# Dislocation Dynamics in Metals at Atomic-scale:

# Interactions between Dislocations and Obstacles with Dislocation Character

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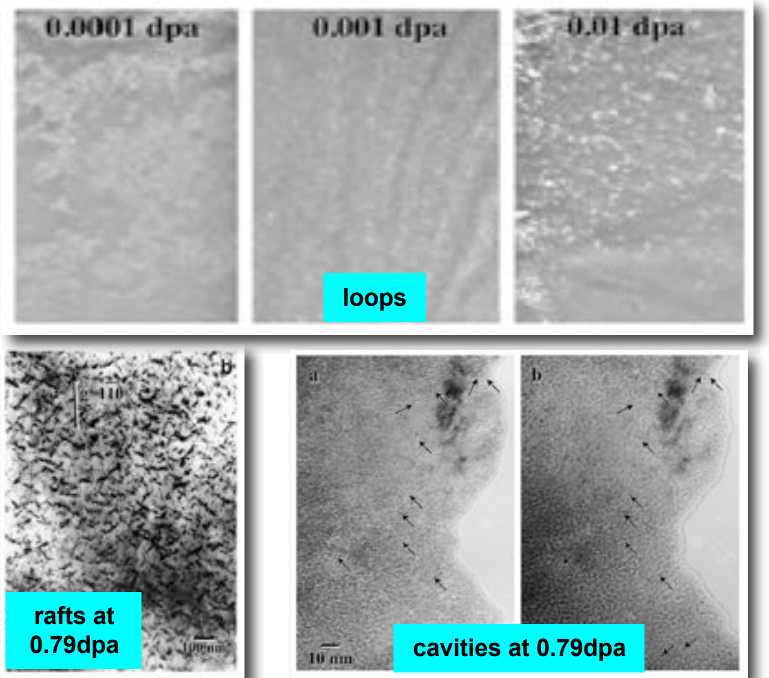
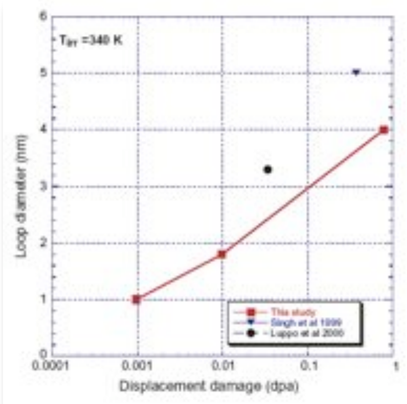
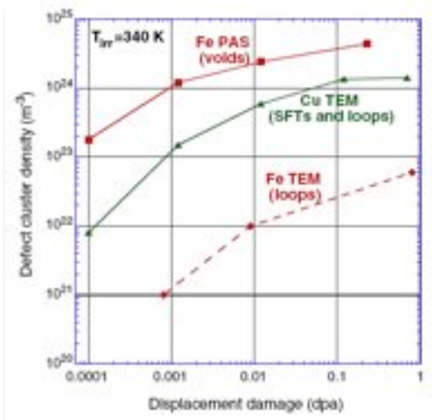
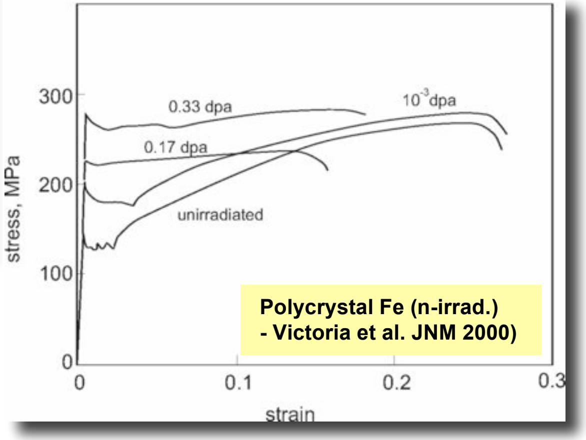
## Motivation: effect of irradiation microstructure on mechanical properties

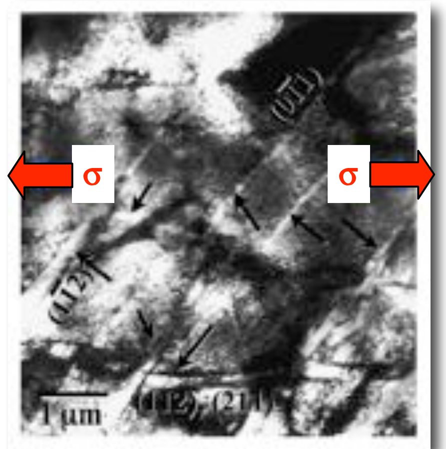



Fe, n-irradiated at 60°C (Zinkle & Singh JNM 2006)



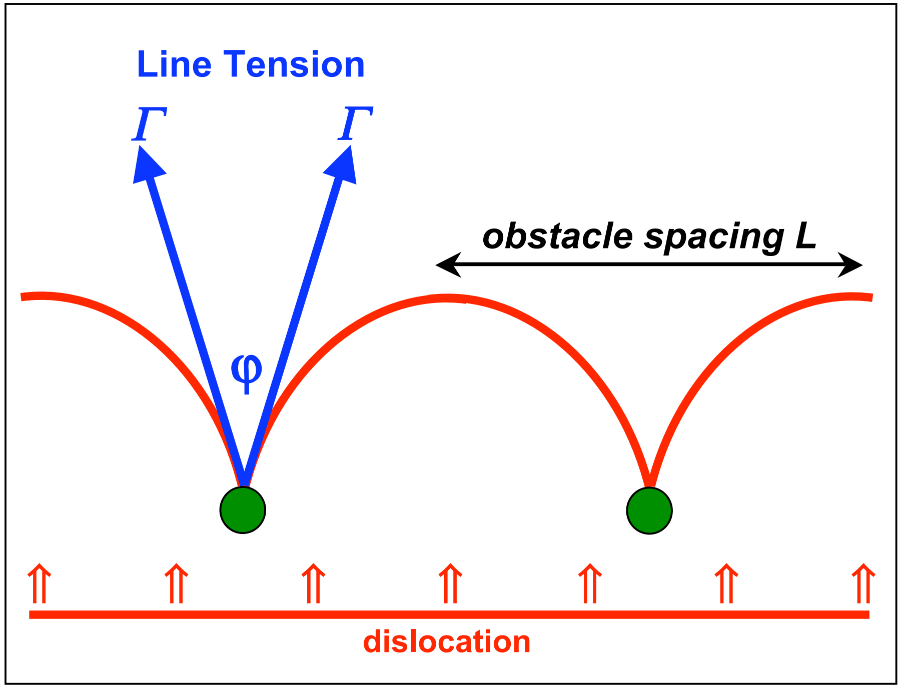




Deformed Fe, n-irrad. 0.4dpa
(Zinkle & Singh JNM 2006)

- dislocations under stress move through field of irradiation-induced obstacles
  - dislocation loops, SFTs, point defect clusters, voids, precipitates, etc.
- yield and flow stress raised, strain to failure reduced

## Continuum modelling of strengthening

### (a) Line tension approximation




- Dislocation overcomes obstacle when $\varphi = \varphi_c$ at $\tau = \tau_c$

$$\tau_c bL = 2\Gamma\cos(\varphi_c/2)$$

- $\Gamma \approx Gb^2/2$

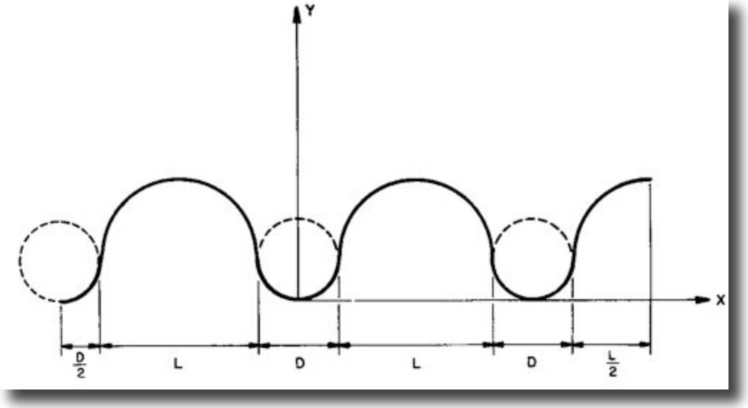
$$\therefore\ \tau_c = \alpha Gb/L$$

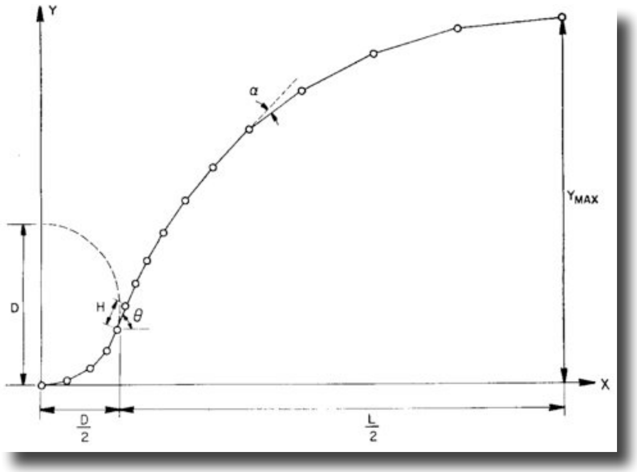
$\alpha = \cos(\varphi_c/2)$
- characterises 'obstacle strength'

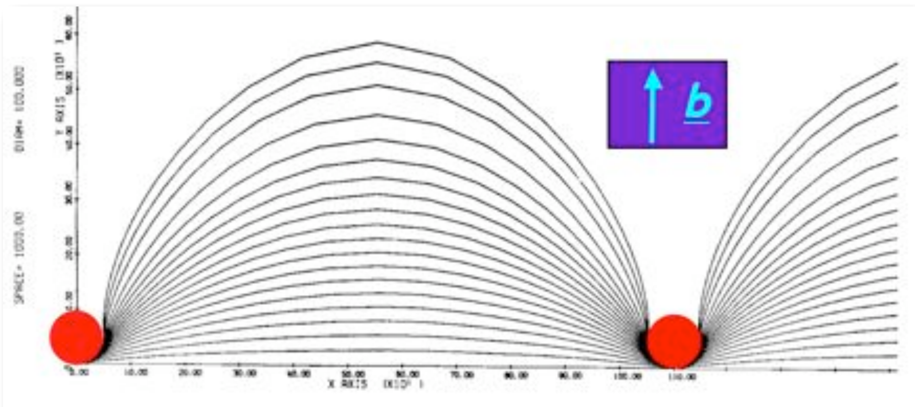
- $\varphi_c$ is largely empirical
- strong obstacles $\varphi_c \sim 0$, but empirically $\alpha \sim 0.2\text{-}0.5$
- LT model ignores dislocation self-interaction
- self-stress is included in 'dislocation dynamics' (DD) modelling (elasticity approximation)

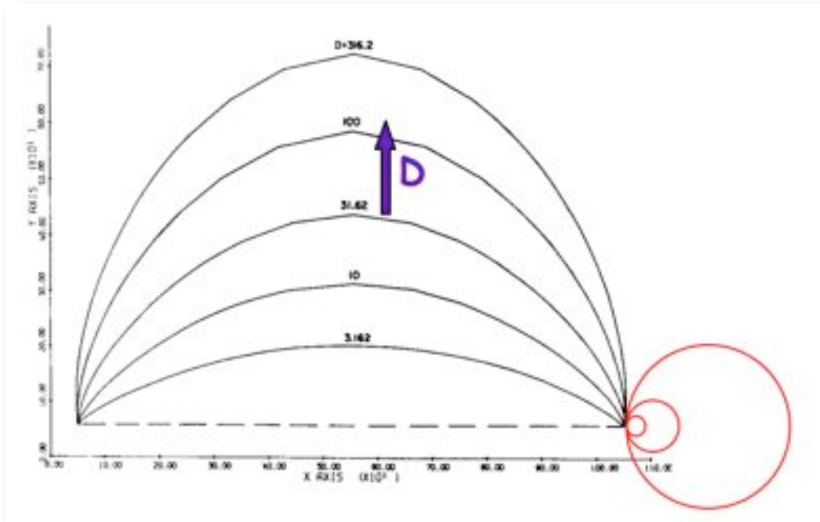
## (b) Dislocation self-stress simulation for strong obstacles

- Orowan strengthening (impenetrable obstacles)



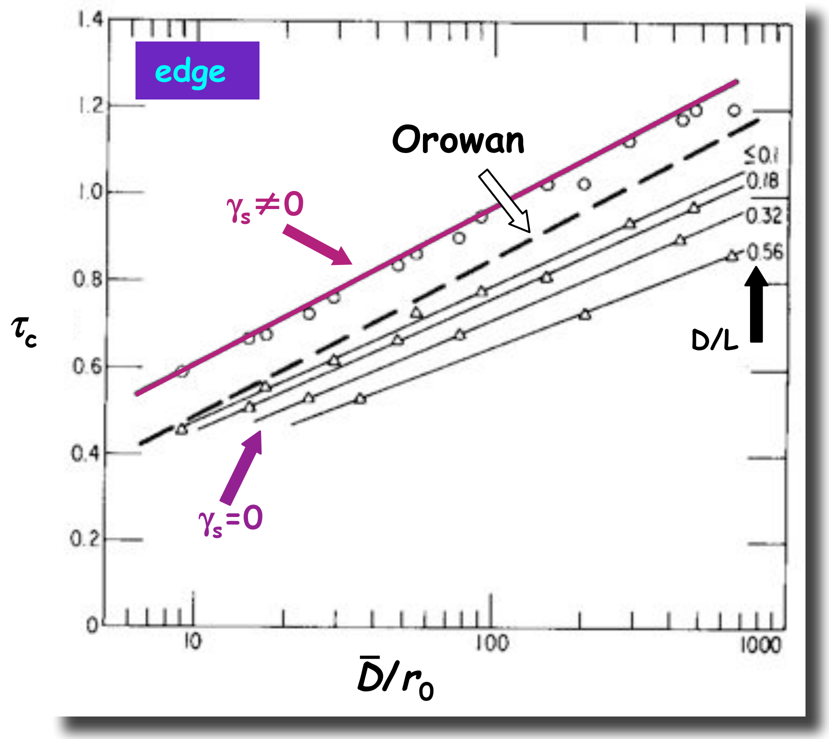

L → D

[Bacon, Scattergood, Kocks (Phil. Mag. 1973-)]

- critical stress for edge dislocation and impenetrable particles or voids:

$$\tau_c \simeq \frac{Gb}{2\pi L}\left[\ln\left(\frac{1}{D^{-1}+L^{-1}}\right)+B\right]$$

where $B$ depends on $\gamma_s$ for voids




- cf line tension: $\tau_c = \alpha Gb/L$
- energy (tension) of dipole $\propto \ln[D]$

$\Rightarrow$ size-dependence for strong obstacles

- dislocation dynamics (DD) requires 'local rules'
  - effects of core structure
  - mobility of segments, strength of junctions
  - dependence on $\tau$, $T$, $\dot{\varepsilon}$

$\Downarrow$ link to atomic scale

- computer simulation of atomic-scale processes by which obstacles affect dislocation motion

$\Rightarrow$ quantitative data on $\tau$, $T$, $\dot{\varepsilon}$

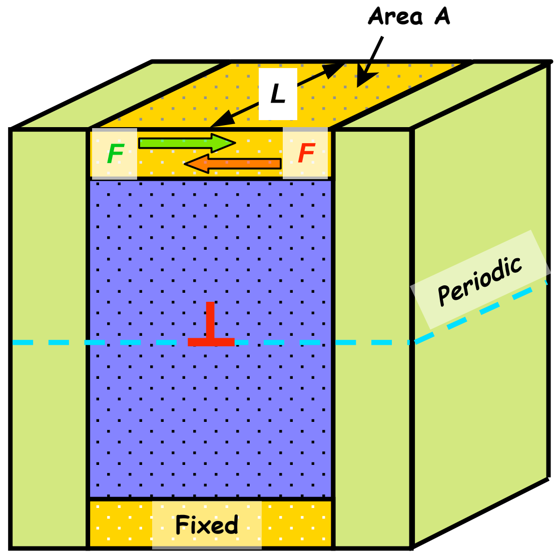
## (c) Atomic-scale simulations of dislocation-obstacle interaction

- System size
  - few M mobile atoms
- Obstacle
  - periodic spacing $L \leq 100$nm
  - size $D \leq 10$nm
  - $\rho_D \sim 10^{14}$-$10^{15}$m$^{-2}$
- Statics (MS) $T$ = 0K
  - apply $\Delta\varepsilon$ incrementally
  - relax to minimum pot'l energy
  - equivalent to elasticity

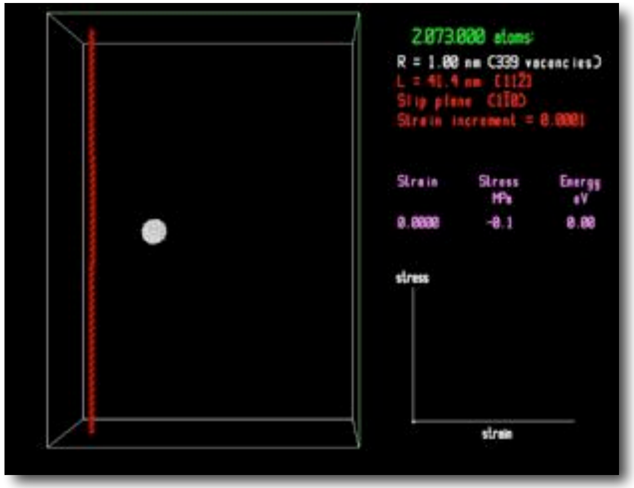
$\tau_{appl} = -F/A$

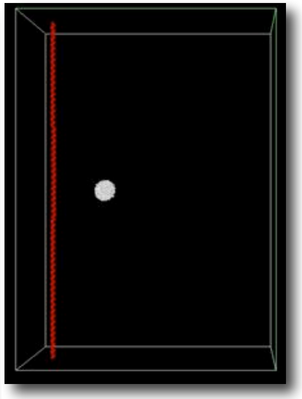
- Dynamics (MD) $T$ > 0K
  - either apply strain rate ~ $10^6$-$10^8$s$^{-1}$
  - dislocation veloc ~ 5-500ms$^{-1}$
  - or apply stress

$\tau_{appl} = F/A$

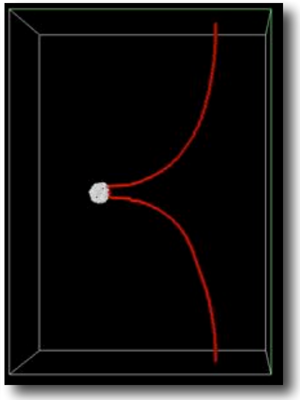


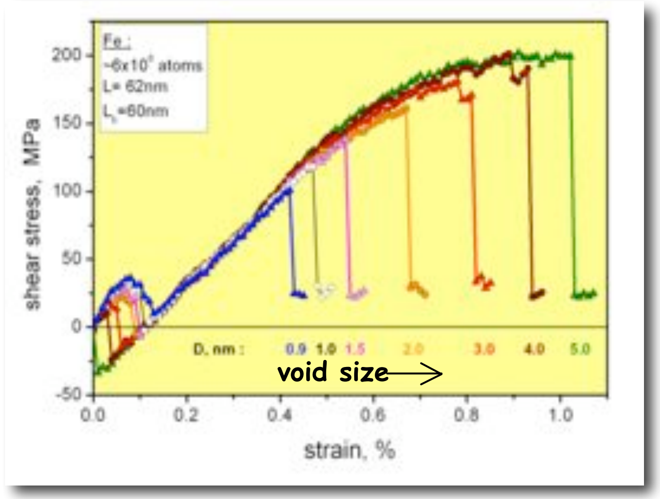
# Void strengthening α-Fe at $T$ = 0K (edge dislocation)

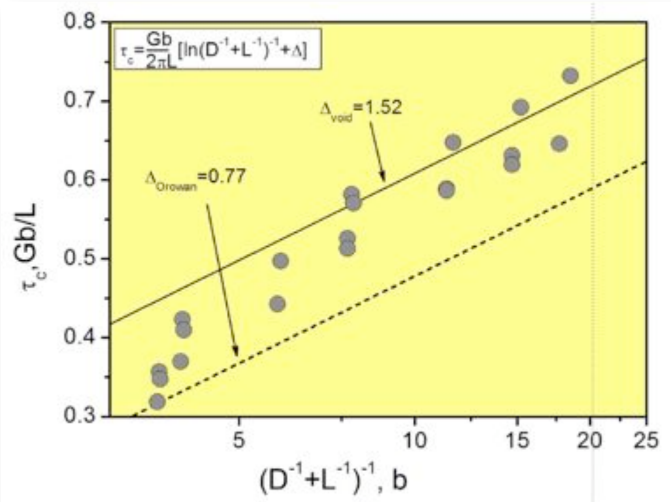


2nm (339v) void in Fe
L=42nm, T=0K





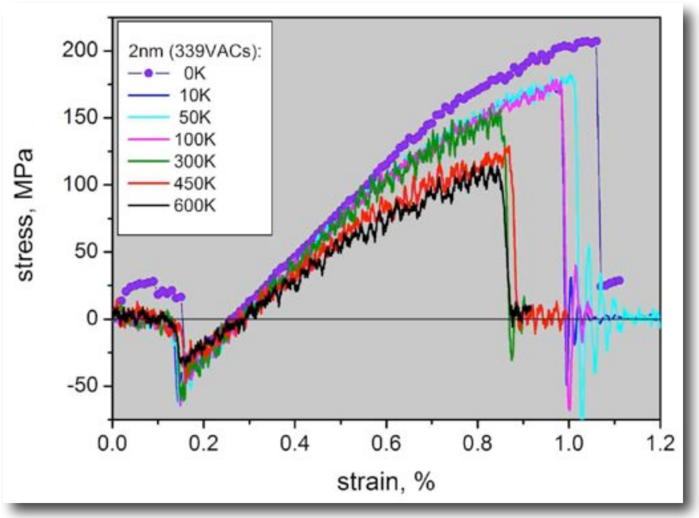




$$\tau_c \simeq \frac{Gb}{2\pi L}\left[\ln\left(\frac{1}{D^{-1}+L^{-1}}\right)+B\right]$$

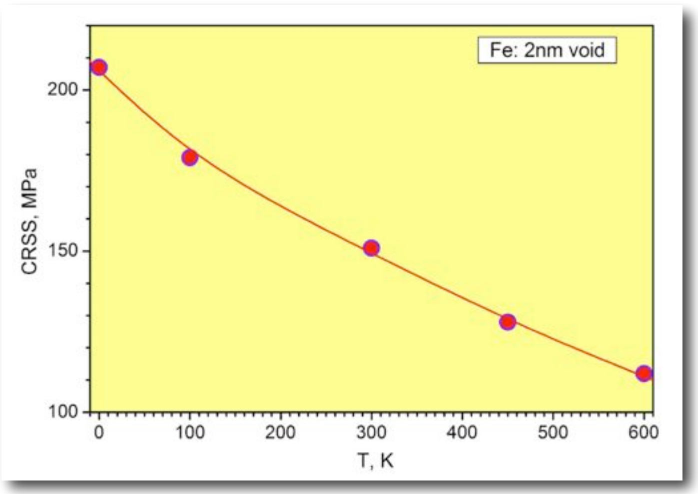
- similar dependence on $L$ and $D$ from atomic-level and continuum treatments

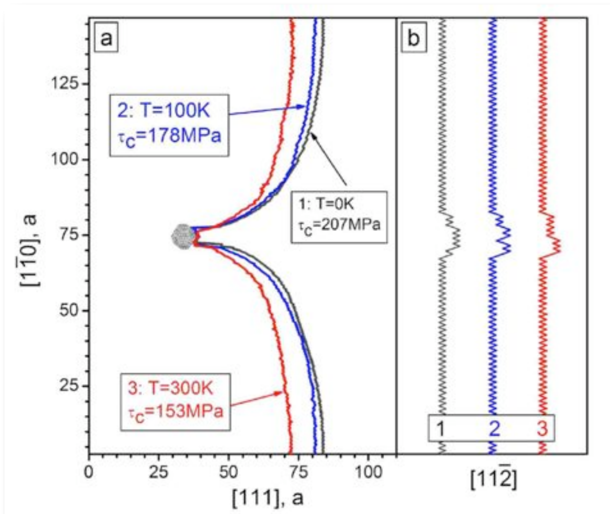
# Void strengthening at *T* > 0K (edge dislocation)

- **motion under constant strain-rate ($10^6$-$10^8 s^{-1}$) - dislocation dynamics at the atomic scale**

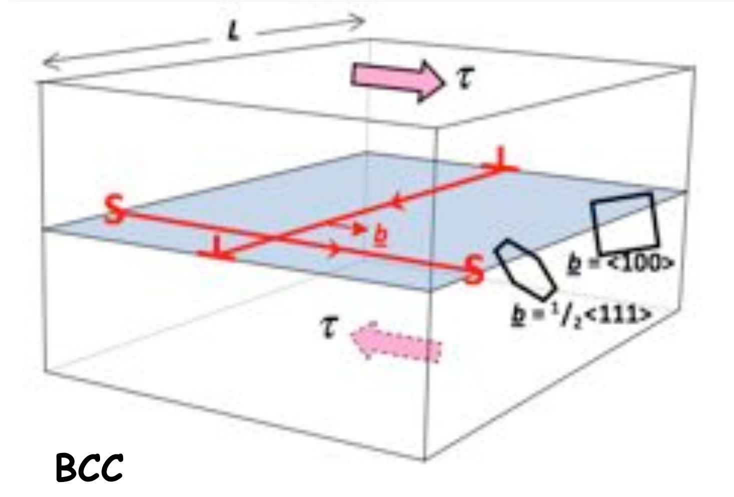


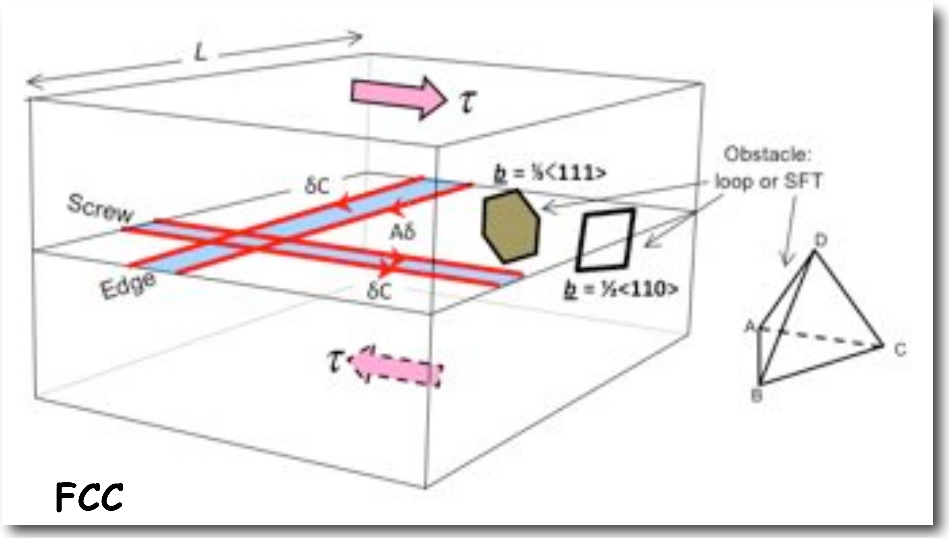

e.g. $\tau_c$: 2nm voids in Fe
- strain rate $5x10^6 s^{-1}$



## (d) Dislocation interaction with nano-scale dislocation obstacles




- Only consider BCC here

- Outcomes
  - R1: dislocation and obstacle unchanged - <u>edge</u> or <u>screw</u>
  - R2: obstacle changed but dislocation unchanged - <u>edge</u> or <u>screw</u>
  - R3: partial or full absorption of obstacle by <u>edge</u> dislocation (superjog formation)
  - R4: temporary absorption of obstacle by <u>screw</u> dislocation (helix formation)
  - loop drag (≡ R1+R3)

**[Bacon, Osetsky & Rodney, in *Dislocations in Solds*, vol. 15 (2009)]**

**No intersection:** Small $\frac{1}{2}[111]$ loop in Fe at 300K

- *edge* dislocation
- parallel *b*s
- loop drag
- breakaway above critical stress


Fe_37SIA: *b*=1/2[111]_300K_100MPa

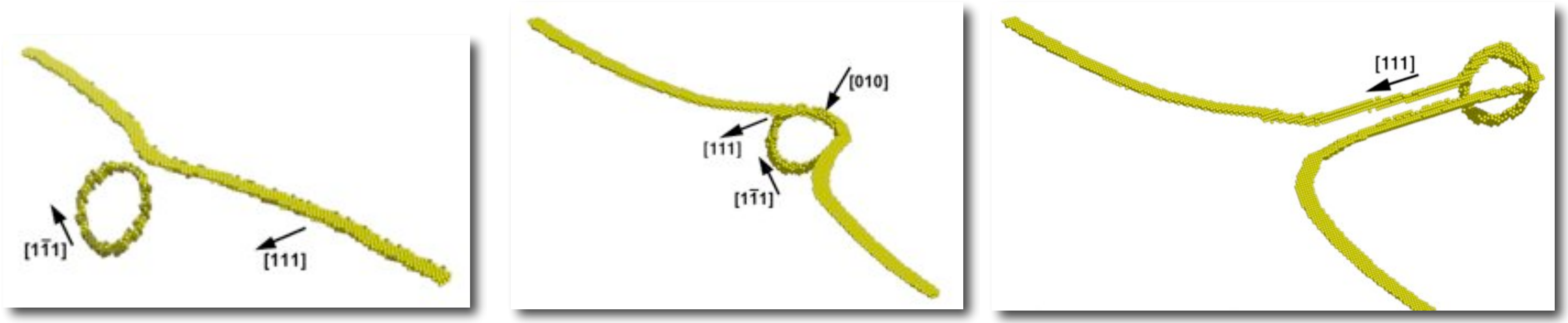
[Rong, Osetsky & Bacon, Phil. Mag. (2005)]

**Intersection:** Frank's rule for energetically-favourable reactions in Fe (BCC) predicts

- $\frac{1}{2}\langle 111 \rangle$ loops acquire $\langle 100 \rangle$ segments
  - e.g. $\frac{1}{2}[111] + \frac{1}{2}[1\bar{1}\bar{1}] = [100]$
- $\langle 100 \rangle$ loops acquire $\frac{1}{2}\langle 111 \rangle$ segments
  - e.g. $\frac{1}{2}[111] + [\bar{1}00] = \frac{1}{2}[\bar{1}11]$

# R1: dislocation and obstacle unchanged

**Intersection:** Large loop (331i) with $\underline{b}$ = ½[1-11] in Fe at 100K
- <u>edge</u> dislocation $\underline{b}$ = ½[111]




- attractive reaction forms [010] segment
- [010] segment has different glide plane and is immobile at low $T$
- screw dipole drawn out
- pinches off by x-slip at $\tau_c$, leaving ½[1-11] loop

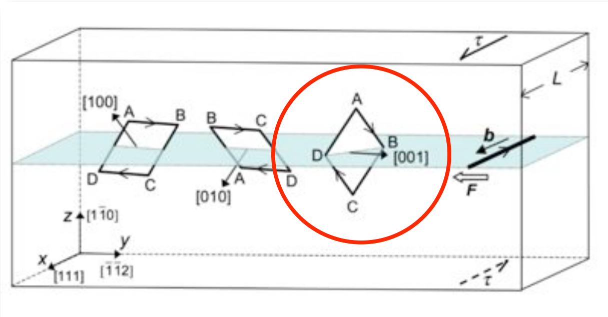
⇒ strong obstacle

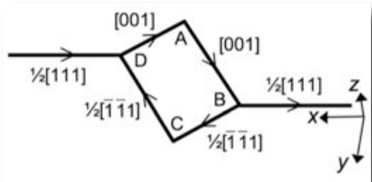
[Bacon, Osetsky & Rong, Phil. Mag. (2006)]

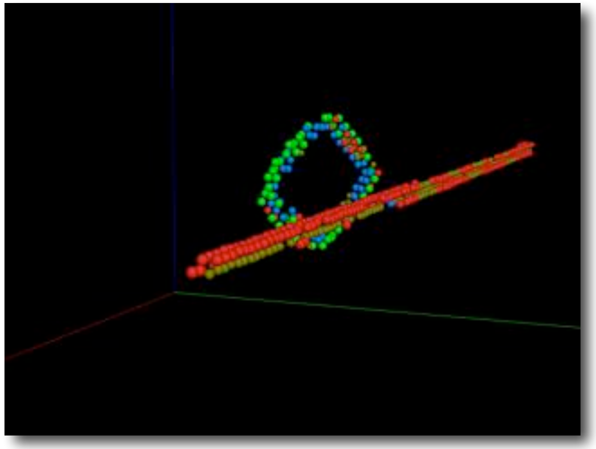
# R1: dislocation and obstacle unchanged (cont'd)

**Intersection:** Large loop (128i) with $\underline{b}$ = [001] in Fe at 300K

- <u>screw</u> dislocation $\underline{b}$ = ½[111]

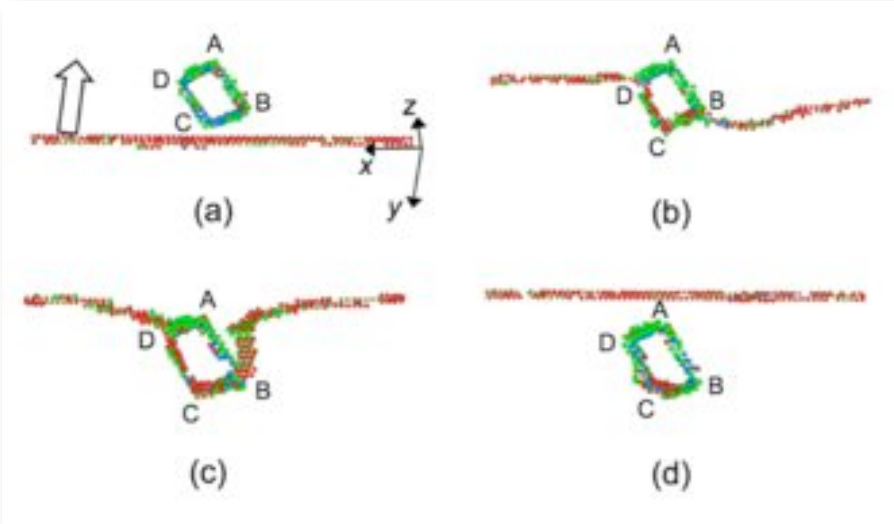


- attractive reaction converts sides BC & CD to ½[-1-11] by x-slip of screw
- screw side arms x-slip to corner C at $\tau_c$ leaving original loop
- screw glide plane now coincident with C (periodic boundaries)

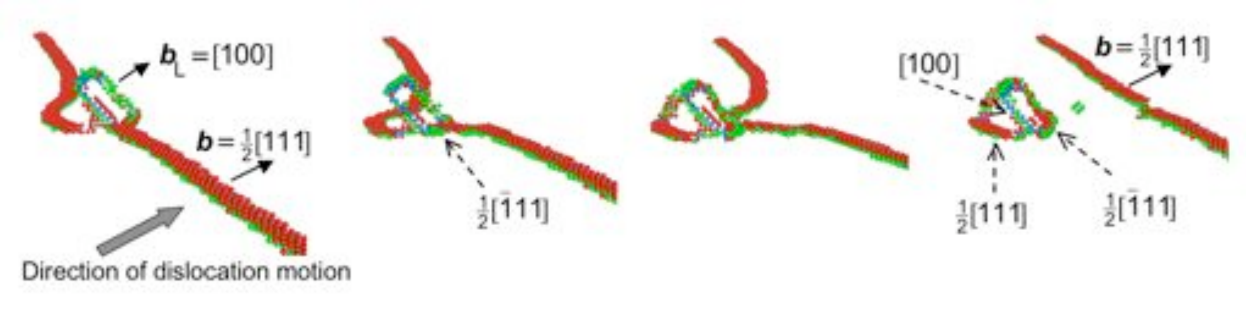
⇒ moderately strong obstacle




[Terentyev, Bacon & Osetsky, Phil Mag, in press]

# R2: dislocation unchanged, obstacle changed

**Intersection:** [100] loop (169i) in Fe at 300K
- ½[111] <u>edge</u> dislocation

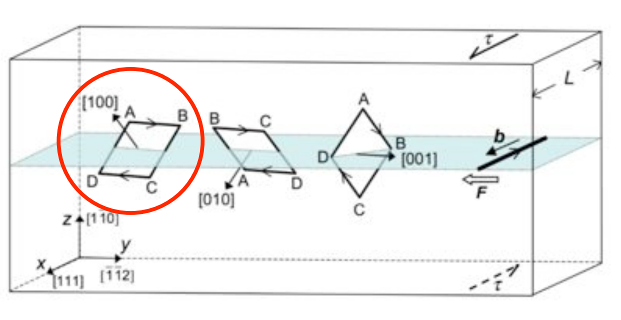


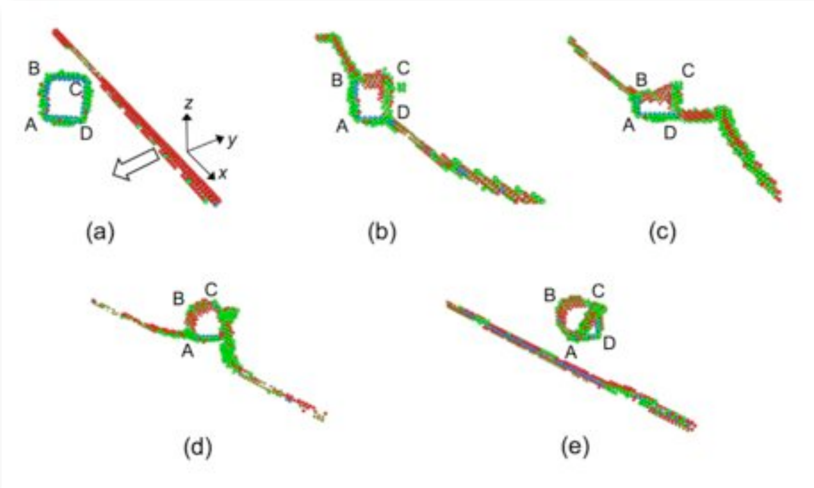

- dislocation repelled but forms ½[-111] segment on contact
- double loop complex remains

[Terentyev, Bacon & Osetsky, Acta Mat. (2008)]

⇒ strong obstacle

- similar complex for [100] loop and ½[111] <u>screw</u>:



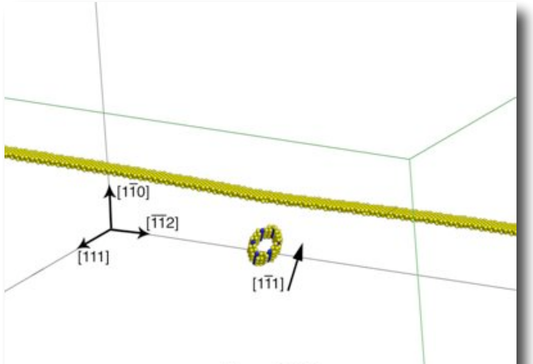




[Terentyev, Bacon & Osetsky, Phil Mag, in press]

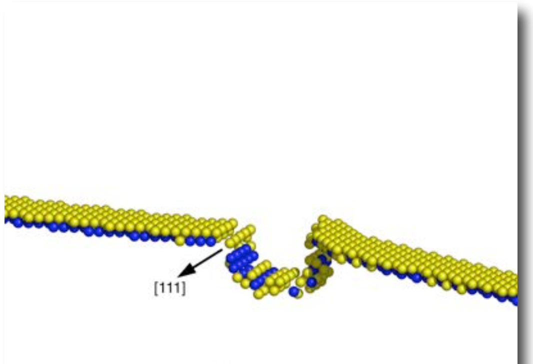
# R3: partial or full absorption of obstacle by edge dislocation (superjog formation)

Small loop (37i) with <u>*b*</u> = ½[1-11] in Fe at 0-600K

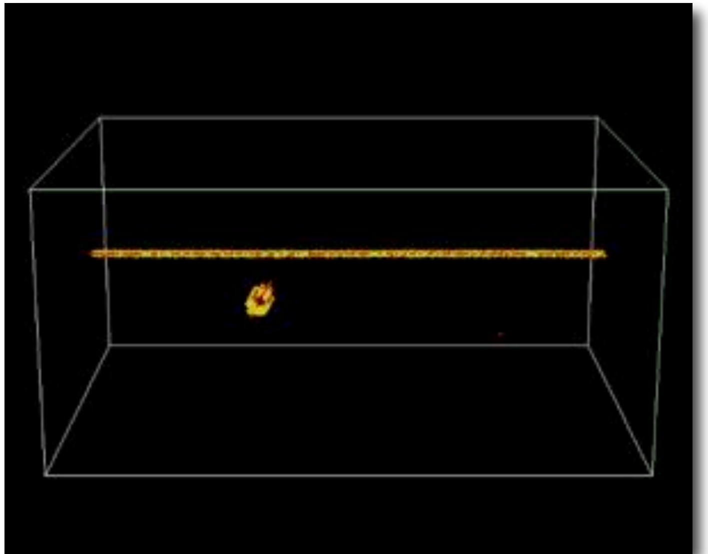
- <u>*edge*</u> dislocation <u>*b*</u> = ½[111]



(a) ε = 0.03%



(b) ε = 0.214%



Fe_37SIA: <u>*b*</u>=1/2[1-11]_300K_SR10

- loop <u>*b*</u> changes on contact

  ⇒ weak obstacle

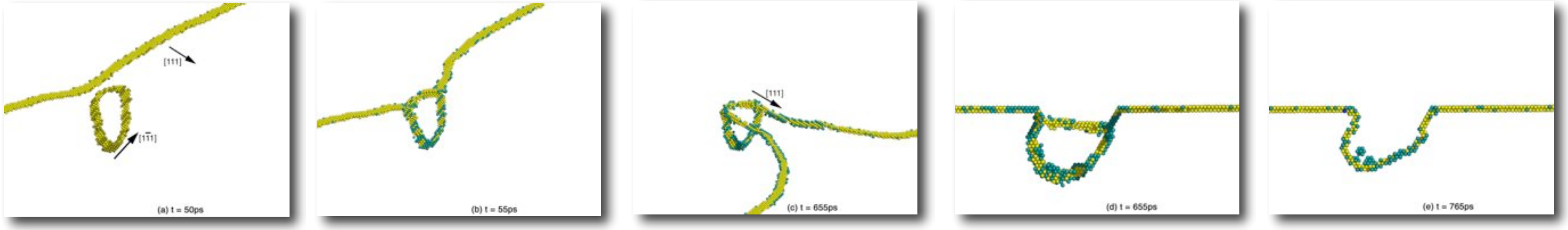
- *efficient absorption of all SIAs*

[Bacon, Osetsky & Rong, Phil. Mag. (2006)]

# R3: partial or full absorption of obstacle by edge dislocation (superjog form$^n$) (cont'd)

Large loop (331i) with $\underline{b}$ = ½[1-11] in Fe at 300-600K

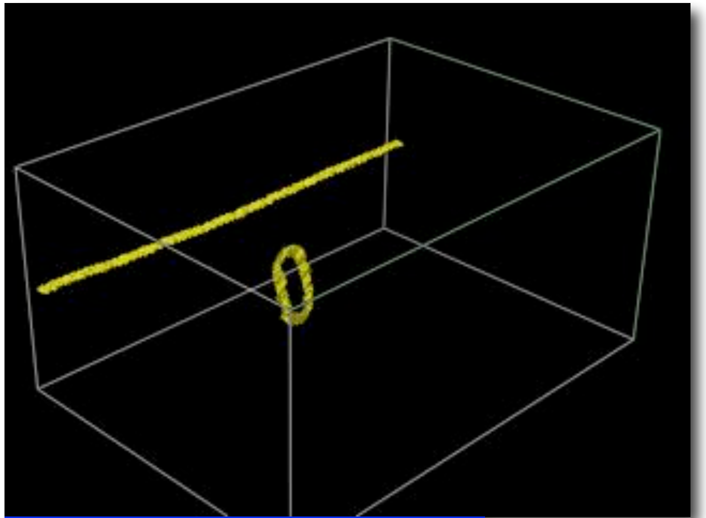
- <u>edge</u> dislocation $\underline{b}$ = ½[111]




- sessile [010] segment forms on contact
- segment has low mobility
- glides over loop converting it to ½[111] as screw side arms x-slip

⇒ strong obstacle

- efficient absorption of all SIAs

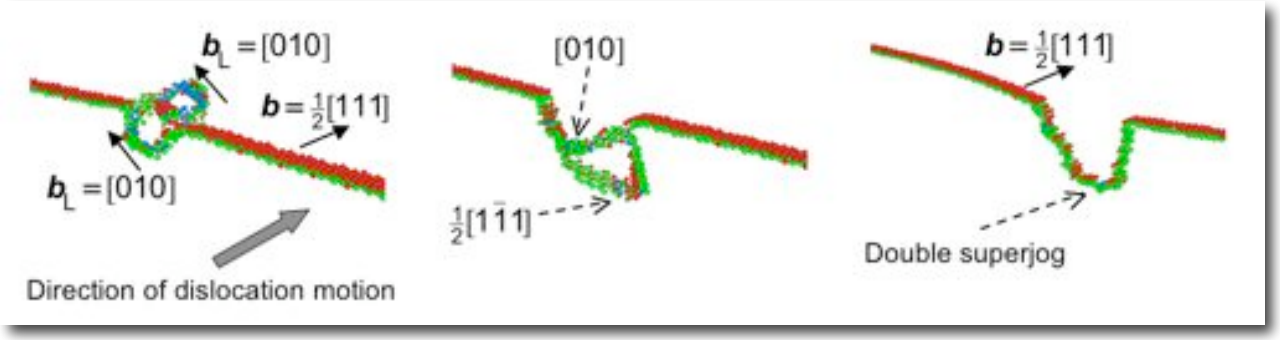


Fe_331SIA: $\underline{b}$=1/2[1-11]_300K_sr20

[Bacon, Osetsky & Rong, Phil. Mag. (2006)]

# R3: partial or full absorption of obstacle by edge dislocation (superjog form$^n$) (cont'd)

[010] loop (169i) in Fe at 300K
- ½[111] edge dislocation




- ½[1-11] segment forms on contact
- segment glides down ⇒ same configuration as interaction with ½[1-11] loop above
- segment glides over loop converting it to ½[111]

⇒ strong obstacle

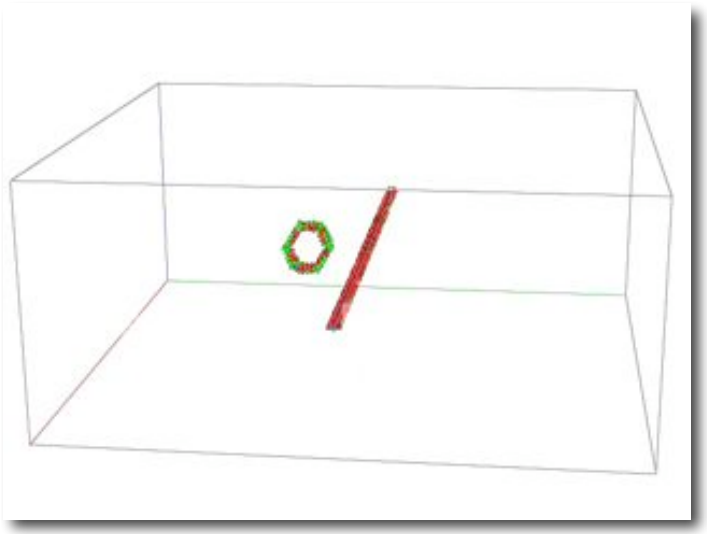
- efficient absorption of all SIAs

[Terentyev, Bacon & Osetsky, Acta Mat. (2008)]

# R4: temporary absorption of obstacle by screw dislocation (helical turn formation)
## - followed by detachment as turn closes

$\frac{1}{2}$[111] loop in Fe at 100K

- screw dislocation $b$ = $\frac{1}{2}$[111]



[Terentyev, unpublished]

- loop absorbed as helical turn
- cannot glide with line
- line released when turn closes and loop restored

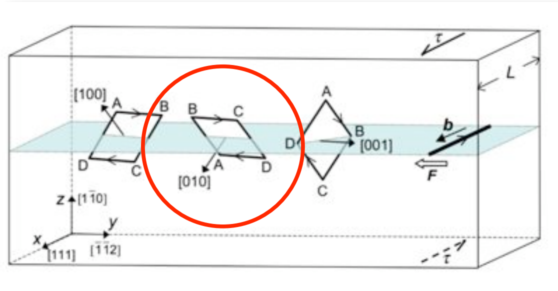
⇒ strong obstacle

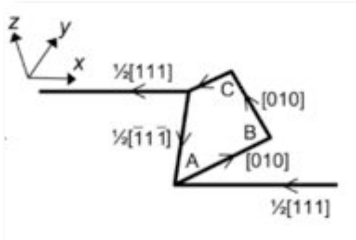
- any net absorption/transport of SIAs is along the line

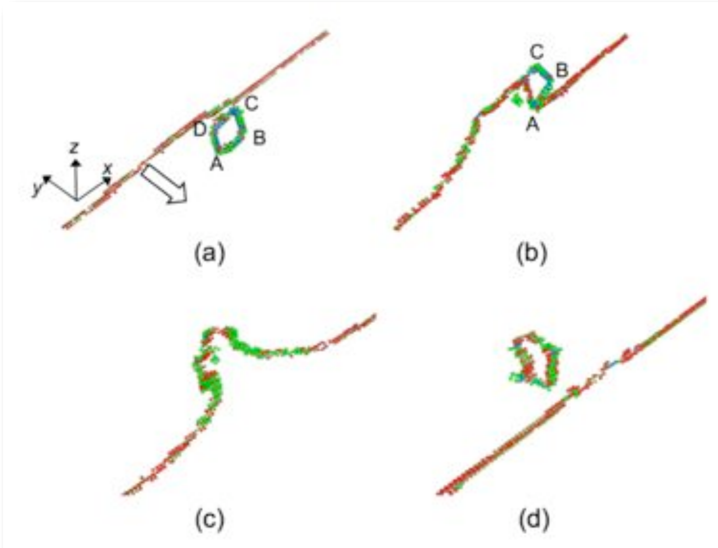
## R4: temporary absorption of obstacle by screw dislocation (helical turn formation)
## - followed by detachment as turn closes (cont'd)

[010] loop in Fe at 300K

- screw dislocation $\underline{b}$ = ½[111]




- screw initially repelled, but x-slips to corner D and converts AD to ½[1-11] segment
- segment sweeps over loop as screw side arms cross-slip, converting other sides to ½[111] ⇒ loop absorbed as helical turn on screw
- ½[111] loop formed when screw breaks away

⇒ strong obstacle

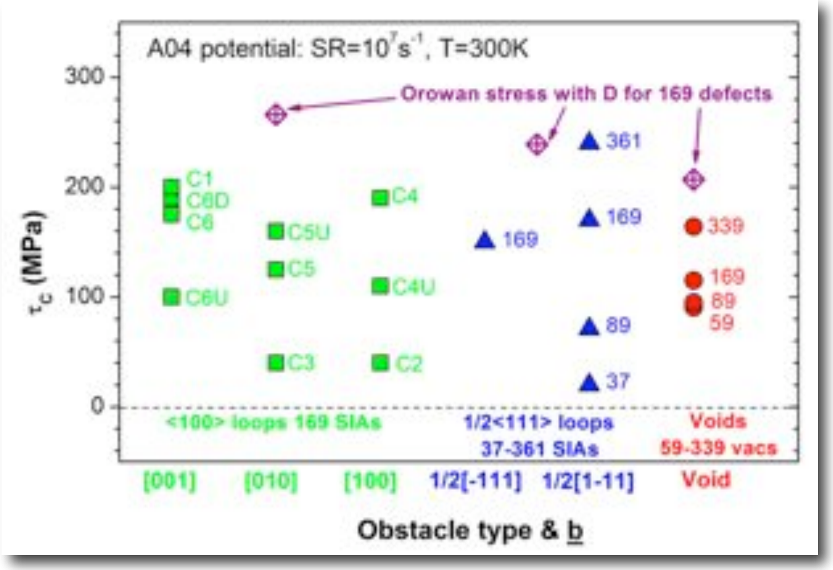
- no net absorption/transport of SIAs

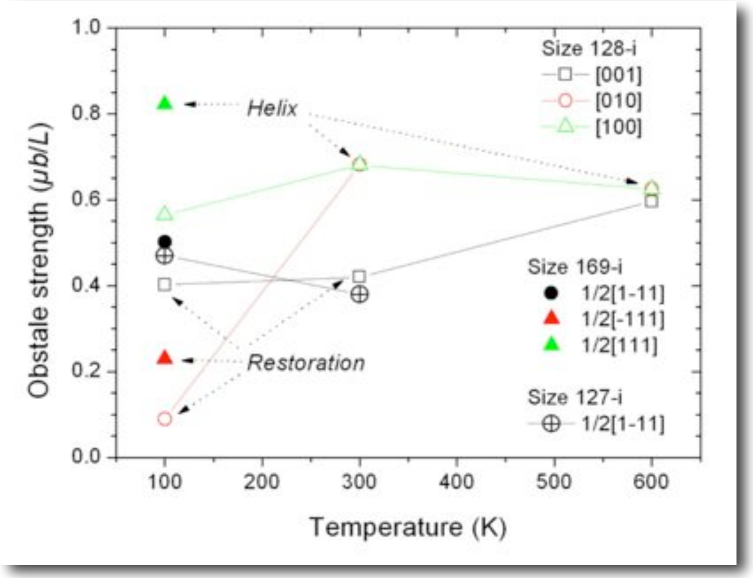
[Terentyev, Bacon & Osetsky, Phil Mag, in press]

## Summary/conclusions for $\tau_c$ in Fe

$\tau_c$ at 300K for edge with $L$ = 41nm

- large variation in $\tau_c$
- large variation in defect absorption on line (0-100%)
- no correlation between $\tau_c$ and absorption



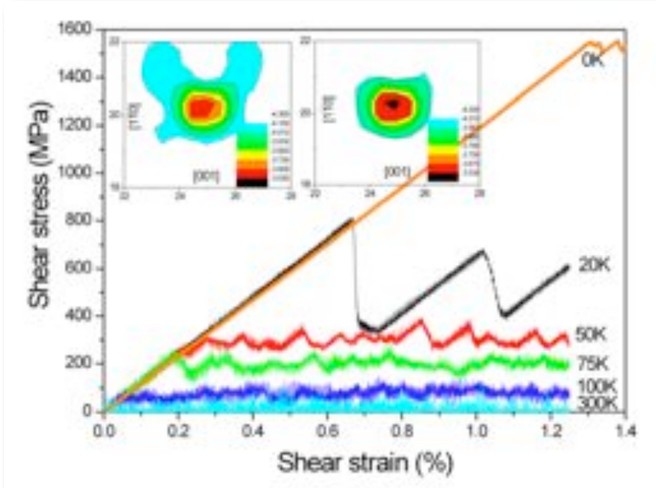

$\tau_c$ for screw at 100-600K for $L$ = 25nm

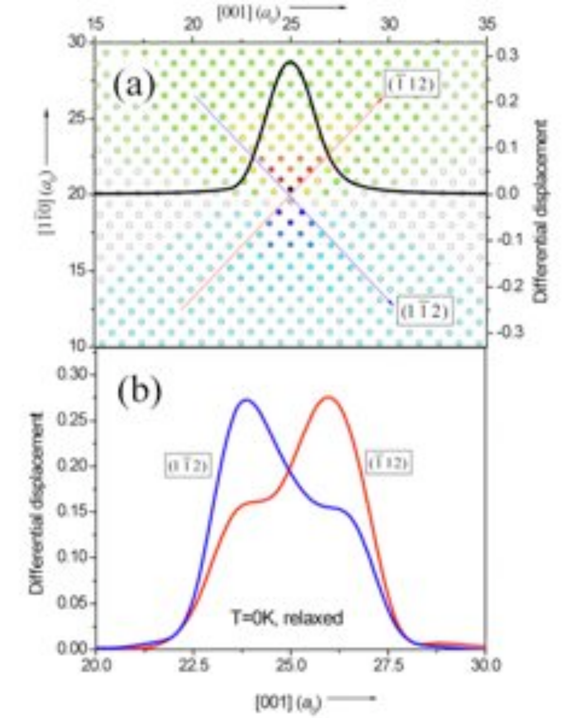
- reactions
  - R1 (loop restored) → lowest $\tau_c$
  - R2 (loop changed) → medium $\tau_c$
  - R4 (loop absorbed in temporary helix) → highest $\tau_c$

[Terentyev, Bacon & Osetsky, Phil Mag, in press; Liu & Biner, Scripta Mat. 2008]

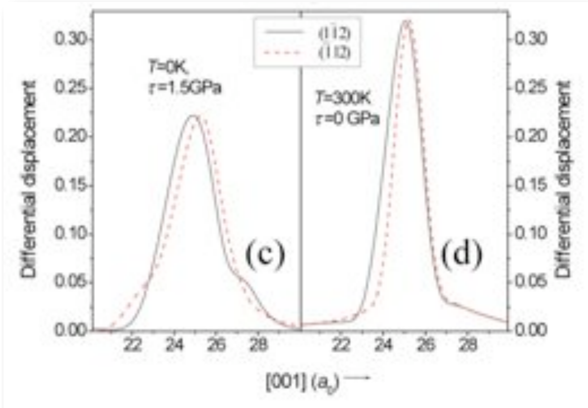
## What else?

- all reactions to form new segments, e.g. <100> on ½<111> loop or ½<111> on <100> loop, satisfy Frank's Rule: $(b_1^2+b_2^2) > b_3^2$ ⇐ even for nm loops
- final outcome depends on mobility of <100> dislocation, and therefore on *T*:




3-D core of <001> edge:
$\underline{b}$ = ½<111> on two {112} planes




3-D core ⇒ 2-D at high τ and/or *T*
$\underline{b}$ = ½[001] on two {112} planes

[Terentyev, Osetsky & Bacon, Acta Mater. in the press]

# Conclusions

## Dislocation Dynamics in Metals at Atomic-scale:

## Interactions between Dislocations and Obstacles with Dislocation Character

- need for predictive computer modelling

- atomic scale simulation can provide unique information on mechanisms
  - qualitative and quantitative
  - wide variety of nano-scale obstacles
  - can validate continuum models
  - increasing understanding of reactions, outcomes, obstacle strength

- future challenges
  - more realistic interatomic potentials, e.g. Fe, alloys
  - multiple dislocation effects, e.g. channelling
  - grain and interphase boundaries
  - strain rate effects
  - local rules and activation parameters for continuum-based dislocation dynamics