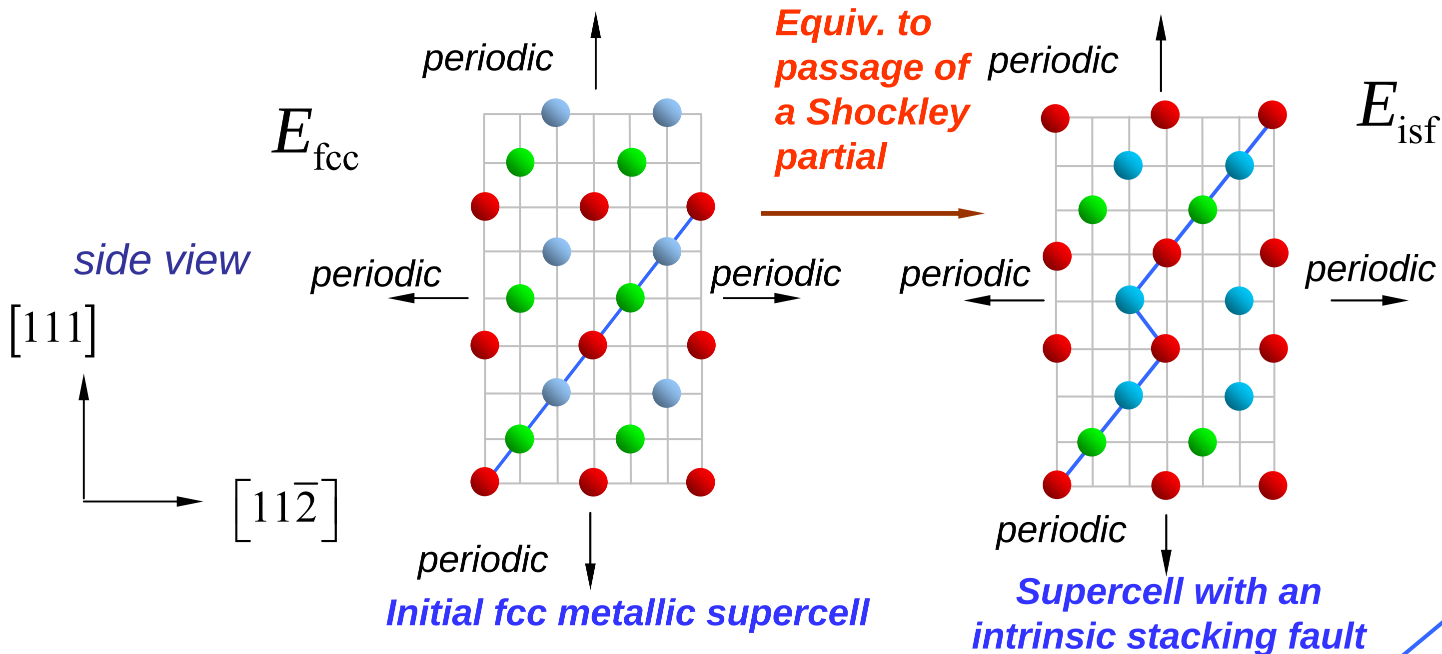


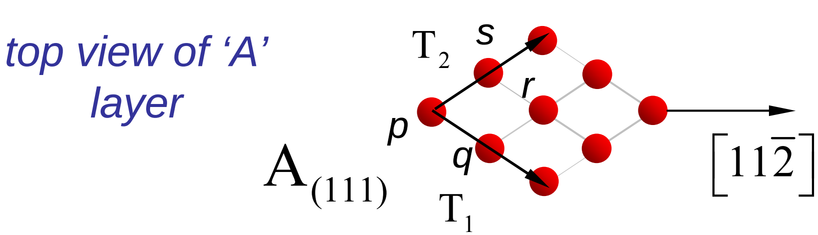
Energy for SF formation during passage of a Shockley partial= area under this surface

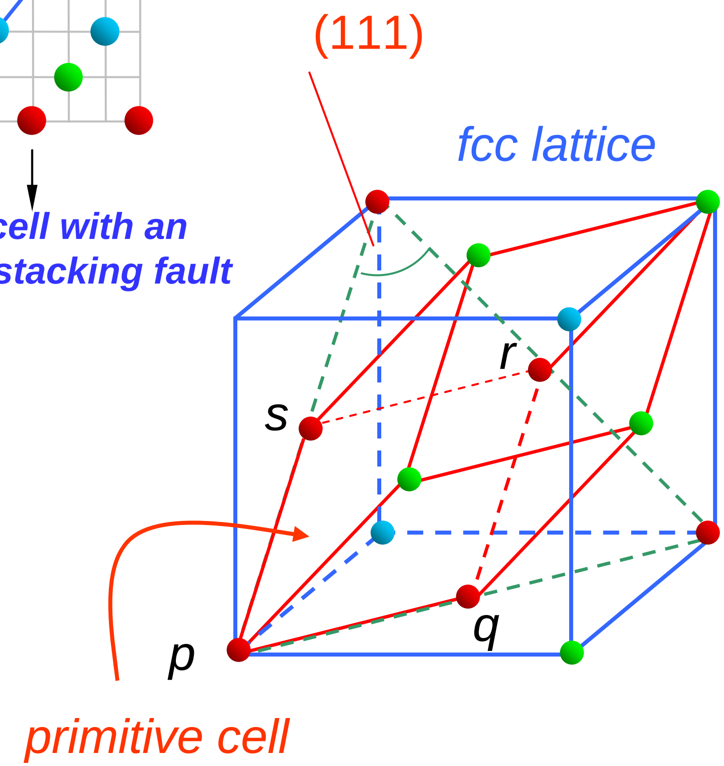
unstable stacking fault energy (*Rice,1992*)

S. Kibey, J.B. Liu, M. W. Curtis, D. D. Johnson and H. Sehitoglu, Acta Mater. 54 (2006) 2991-3001

Calculating the energy required to shear the lattice

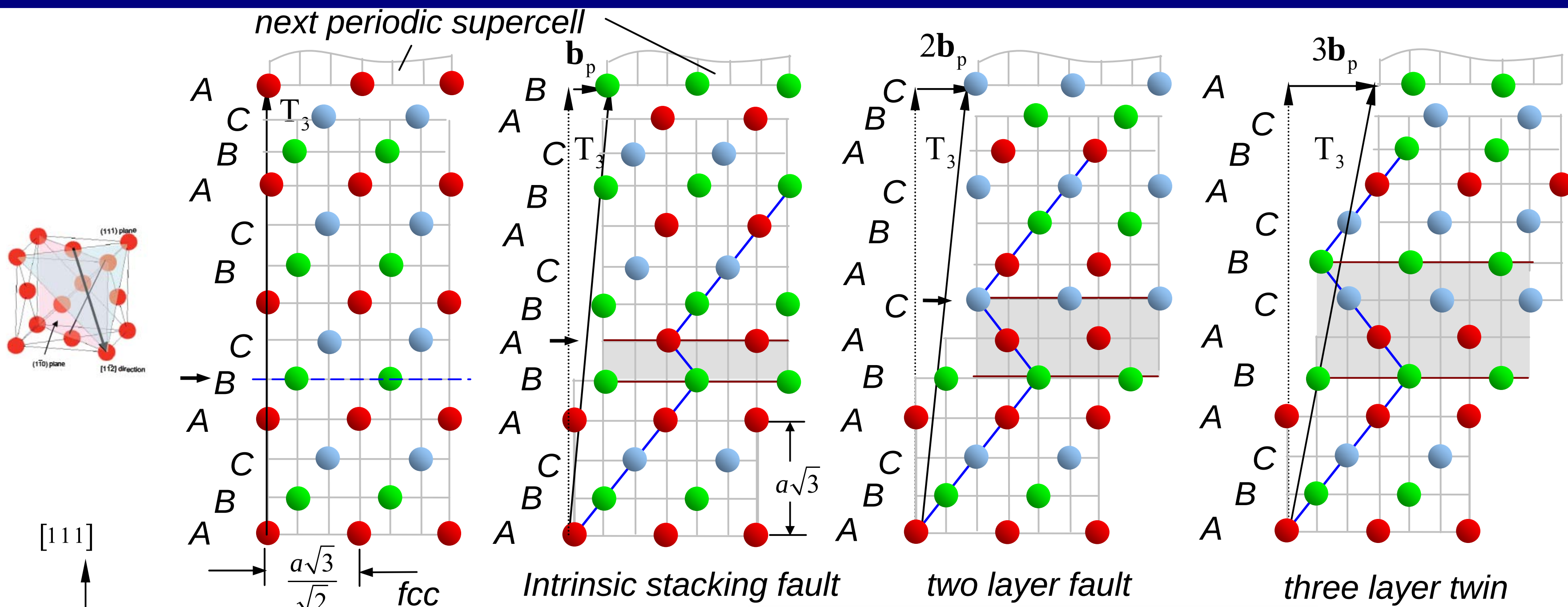


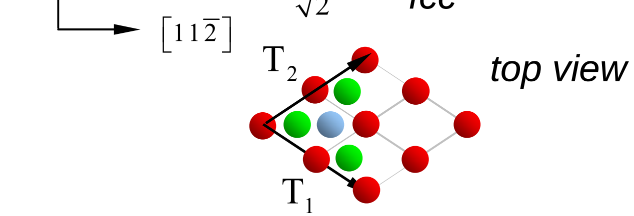


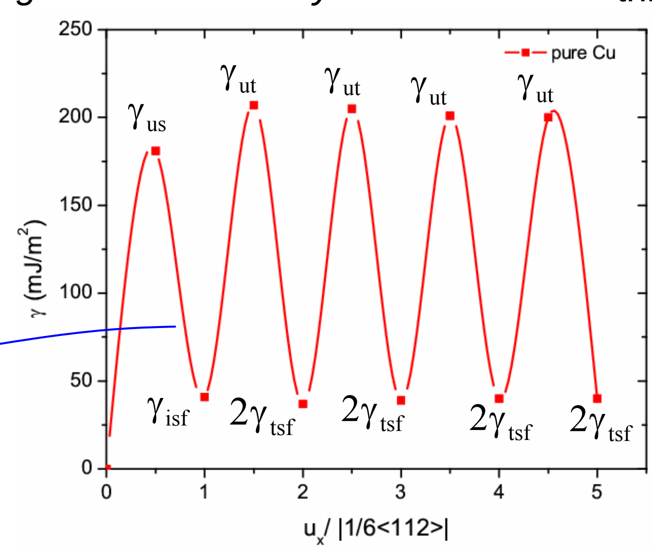


stacking fault energy $$\gamma_{isf} = \frac{E_{isf} - E_{fcc}}{A_{(111)}}$$

Energy required to twin the lattice

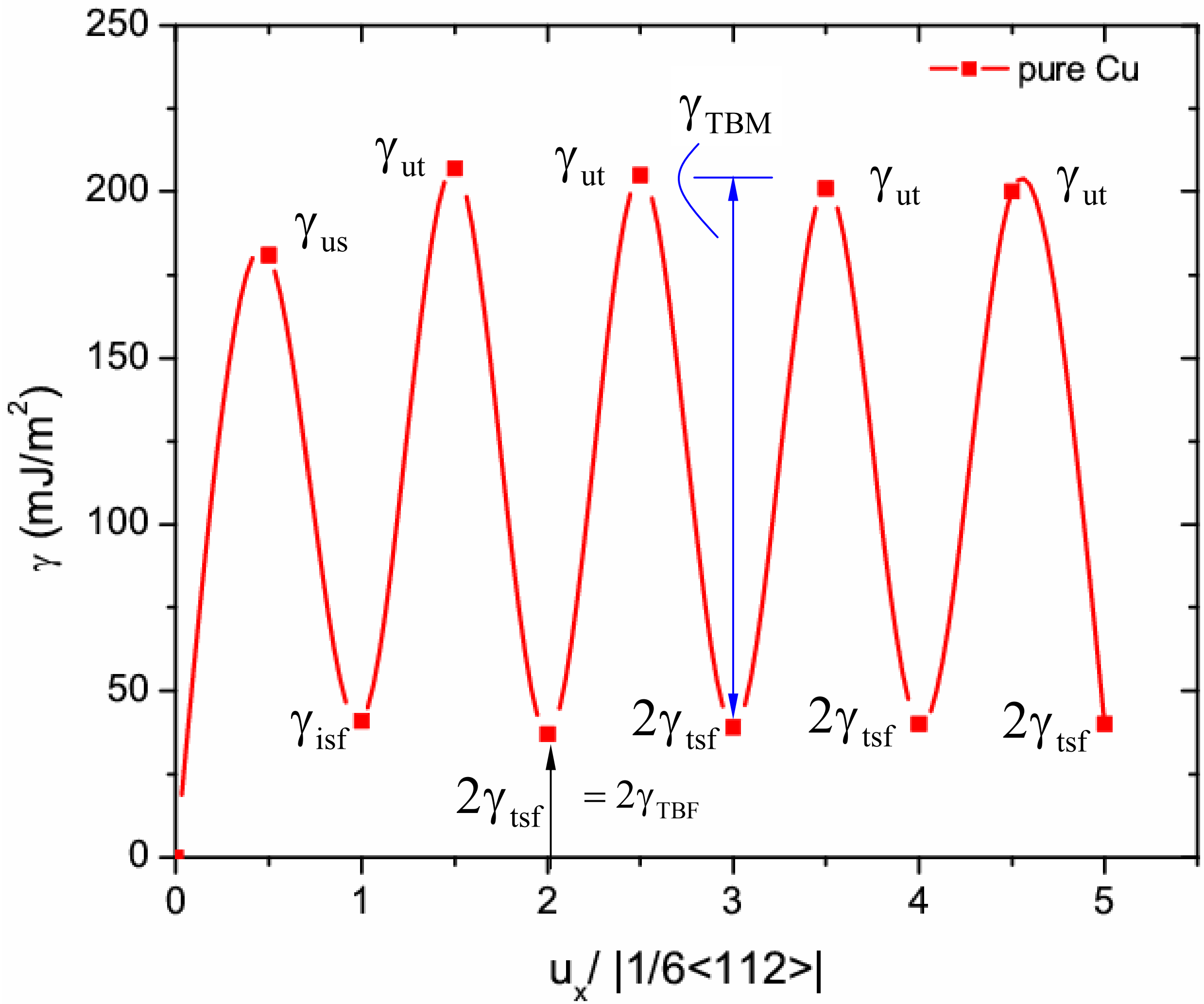






Area under this curve is the required energy to twin the lattice by successive shear

Energy pathway for twinning : pure Cu

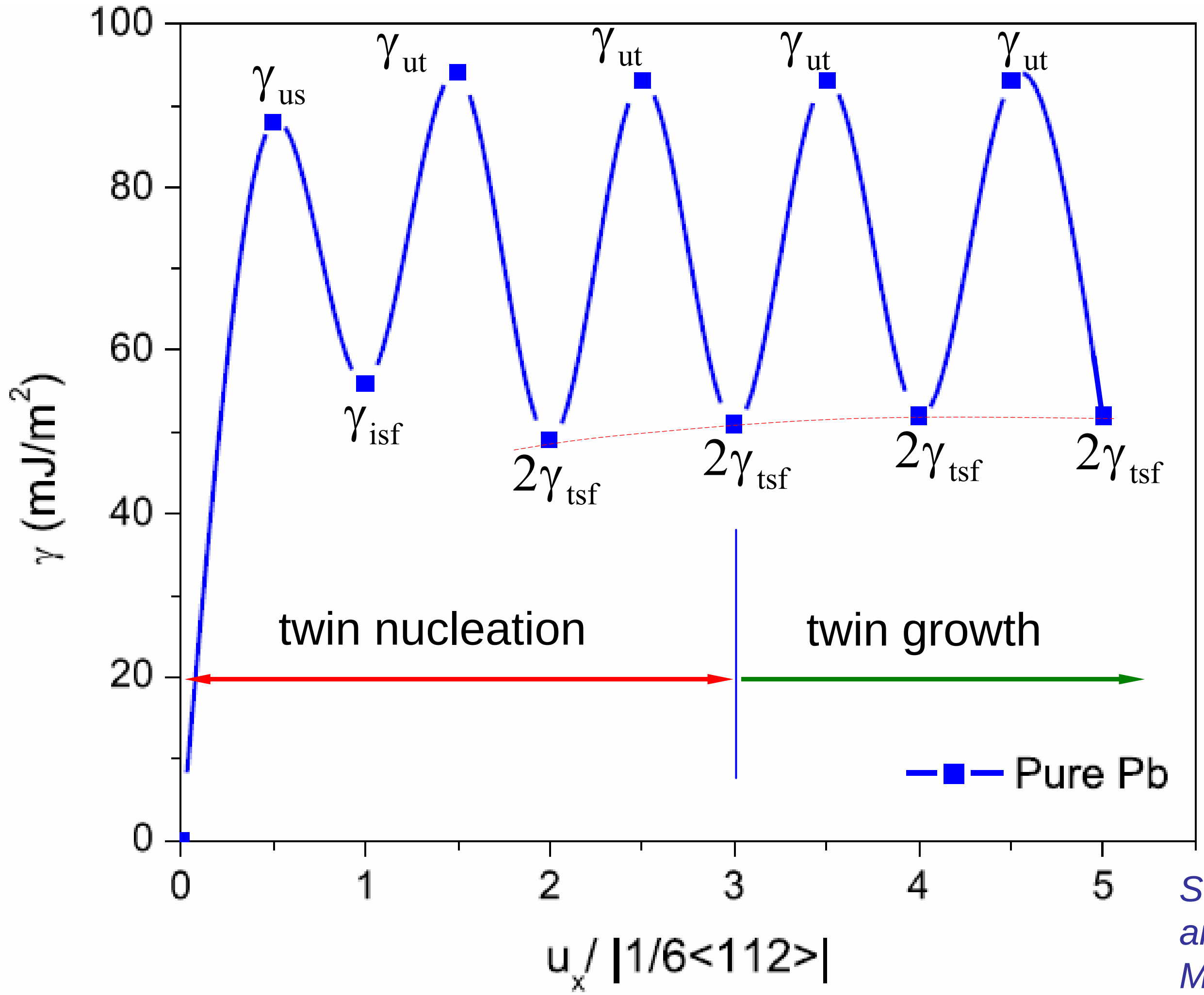


- VASP-PAW-GGA
- 8 x 8 x 4 k-point mesh
- 273.2 eV energy cutoff.

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Appl. Phys. Lett. 89 (2006) 191911.

Fault energies converge after third layer sliding indicating the completion of twin nucleation.

Energy pathway for twinning : pure Pb



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

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Convergence occurs after the third layer sliding for Pb as well. Hence, a three-layer twin is considered as the basic nucleus in fcc metals.

Computed fault energies for fcc metals

Metal	γ_{us}	γ_{isf}		γ_{ut}	$2\gamma_{tsf}$	
	Theory	Theory	Expt.	Theory	Theory	Expt.[a]
Pb (4.95 Å)	87	49	—	92	44	—
Ag (4.09 Å)	133	18	16[a]	143	18	16
Au (4.08 Å)	134	33	32[a]	148	31	30
Cu (3.61 Å)	180	41	45[a]	200	40	48
Ni[b] (3.51 Å)	273	110	125[a]	324	110	86
Pd (3.89 Å)	287	168	180[a]	361	172	—
Pt (3.92 Å)	339	324	322[a]	486	321	322
Al (4.05 Å)	162	130	120[c]	215	113	150

[a] *fault energies from individual Refs. in Table A-1, Hirth and Lothe (1982).*

(all energies in mJ/m^2)

[b] *fault energies* computed using SP-PAW-GGA**.** *Siegel, Appl. Phys. Lett. (2005)*

[c] *pair potential. Rautioaho, Phys. Status Sol. (1982).*

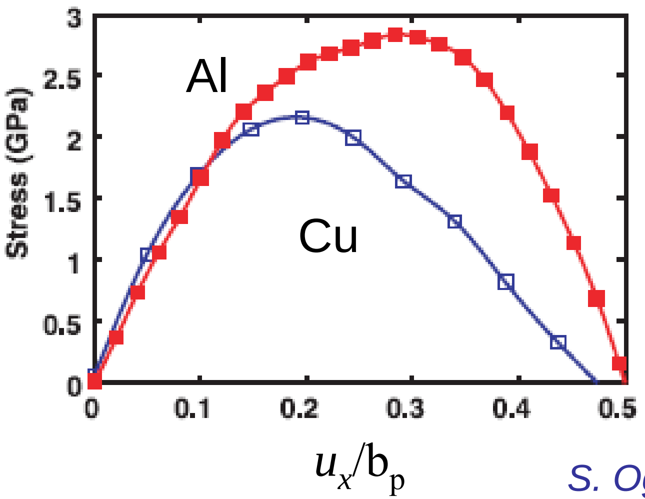
The above table represents the most complete set of DFT-based theoretical calculations of fault energies for fcc metals.

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Ideal strength prediction from GPFE

Ideal twinning stress can be related to the GPFE curves as follows:

$$\tau_{\mathrm{ideal}} = -\frac{\partial \gamma(u_x)}{\partial u_x} = \frac{(\gamma_{\mathrm{ut}} - 2\gamma_{\mathrm{tsf}})}{\pi b_{\mathrm{twin}}}$$



S. Ogata, J. Li and S. Yip, Science (2002).

Simple shear case

However, non-ideal (real) twinning stresses of materials are of the order of MPa due to presence of defects.

Can we predict realistic critical stresses using mesoscale models in conjunction with defect energy landscapes?

Classical twin nucleation model

Classical twinning stress equation:

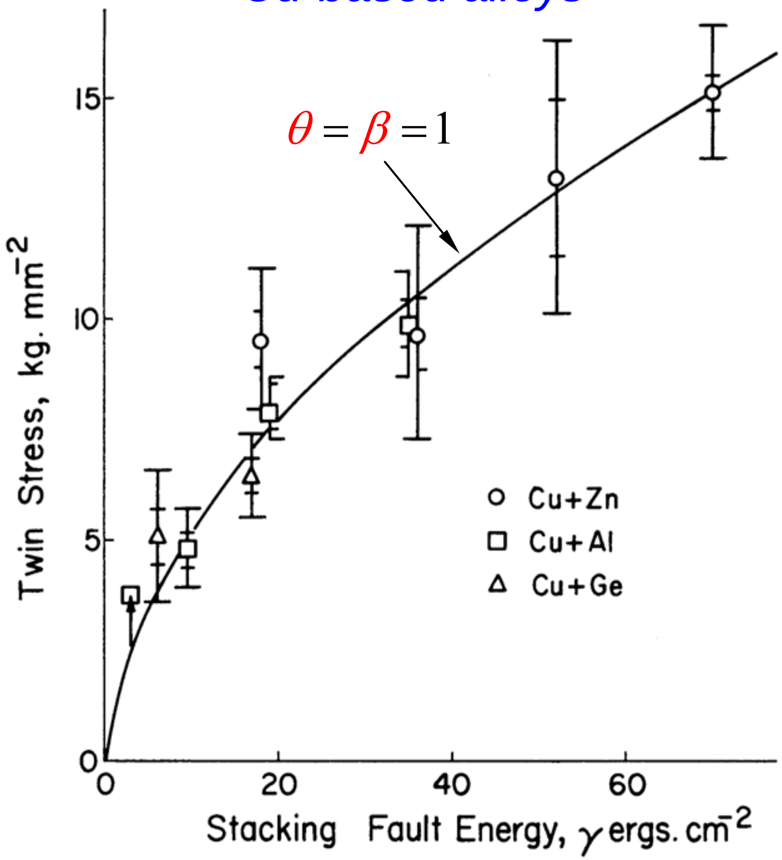
$$\left[\left(\frac{1-2\theta}{2\beta}\right)+K\theta^{2}\tau_{crit}\right]\tau_{crit}=\frac{\gamma_{isf}}{b_p}$$

fitting parameters: K, θ and β

Calibration of fitting parameters for different alloys is required.

need a more fundamental approach to predict twinning stress.

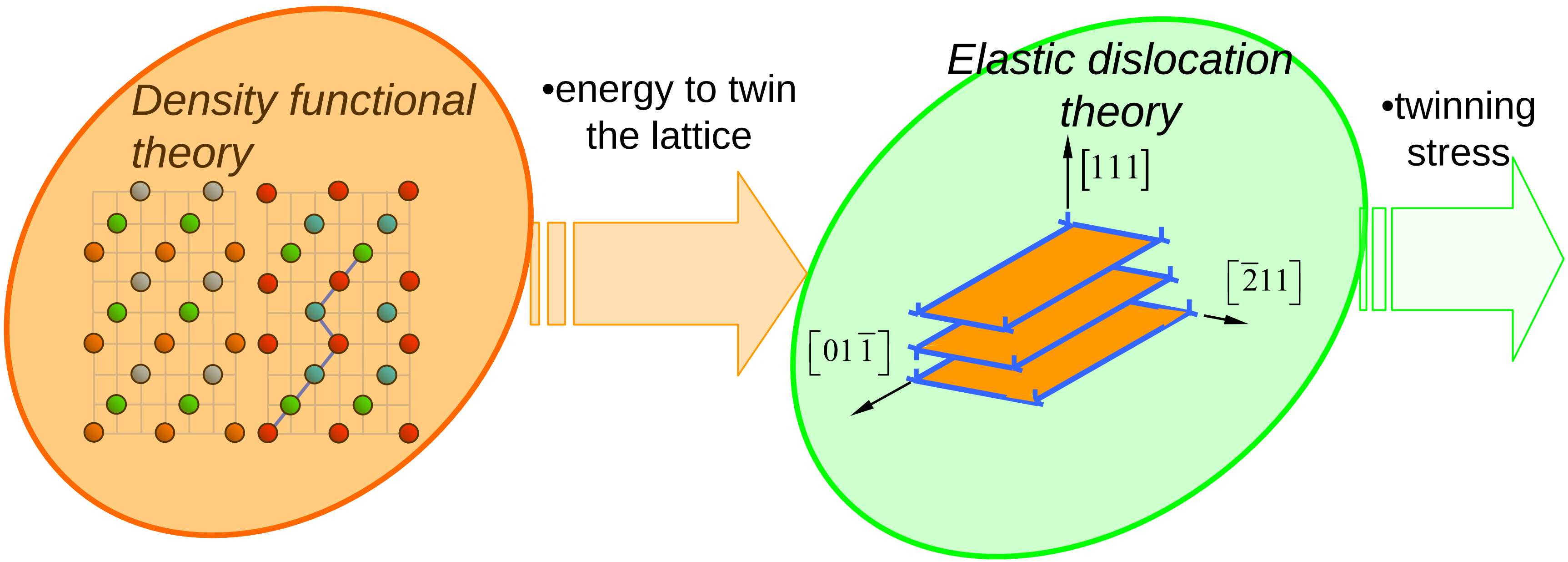
Cu-based alloys



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

Present Approach

atomic scale *mesoscale*

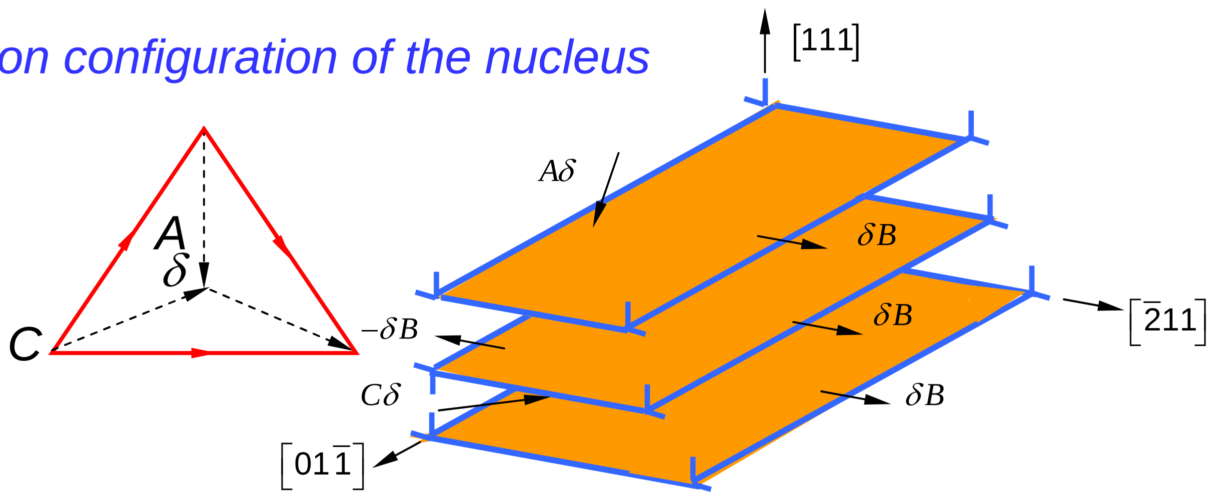


Mesoscale model for fcc twins

Total energy of the twin nucleus:

$$E_{total} = \underbrace{E_{edge}}_{\text{energy contribution of edge components}} + \underbrace{E_{screw}}_{\text{energy contribution of screw components}} - \underbrace{W_{\tau}}_{\text{work done by applied stress}} + \underbrace{E_{GPFE}}_{\text{energy associated with twin-energy pathway}}$$

Dislocation configuration of the nucleus



Mahajan and Chin, Acta Metallurgica (1973)

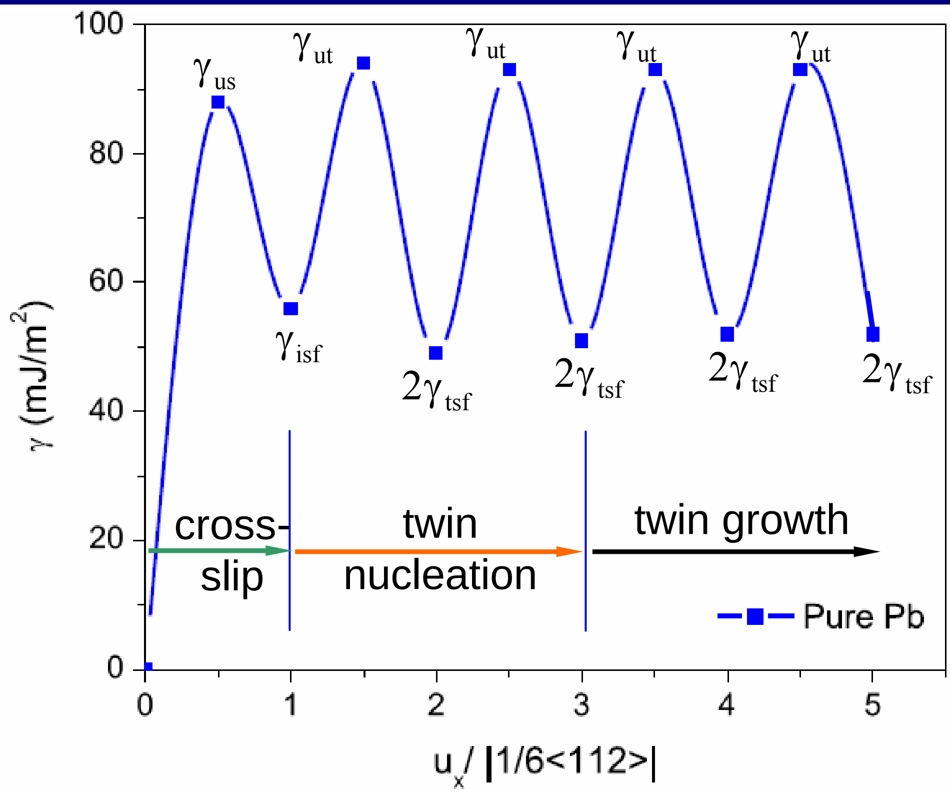
Total energy:

$$E_{total}(d,N) = \frac{Gb_e^2 d}{4\pi(1-\upsilon)}\left[N^2\left\{ln\left(\frac{d}{N}\right)+\frac{1}{2}\right\} - N\,ln\left(\frac{d}{r_0}\right) - \frac{1}{6}ln(N)\right] + \frac{Gb_s^2}{9\pi}dN^2\left[ln\left(\frac{d}{N}\right)-\frac{1}{2}\right]$$

$$-N\tau d^2 b_{twin} + E_{GPFE}$$

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Total energy of the twin nucleus



Energy contribution of GPFE:

$$\underbrace{E_{GPFE}}_{\text{energy associated with twin-energy pathway}} = \underbrace{E_{\gamma\text{-}twin}}_{\text{energy required to twin the lattice}} - \underbrace{E_{\gamma\text{-}SF}}_{\text{energy required to cross-slip}}$$

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

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

Total energy:

$$E_{total}(d,N) = \frac{Gb_e^2 d}{4\pi(1-\upsilon)}\left[N^2\left\{ln\left(\frac{d}{N}\right)+\frac{1}{2}\right\} - N\,ln\left(\frac{d}{r_0}\right) - \frac{1}{6}ln(N)\right] + \frac{Gb_s^2}{9\pi} dN^2\left[ln\left(\frac{d}{N}\right)-\frac{1}{2}\right]$$
$$+(N-1)\,d\int_0^d \gamma_{twin}\,dx - d\int_0^d \gamma_{SF}\,dx - N\tau d^2 b_{twin}$$

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Twinning stress equation

For a stable twin configuration:

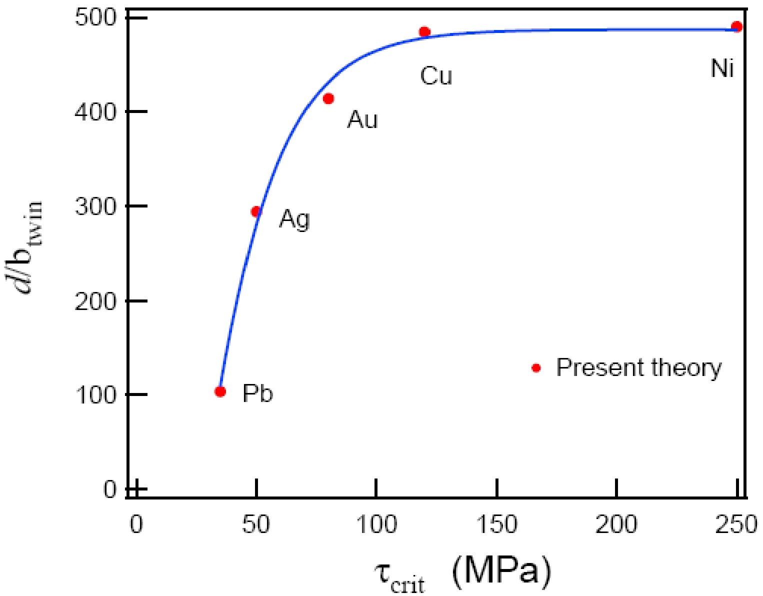
$$\frac{\partial E_{total}}{\partial d} = 0 \; , \; \frac{\partial E_{total}}{\partial N} = 0 \Rightarrow \tau = \tau(\gamma_{\mathrm{isf}}, \gamma_{\mathrm{tsf}}, \gamma_{\mathrm{us}}, \gamma_{\mathrm{ut}}, G_{\{111\}}, N, d)$$

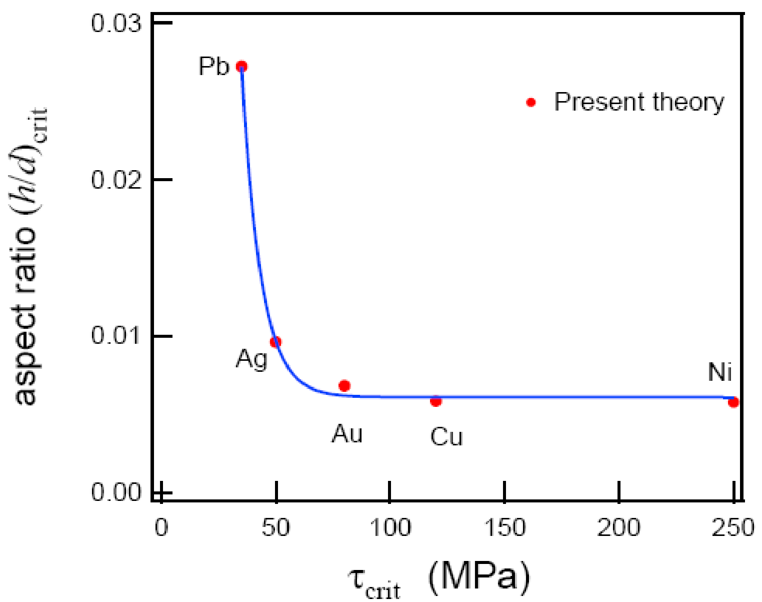
$$\begin{aligned}\tau(d) = & \frac{G_{\{111\}}N}{\pi d}\left[\frac{\mathrm{b}_{\mathrm{e}}^2}{4(1-\nu)} + \frac{\mathrm{b}_{\mathrm{s}}^2}{9}\right] + \frac{2}{3N\mathrm{b}_{\mathrm{twin}}}\left(\frac{3N}{4} - 1\right)\left[\gamma_{\mathrm{ut}} + \frac{(2\gamma_{\mathrm{tsf}} + \gamma_{\mathrm{isf}})}{2}\right] \\ & + \frac{1}{6\mathrm{b}_{\mathrm{twin}}}\left[\gamma_{\mathrm{ut}} - \frac{(2\gamma_{\mathrm{tsf}} + \gamma_{\mathrm{isf}})}{2}\right]\left(\frac{w}{d}\right)\left[\ln\left(\frac{d + \sqrt{d^2 + w^2}}{w}\right) + \frac{d}{\sqrt{d^2 + w^2}}\right] \\ & - \frac{2}{3N\mathrm{b}_{\mathrm{twin}}}(\gamma_{\mathrm{us}} + \gamma_{\mathrm{isf}}) + \frac{1}{3N\mathrm{b}_{\mathrm{twin}}}(\gamma_{\mathrm{us}} - \gamma_{\mathrm{isf}})\left(\frac{w}{d}\right)\left[\ln\left(\frac{d + \sqrt{d^2 + w^2}}{w}\right) + \frac{d}{\sqrt{d^2 + w^2}}\right]\end{aligned}$$

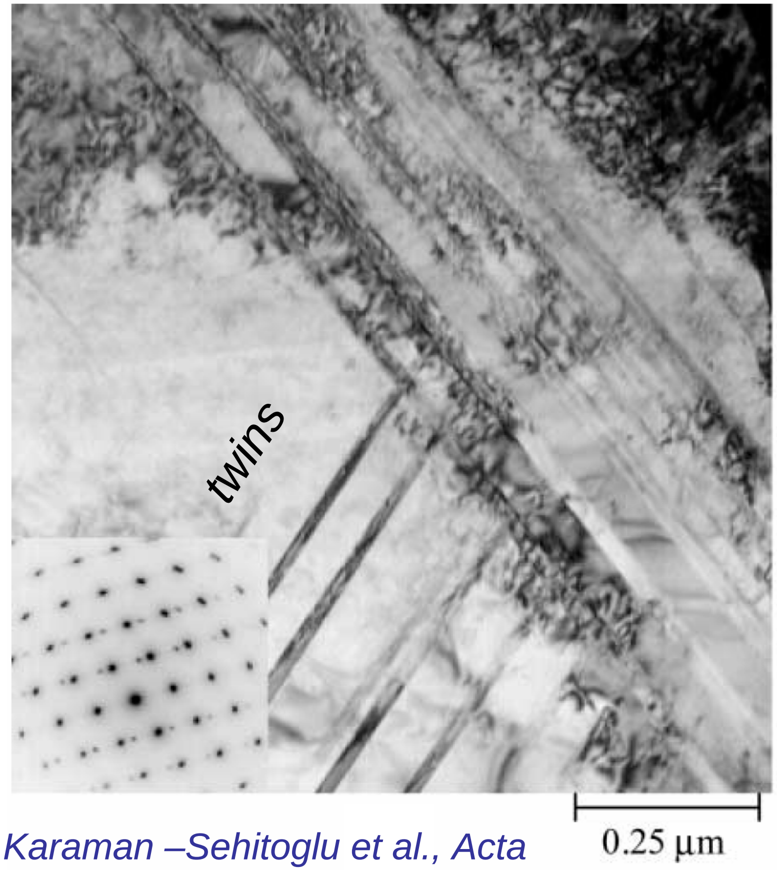
$$\tau_{\mathrm{crit}} = \begin{cases} \text{Minimize} & \tau(d) \\ \text{subject to} & d \geq \mathrm{b}_{\mathrm{twin}}. \end{cases}$$

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Twin nucleus shape







Karaman –Sehitoglu et al., Acta Mater (2001)

316 stainless steel at 3% strain

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

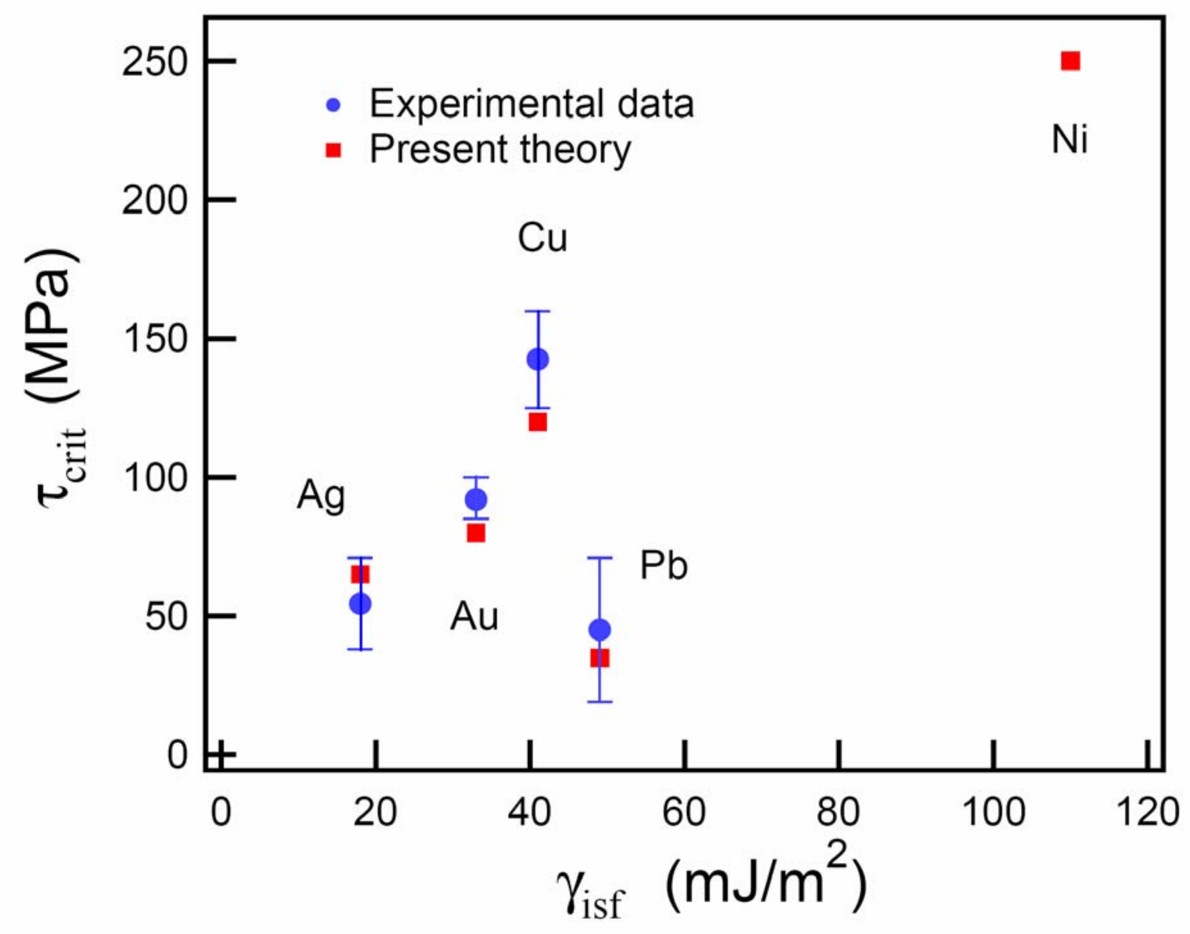
For Thin twins

$$\tau_{crit} = \frac{2}{3N b_{twin}}\left(\frac{3N}{4}-1\right)\left[\gamma_{ut} + \frac{(2\gamma_{tsf}+\gamma_{isf})}{2}\right] - \frac{2}{3N b_{twin}}(\gamma_{us}+\gamma_{isf})$$

Increases Critical Twin Stress

Decreases Critical Twin Stress

Predicted twinning stresses for fcc metals



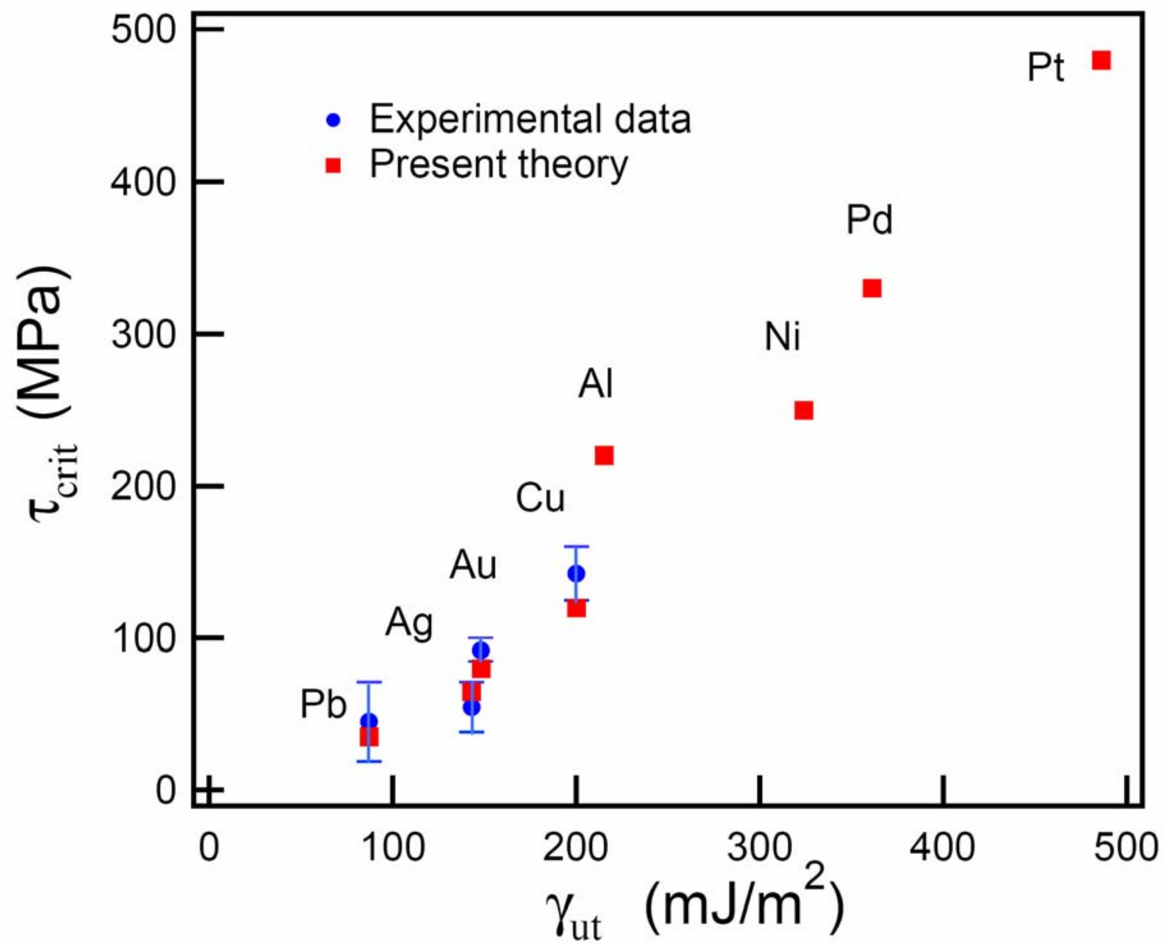
$$\tau_{crit} \sim K \frac{\gamma_{isf}}{b_{twin}}$$

does not hold !

Twinning stress depends non-monotonically on stacking fault energy.

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Predicted twinning stresses for fcc metals (contd.)



Twinning stress depends monotonically on unstable twin SFE .

γ_{ut} *governs the physics of twin nucleation.*

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Predicted twinning stresses for fcc metals (contd.)

Metal	τ_{crit}^{theory} (MPa) (predicted)	τ_{crit}^{expt} (MPa) (expt.)	τ_{ideal}^{theory} (MPa)	Deformation mechanism
Pb	40	19 – 71[b]	660	twinning
Ag	65	38 – 71[c]	1910	twinning
Au	80	85 – 100[d]	2210	twinning
Cu	120	125 – 160[e]	3380	twinning
Ni	250	—	4680	twinning
Al	220	—	1940	cross-slip
Pd	330	—	5260	cross-slip
Pt	480	—	3240	cross-slip

[b] *Bolling, Casey and Richman, Phil. Mag. (1965).*

[c] *Suzuki and Barrett, Acta Metall. (1958).*

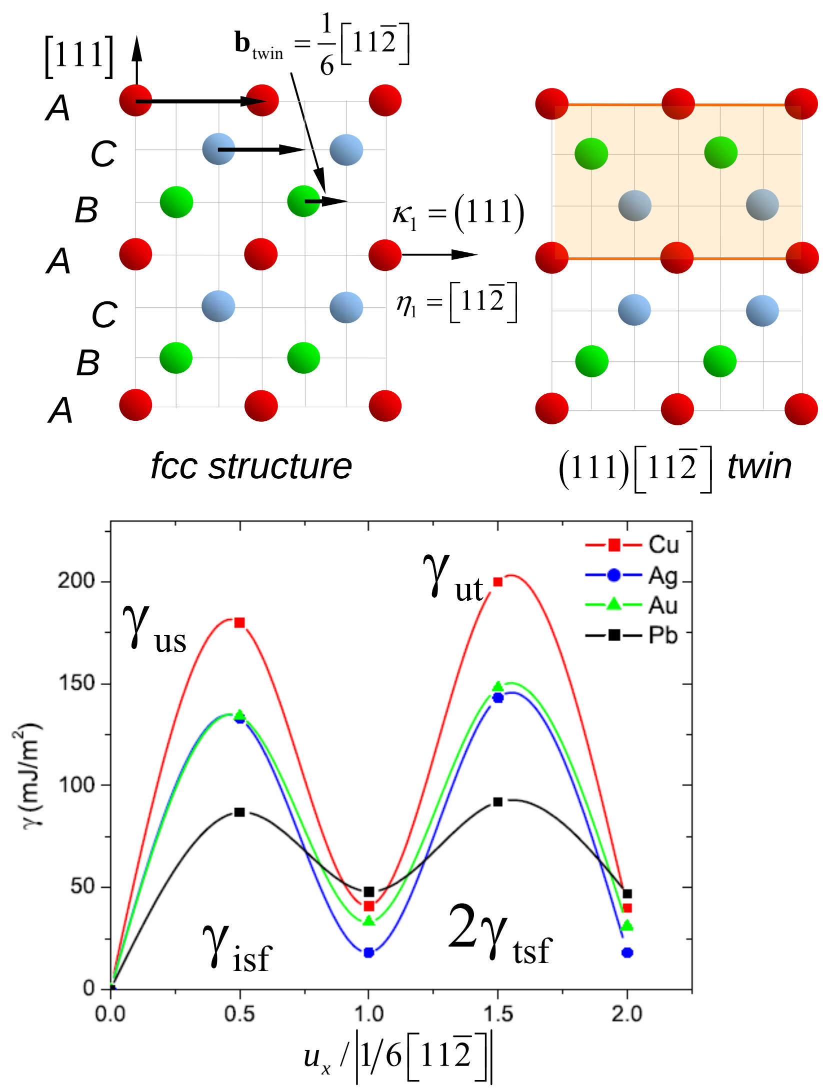
[d] *Narita et al., J. Japan Inst. Metals (1978).*

[e] *Yamamato et al., J. Japan Inst. Metals (1983).*

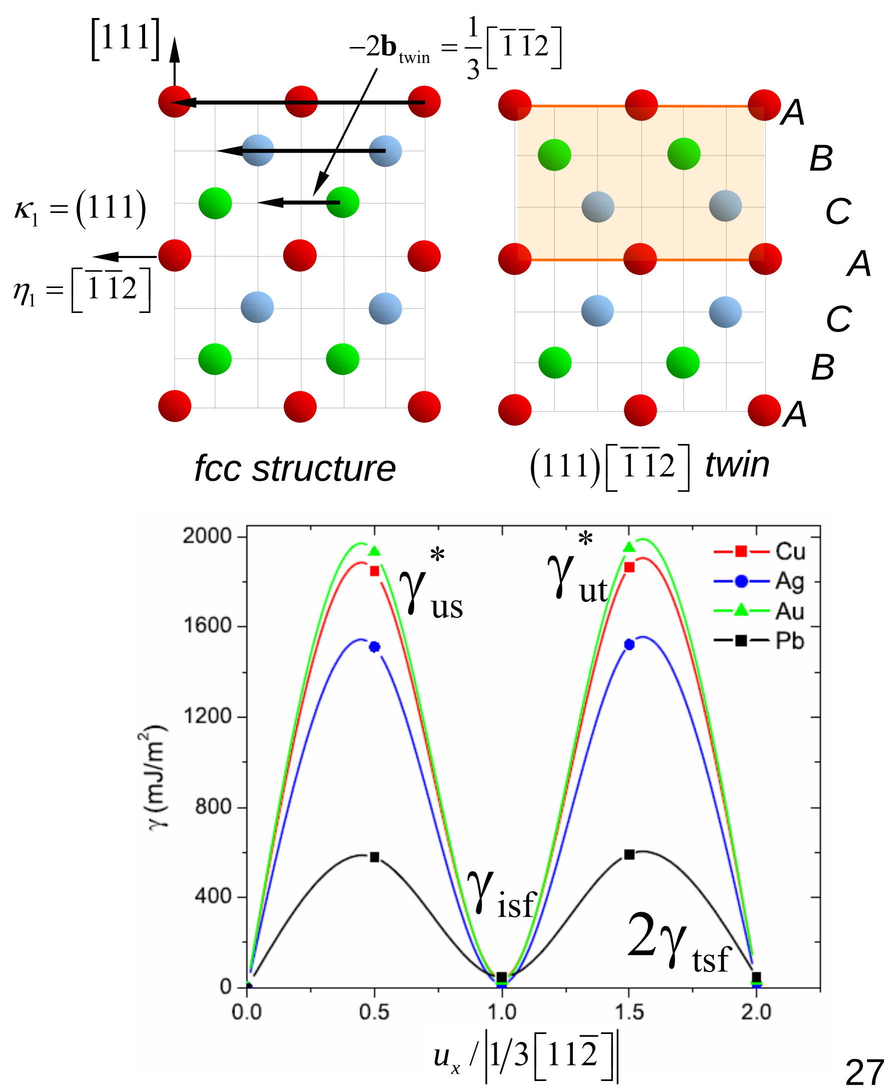
S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, Acta Materialia 55 (2007) 6843-6851

Twinning is directional

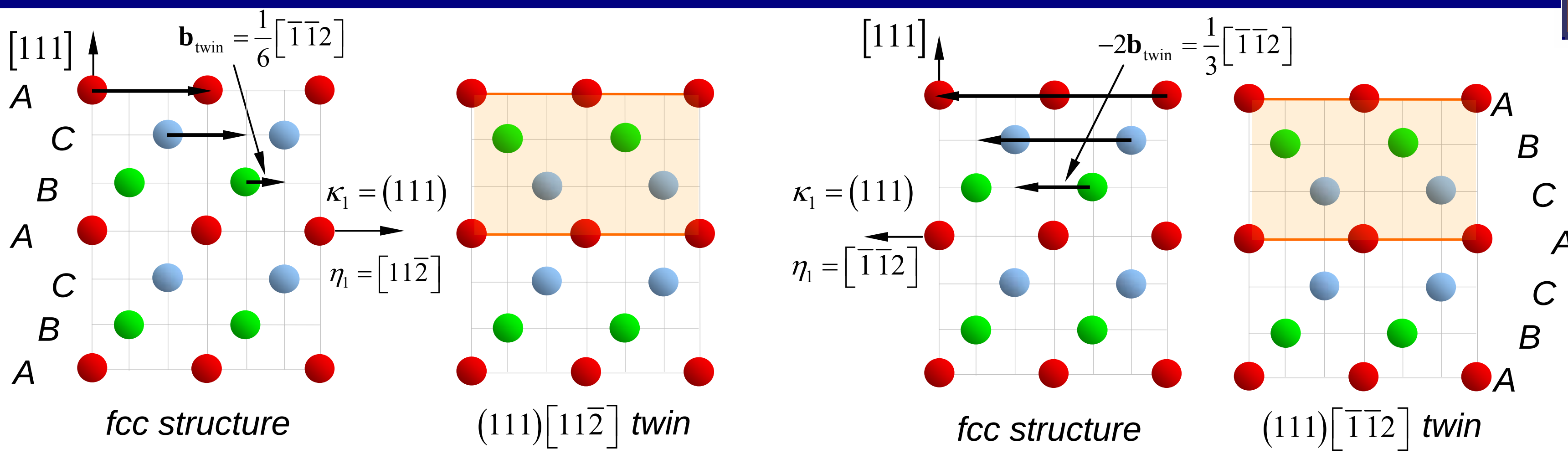
Energetically favorable and observed



Energetically unfavorable and not observed



Twinning directionality



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

$T \geq 1 \Rightarrow$ *twin nucleation*

Bernstein and Tadmor
Phys. Rev. B (2004)

twinning mode				$(111)[11\bar{2}]$					$(111)[\bar{1}\bar{1}2]$			
Metal	a_0(Å)	γ_{isf}	$2\gamma_{\text{tsf}}$	γ_{us}	γ_{ut}	T	τ_{crit}	τ_{expt}	γ^*_{us}	γ^*_{ut}	T^*	τ^*_{crit}
Pb	4.95	48	47	87	92	1.02	40	19-71[a]	578	592	1.11	170
Ag	4.09	13	12	133	143	1.09	65	38-71[b]	1512	1522	1.13	310
Au	4.08	33	31	134	148	1.05	80	85-100[c]	1930	1947	1.13	400
Cu	3.61	41	40	180	200	1.05	120	125-160[d]	1847	1865	1.13	370

(all energies in mJ/m^2 & stresses in MPa)

S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu, APL,91,181916 (2007)

Summary

- *Presented a hierarchical, multiscale, adjustable parameter-free approach for twin nucleation in fcc metals and alloys.*
- *Predicted twinning stresses are in excellent agreement with available experimental data.*
- *Our theory inherently accounts for directional nature of twinning.*

Outline

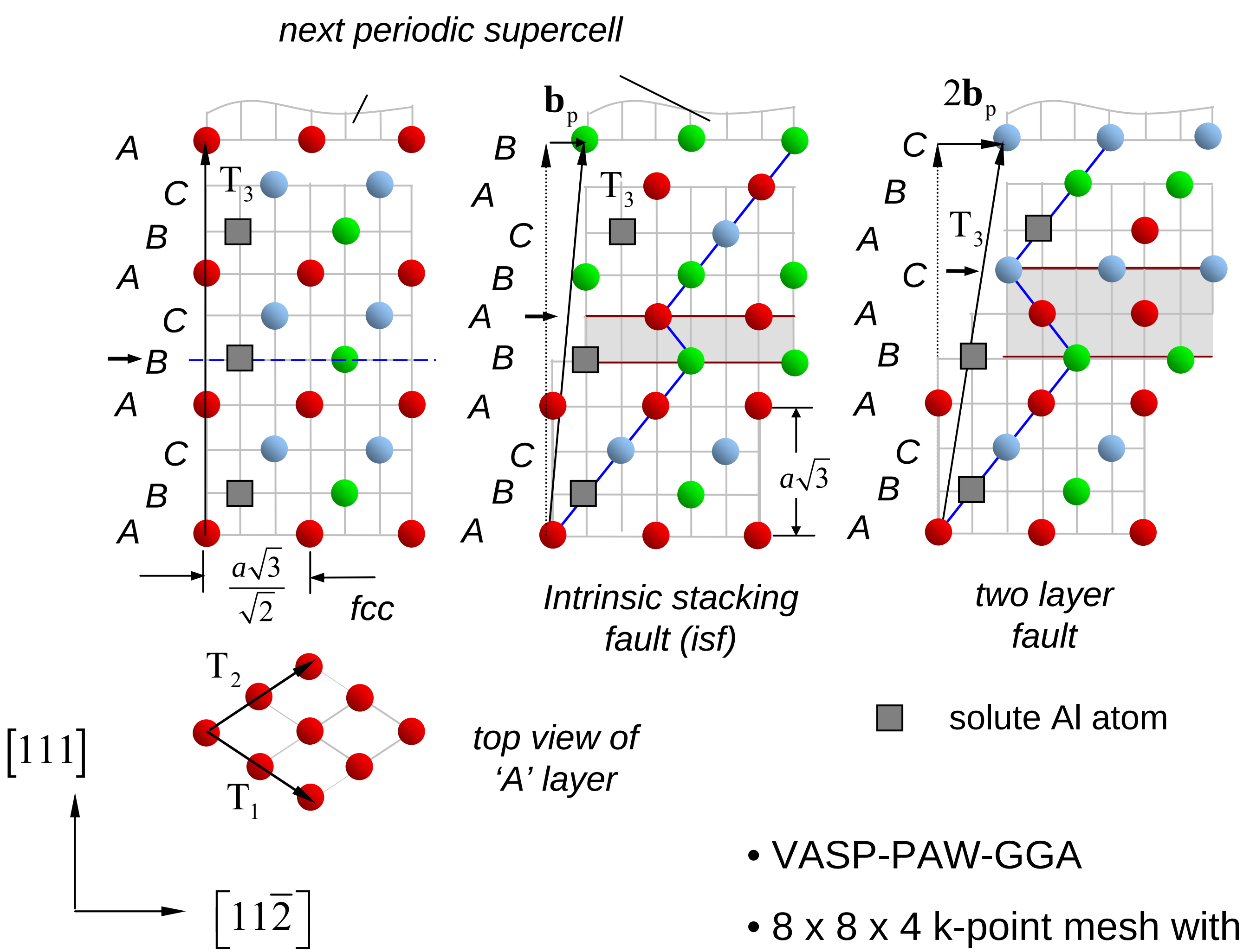
- Stacking faults in fcc materials.
  - Energy landscape/pathway (GSFE) – atomic level.

- Deformation twinning in fcc metals.
  - Energy landscape/pathway (GPFE).
  - Mesoscale twinning stress model

- Material Design (Cu-Al, Hadfield Steel with Nitrogen)

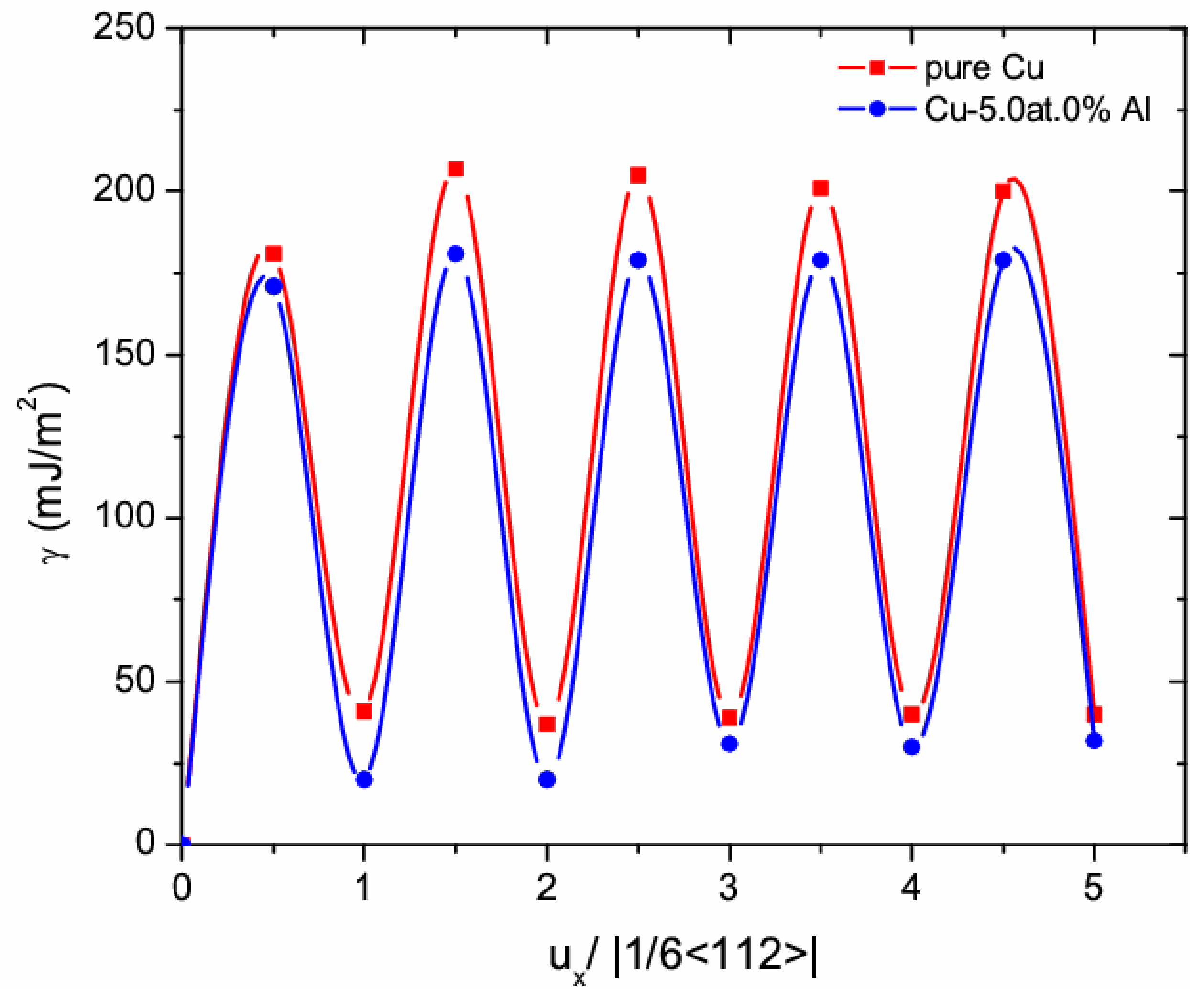
- Summary

Supercell for Cu-8.3at.%Al



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

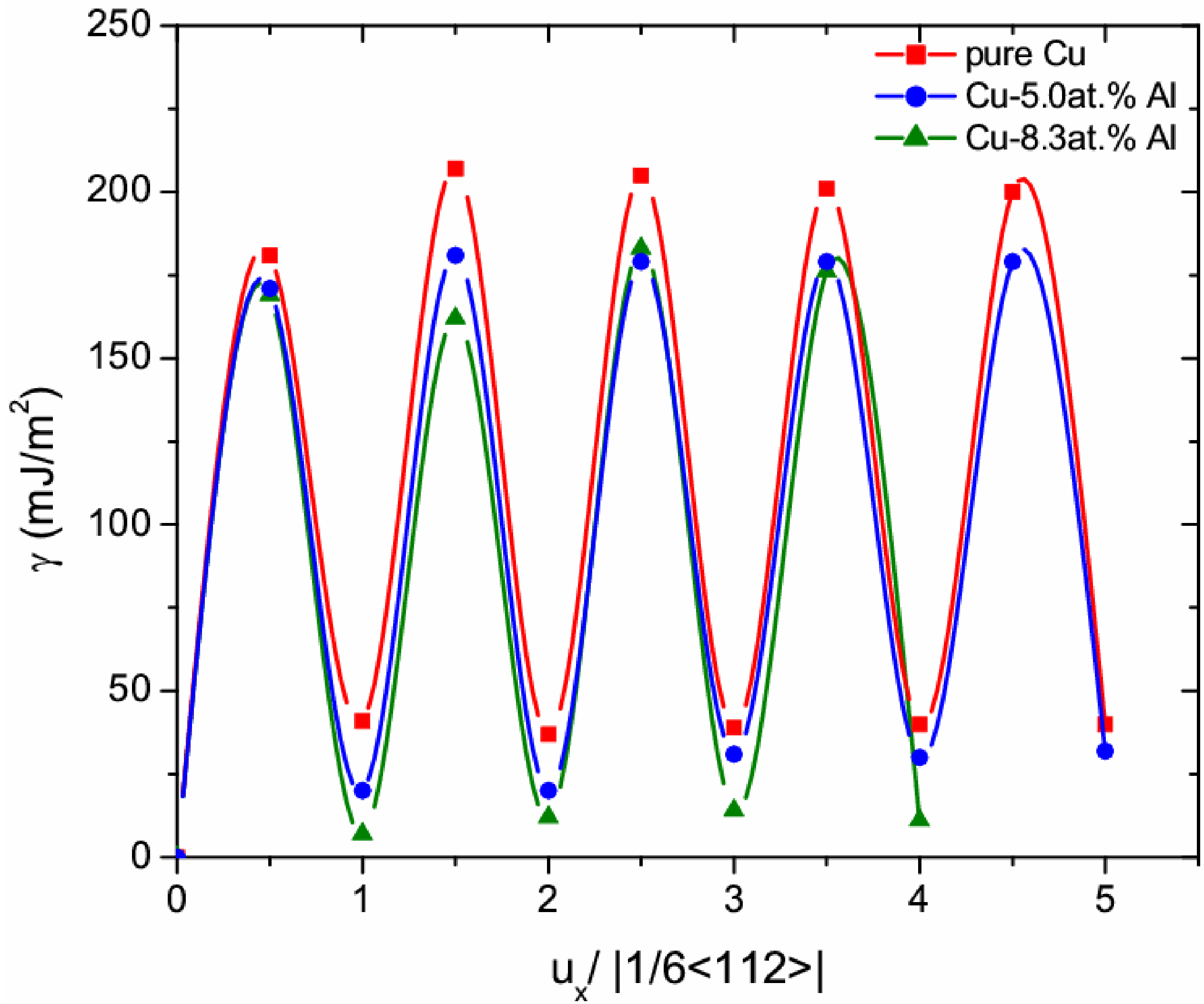
GPFE curves for Cu-Al alloys



Convergence at the third layer sliding is seen for Cu-5.0at.% Al as well. Hence, a three-layer twin is the basic nucleus in fcc alloys.

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

GPFE curves for Cu-Al alloys (contd.)



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

Predicted fault energies for Cu-xAl

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

(all energies in mJ/m^2)

The only ab initio calculations reported for fcc Cu-Al alloys.

[a] *Murr, Interfacial Phenomena in Metals and Alloys (1975).*

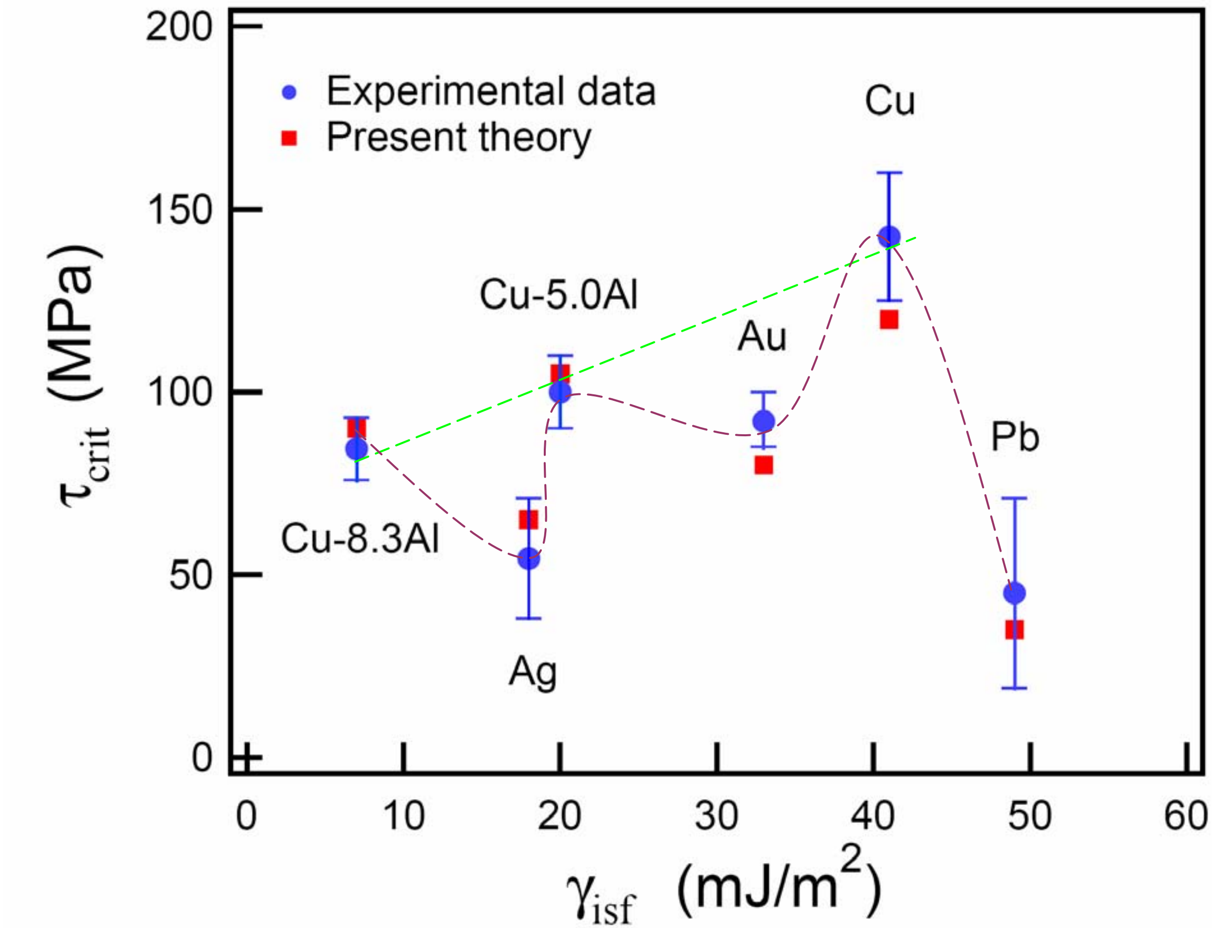
[b] *Ogata, Li and Yip Phys. Rev. B (2005).*

[c] *Carter and Ray, Phil. Mag. (1977).*

[d] *Pearson In: A Handbook of Lattice Spacings and Structures of Metals and Alloys (1958)*

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

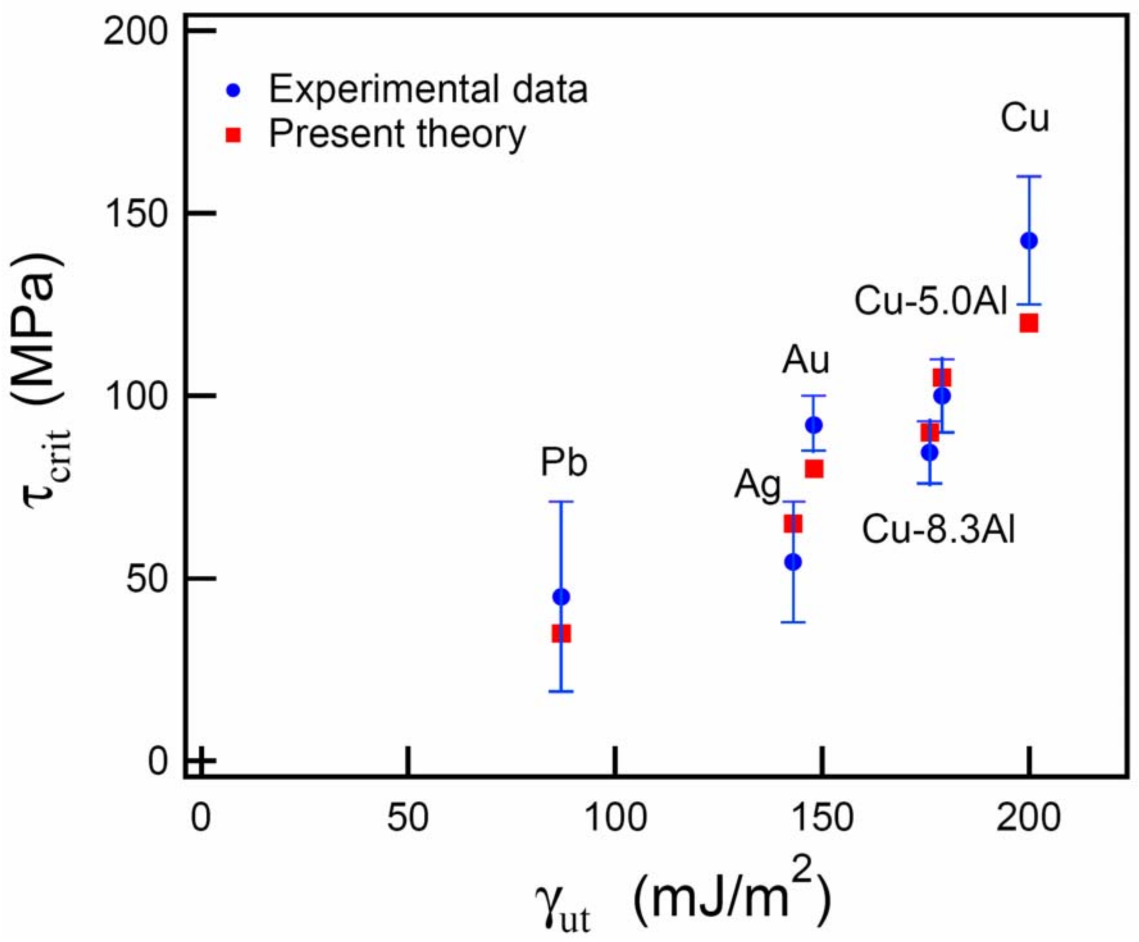
Prediction of twinning stresses in alloys



Twinning stress depends non-monotonically on intrinsic SFE. However, within Cu-xAl, the variation is monotonic. The present hierarchical, theory of twinning stress holds for fcc metals and alloys.

S. Kibey, L. L. Wang, J.B. Liu, D.D. Johnson, H. T. Johnson and H. Sehitoglu, manuscript in preparation.

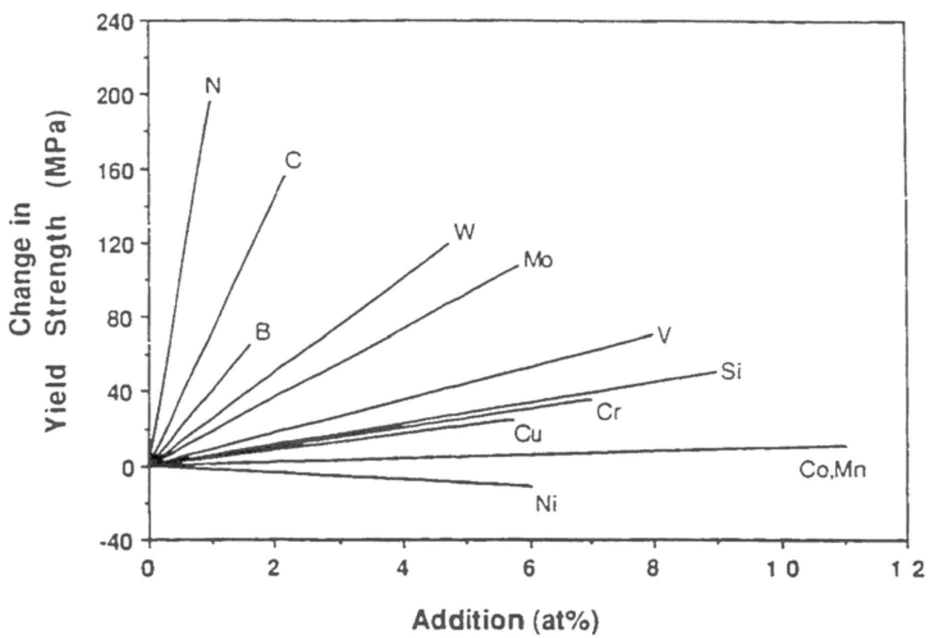
Prediction of twinning stresses in alloys (contd.)



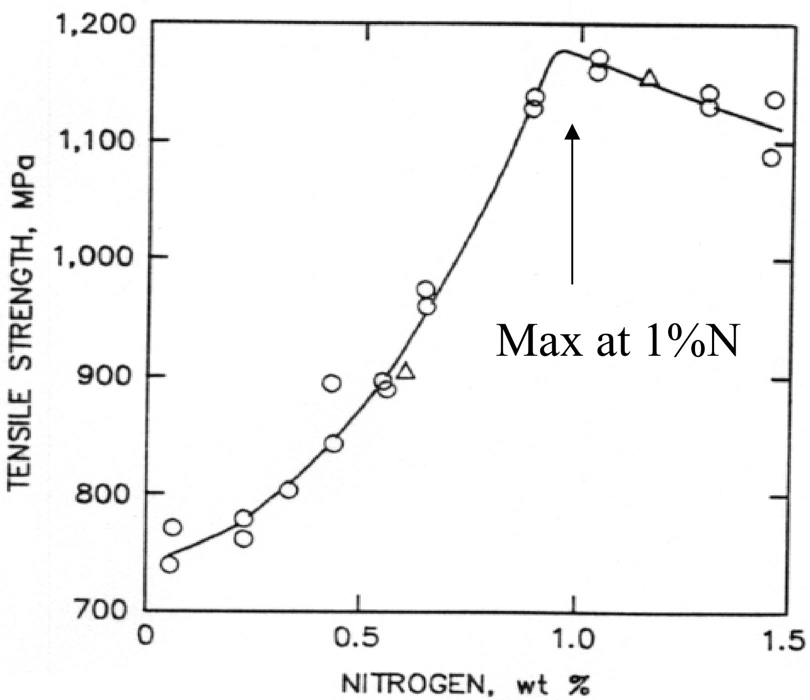
Twinning stress for Cu-xAl depends monotonically on unstable twin SFE.

S. Kibey, L. L. Wang, J.B. Liu, D.D. Johnson, H. T. Johnson and H. Sehitoglu, manuscript in preparation.

Addition of nitrogen to Fe-based materials

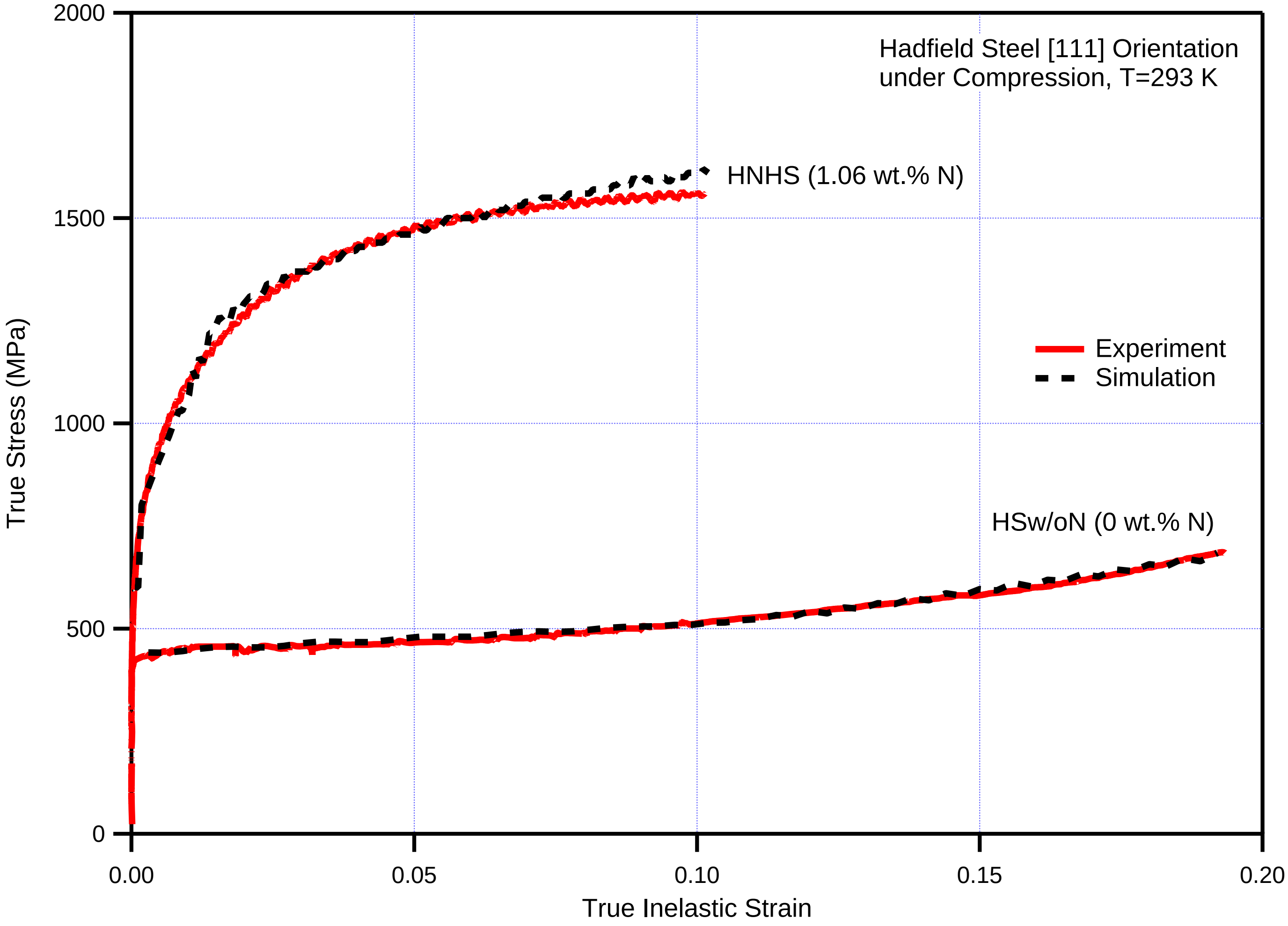


J. Reed, J.Metals, 1989.

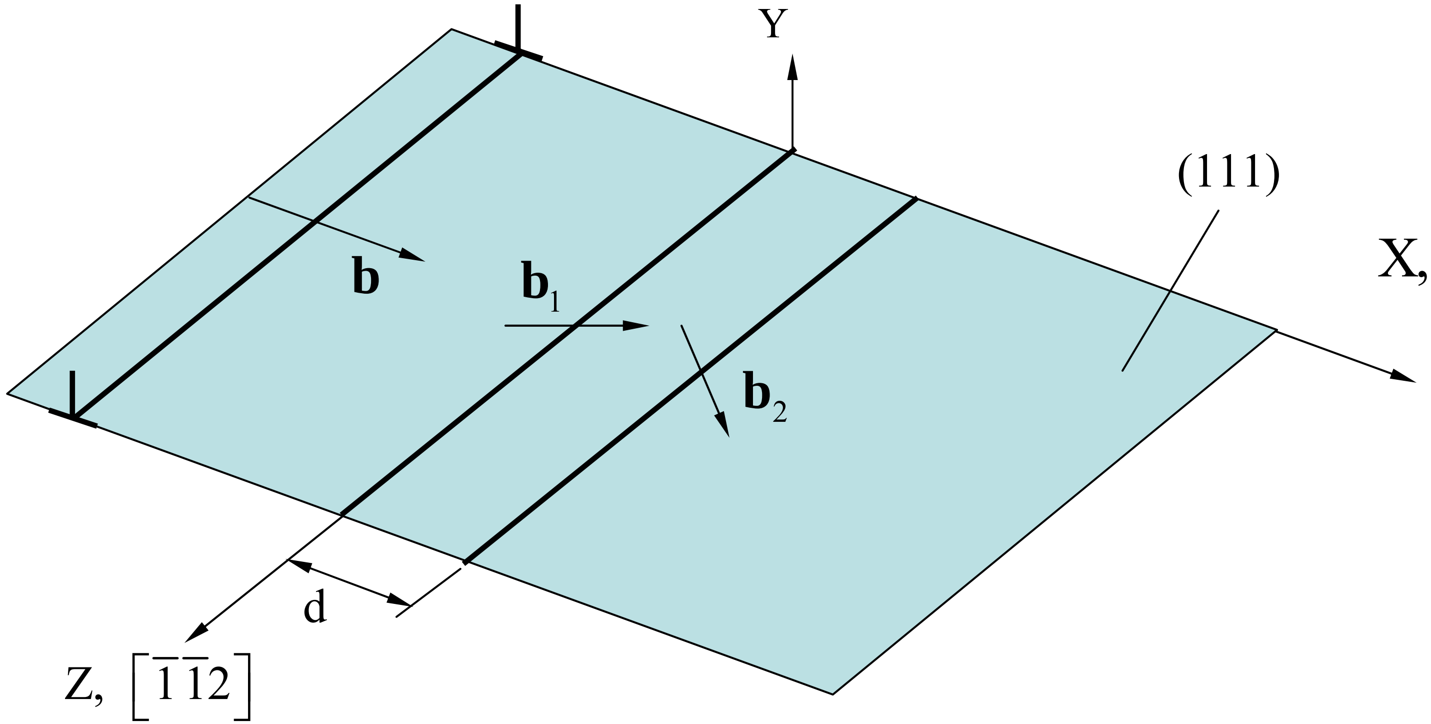


Rawers and Slavens (1995)

FeMnN-Theory vs. Experiment - [111] Orientation



Extended edge dislocation



$$\mathbf{b} = \mathbf{b}_1 + \mathbf{b}_2$$

$$\frac{1}{2}\left[1\bar{1}0\right] = \frac{1}{6}\left[2\bar{1}\bar{1}\right] + \frac{1}{6}\left[1\bar{2}1\right]$$

Z direction is equivalent to <112> direction for GSFE

X direction equivalent to <110> direction for GSFE

Generalized P-N model

- Generalize to extended dislocations
- Edge components:

$$u_x = \frac{-1}{2\pi}\left[b_{e1}\, tan^{-1}\left(\frac{x}{w}\right) + b_{e2}\, tan^{-1}\left(\frac{x-d}{w}\right)\right]$$

$$\sigma_{xy}(x,0) = -\frac{\mu b}{2\pi(1-\nu)}\left[\frac{b_{e1}x}{x^2+w^2} + \frac{b_{e2}(x-d)}{(x-d)^2+w^2}\right]$$

- Screw components:

$$u_z = \frac{-1}{2\pi}\left[b_{s1}\, tan^{-1}\left(\frac{x}{w}\right) + b_{s2}\, tan^{-1}\left(\frac{x-d}{w}\right)\right]$$

$$\sigma_{yz}(x,0) = -\frac{\mu b}{2\pi}\left[\frac{b_{s1}x}{x^2+w^2} + \frac{b_{s2}(x-d)}{(x-d)^2+w^2}\right]$$

Generalized P-N model (contd.)

$$E_{total}(d) = E_{elastic}(d) + E_{misfit}(d)$$

$$E_{elastic}(d) = \int_{-r}^{r} \left(\sigma_{xy}u_x + \sigma_{yz}u_z\right)dx$$

$$= \frac{\mu}{4\pi}\left(\frac{b_{e1}^2}{(1-\nu)} + b_{s1}^2\right) ln\left[\frac{r}{2w}\right] + \frac{\mu}{4\pi}\left(\frac{b_{e2}^2}{(1-\nu)} + b_{s2}^2\right) ln\left[\frac{r-d}{2w}\right]$$

$$+ \frac{\mu}{4\pi}\left(\frac{b_{e1}b_{e2}}{(1-\nu)} + b_{s1}b_{s2}\right) ln\left[1 + \frac{r^2}{w^2}\right] tan^{-1}\left(\frac{r-d}{w}\right)$$

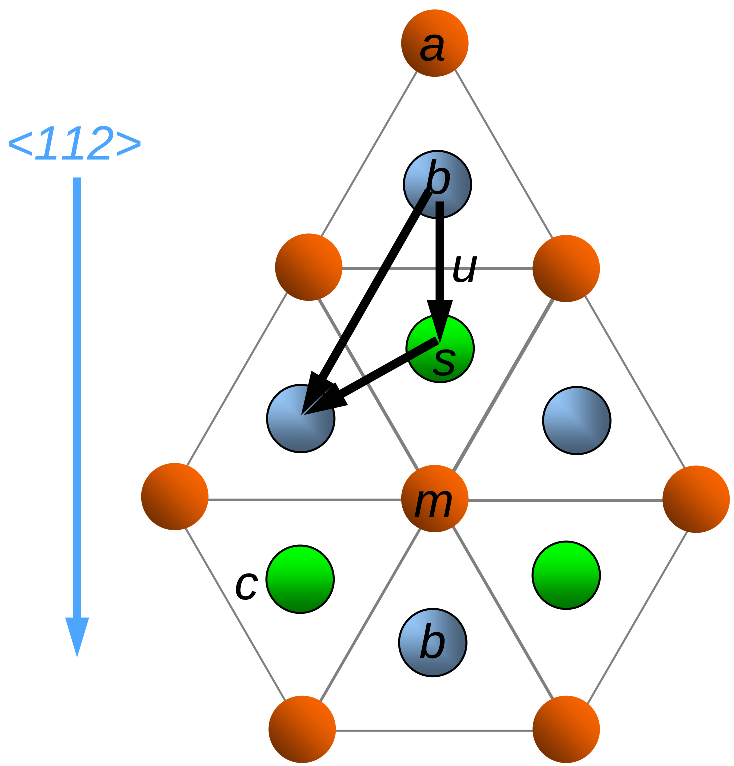
$$+ \frac{\mu}{8\pi}\left(\frac{b_{e1}b_{e2}}{(1-\nu)} + b_{s1}b_{s2}\right)\left\{ ln\left[1 + \frac{(r-d)^2}{w^2}\right] tan^{-1}\left(\frac{r-d}{w}\right) + ln\left[1 + \frac{(r-d)^2}{w^2}\right] tan^{-1}\left(\frac{r+d}{w}\right)\right\}$$

$$E_{misfit} = \int_{-r}^{r} \gamma(u_x, u_z)dx$$

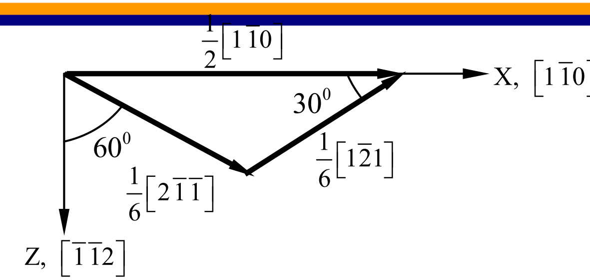
Generalized SFE

Minimize $E_{total}(d)$ **to obtain stable stacking fault width.**

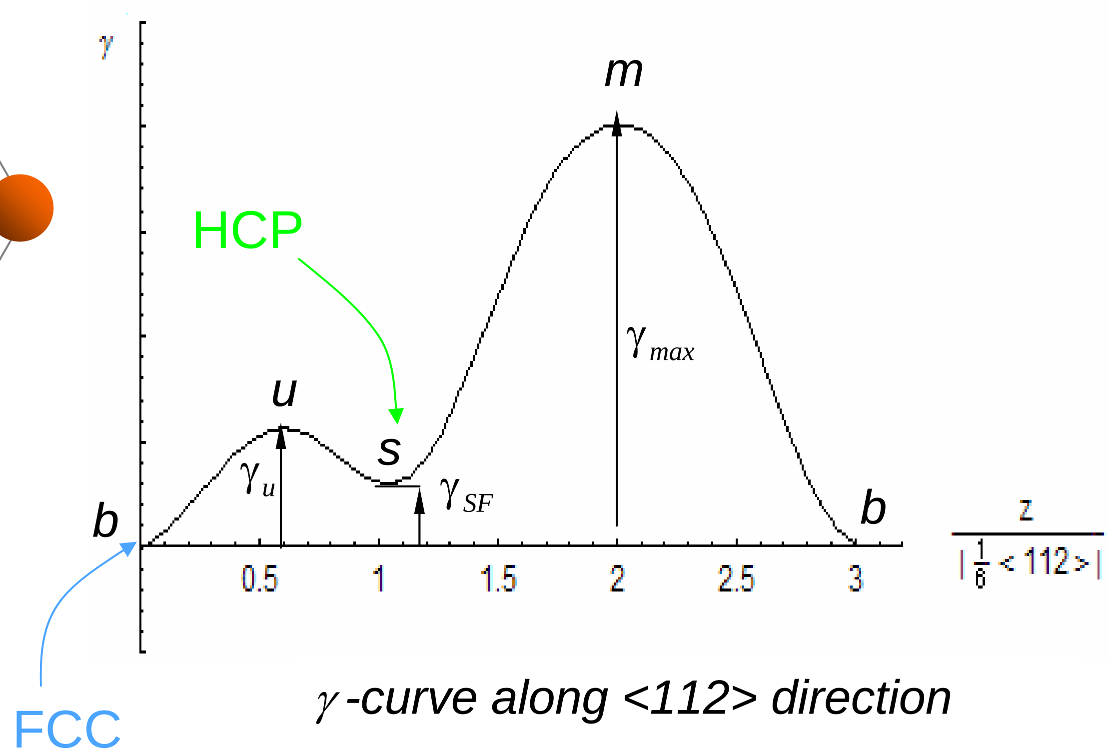
GSFE curve along <112>



FCC lattice

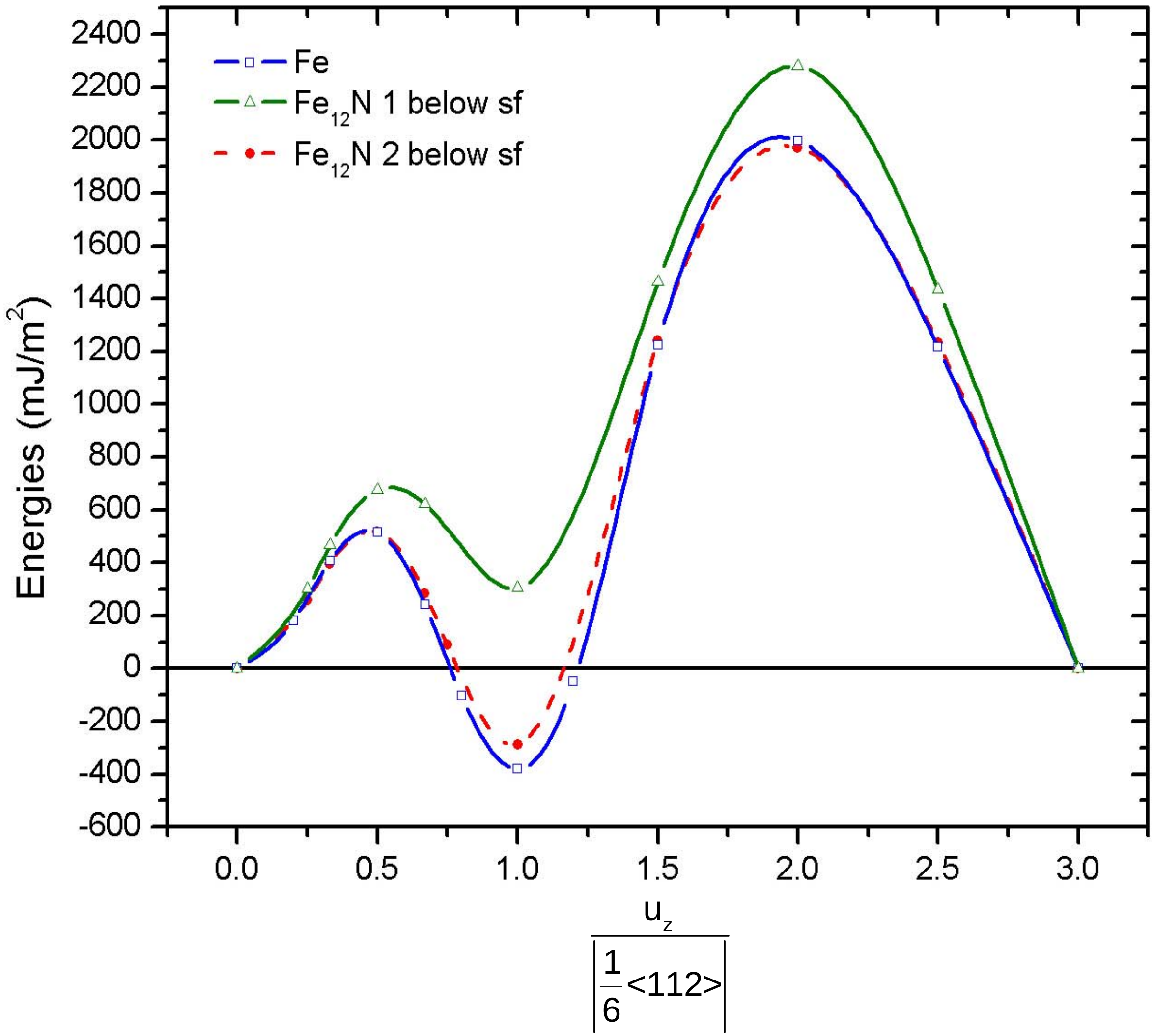


60^0 symmetry of γ surface



γ-curve along <112> direction

Results of atomistic calculations

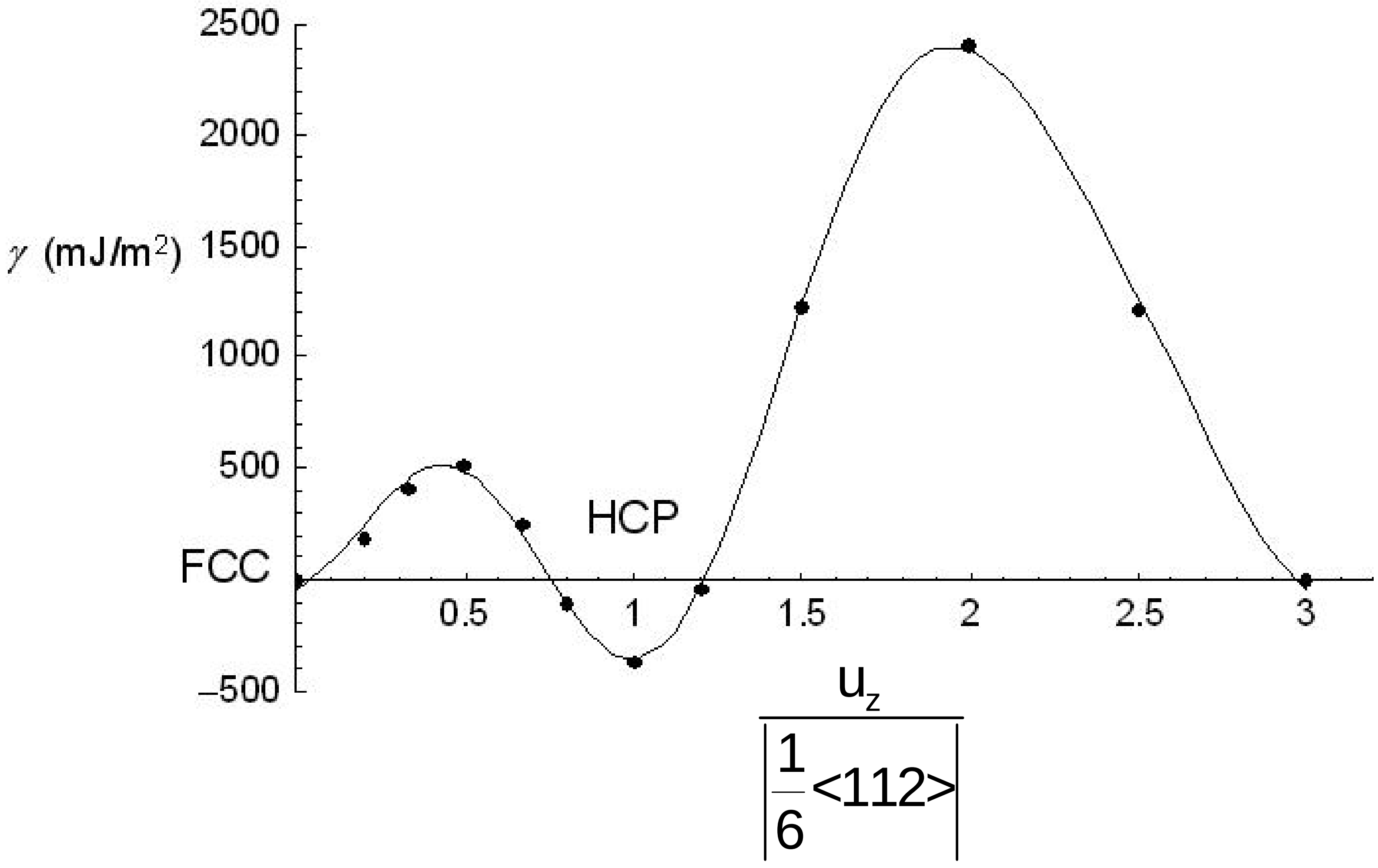


Pure iron

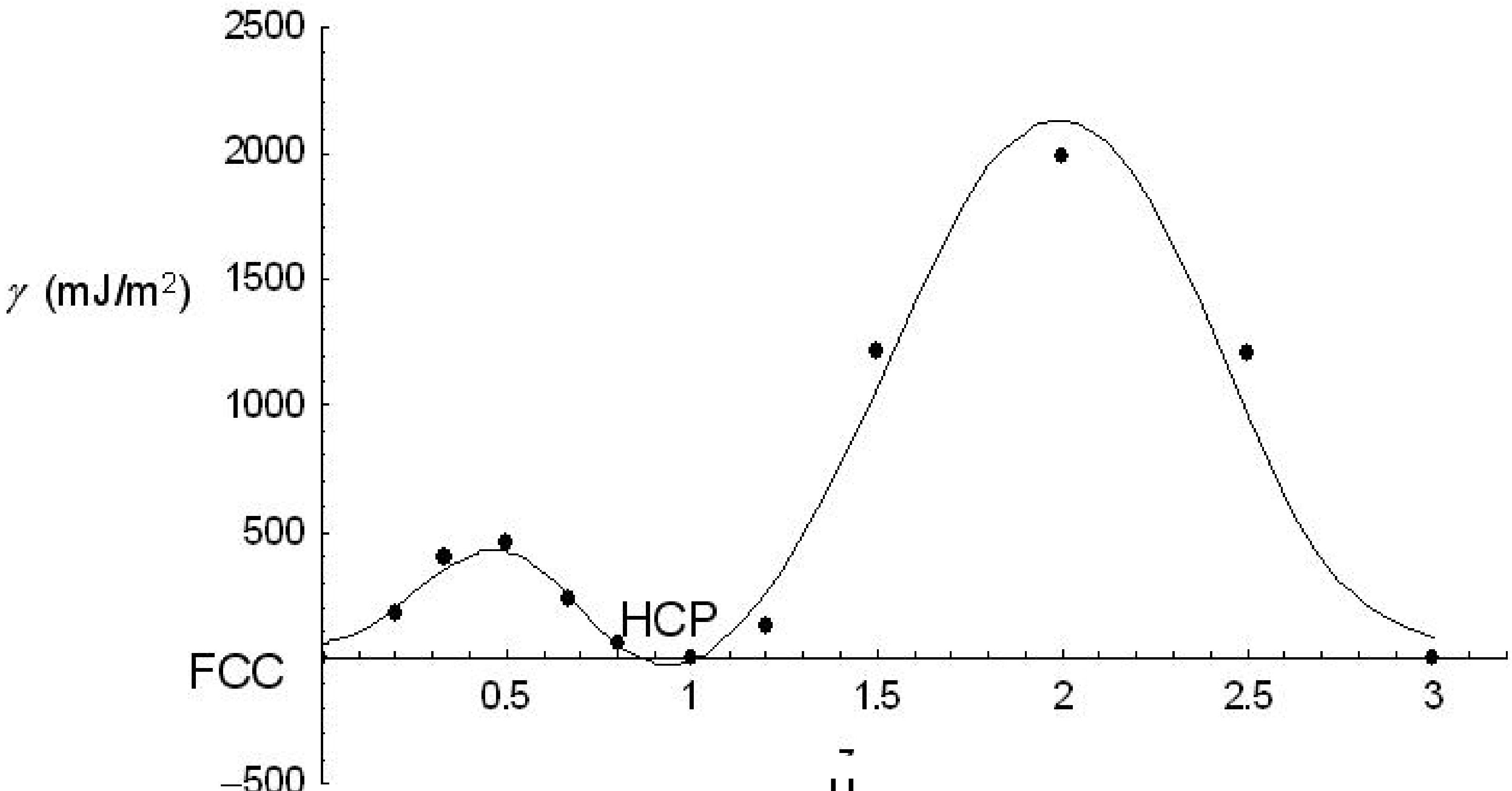
Nitrogen 1 layer away from stacking fault

Nitrogen 2 layers away from stacking fault

Fourier fit for γ-curve : pure Fe

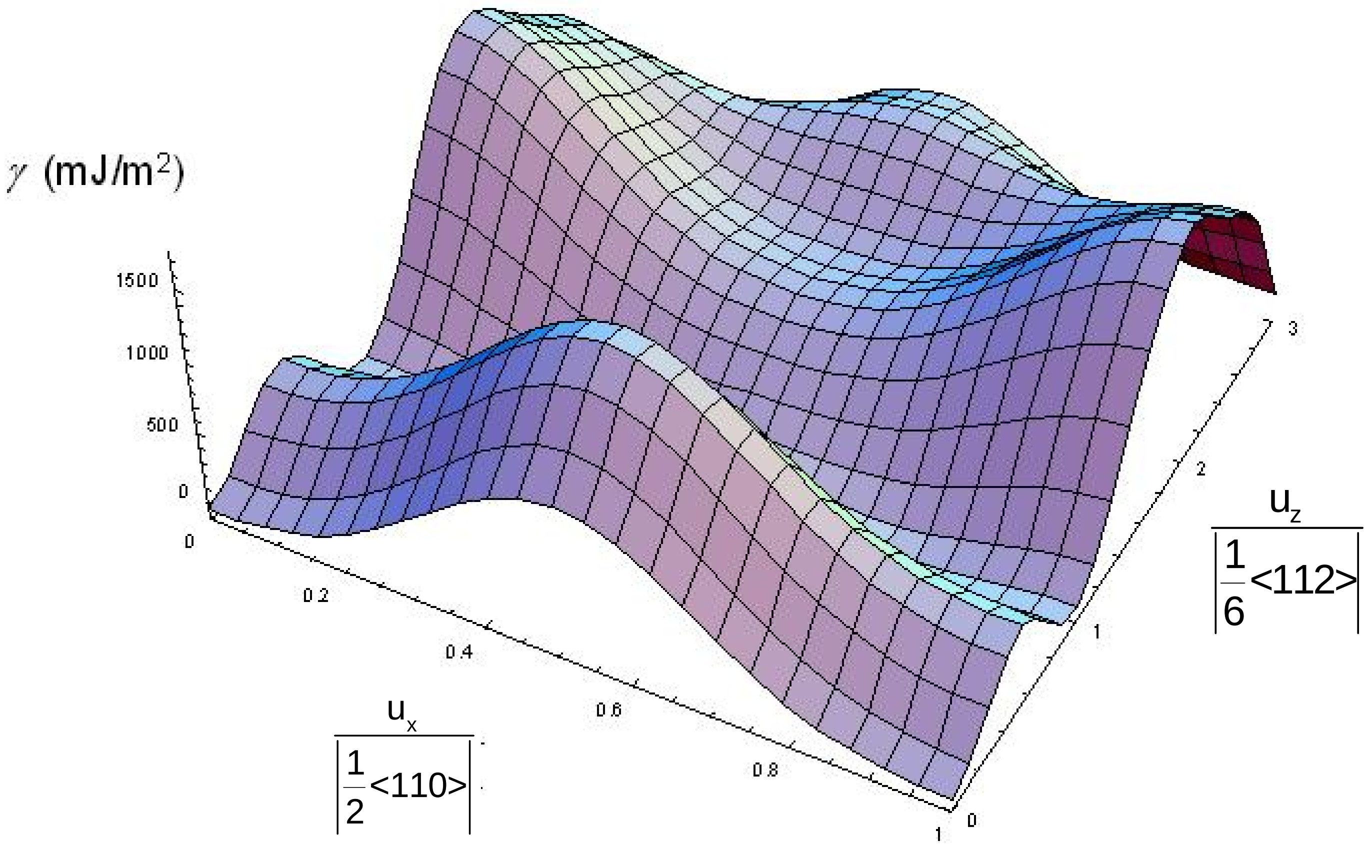


Fourier fit for γ-curve : Fe-4 at.%N

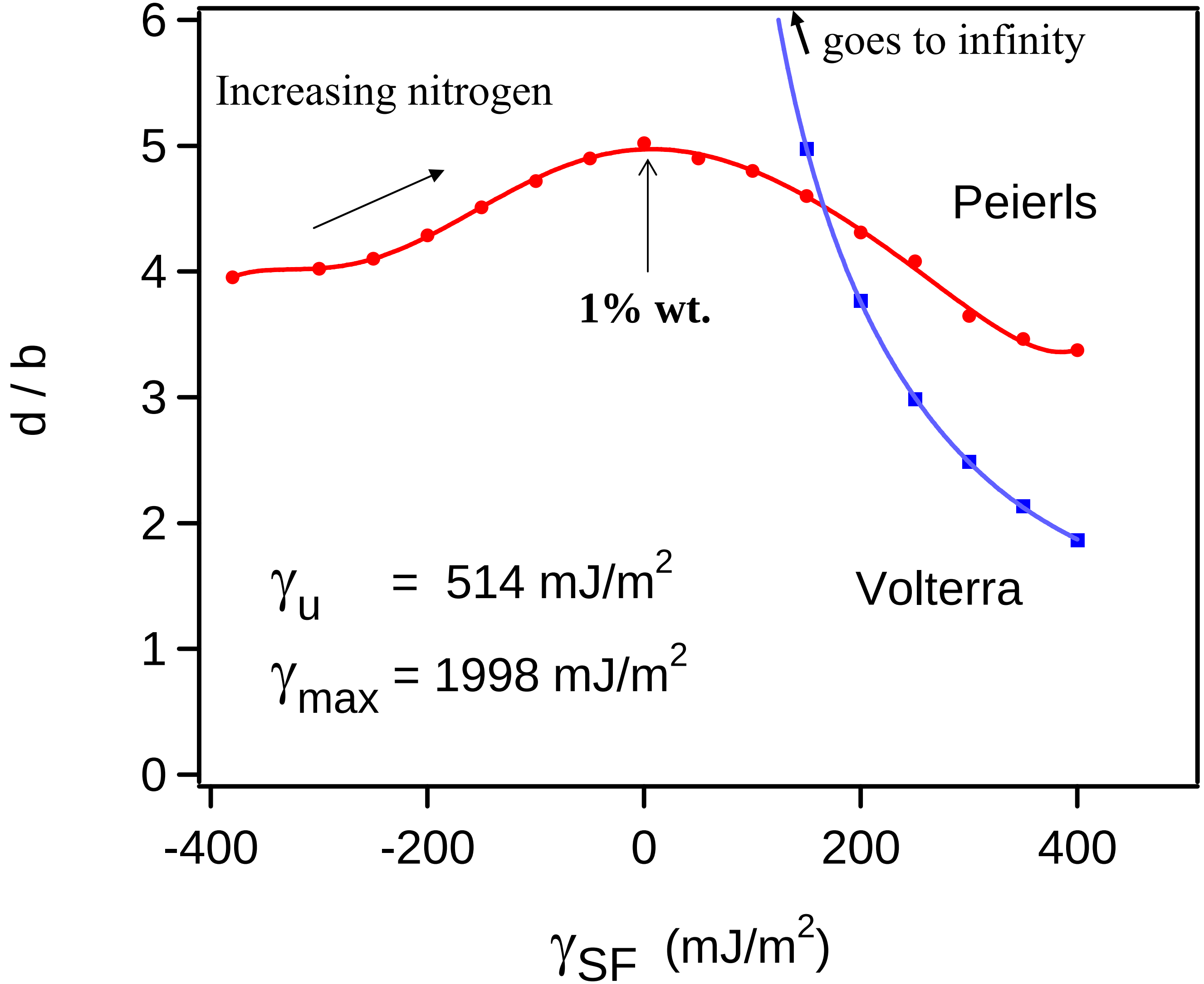


$$\frac{\bar{u}_z}{\left|\frac{1}{6}<112>\right|}$$

Fourier fit for GSFE Fe-4 at.%N



Effect of stable SFE (note finite separation for negative values)



Summary (ctd.)

•Stacking fault width is determined by γ–surface, not by intrinsic stacking fault energy alone.

•The models developed for twinning stress and stacking fault widths can be utilized to design new alloys.