Dislocation Modelling
Atomic-scale to the Continuum

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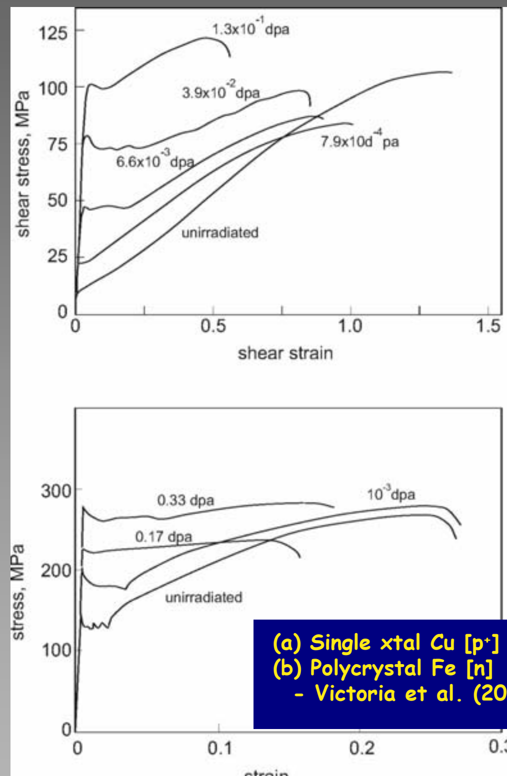
Issues:

- how to model strengthening effects, yield phenomena, obstacle absorption, defect motion, etc.?
- models able to give quantitative information?
- models able to describe candidate materials?
- periodic boundary conditions?
- dislocation density?
- statics or dynamics?
- are results for dislocation shape and critical stress comparable with elasticity theory?
- is high strain rate unavoidable? - is it realistic?
- how good is simulation based on elasticity theory?
- what shape should be taken from MD or experiment for DD?
- incorporation of atomic-scale information from statics and/or dynamics into models based on elasticity theory?
- other areas: solutes, cracks

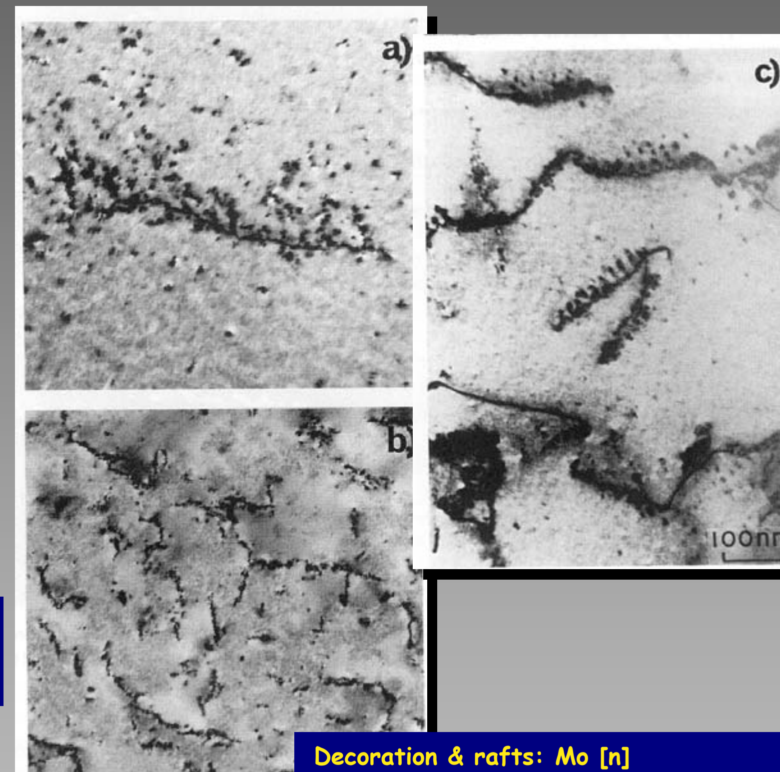
Irradiation microstructure - effect on mechanical properties

- dislocations under stress move through field of irradiation-induced obstacles - dislocation loops, SFTs, point defect clusters, voids, precipitates, etc.

Channelling: Pd [p^+; 0.12dpa] - Victoria et al. (2000)



(a) Single xtal Cu [p^+]
(b) Polycrystal Fe [n]
- Victoria et al. (2000)



Decoration & rafts: Mo [n]
- Singh & Evans (1997)
- Yamakawa & Shimomura (1998)

<u>Issue</u>: how to model strengthening effects, yield phenomena, defect absorption, defect motion, etc.?

- Multiscale modelling approach is necessary
  - continuum scale for strength, stress-strain characteristics, obstacle statistics effects, etc.
  - atomic scale for dislocation-obstacle interaction mechanisms, strength parameters, etc. (not obvious *a priori*)
  - nano- → micro- → meso-mechanics

- continuum scale for strength, stress-strain characteristics, obstacle statistics effects, etc.

Institute of Physics Publishing — Modelling and Simulation in Materials Science and Engineering
Modelling Simul. Mater. Sci. Eng. 11 (2003) R33–R68 — PII: S0965-0393(03)21576-X

TOPICAL REVIEW

Atomistic/continuum coupling in computational materials science

W A Curtin[1] and Ronald E Miller[2]

ELSEVIER — Journal of Nuclear Materials 276 (2000) 154–165 — journal of nuclear materials — www.elsevier.nl/locate/jnucmat

3D dislocation dynamics: stress–strain behavior and hardening mechanisms in fcc and bcc metals

Hussein M. Zbib[a,*], Tomas Díaz de la Rubia[b], Moono Rhee[b], John P. Hirth[a]

Philosophical Magazine, 1 Nov–1 Dec 2003
Vol. 83, Nos. 31–34, 3475–3528 — Taylor & Francis, Taylor & Francis Group

Multiscale modelling of nanomechanics and micromechanics: an overview

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ELSEVIER — Available online at www.sciencedirect.com — SCIENCE DIRECT — Journal of Nuclear Materials 323 (2003) 290–303 — journal of nuclear materials — www.elsevier.com/locate/jnucmat

On dislocation–defect interactions and patterning: stochastic discrete dislocation dynamics (SDD)

M. Hiratani[a], H.M. Zbib[b,*]

Pergamon — Available online at www.sciencedirect.com — SCIENCE DIRECT — Acta Materialia 51 (2003) 5499–5518 — Acta MATERIALIA — www.actamat-journals.com

A level set method for dislocation dynamics

Yang Xiang[a,*], Li-Tien Cheng[b], David J. Srolovitz[c], Weinan E[d]

Philosophical Magazine, 2003, Vol. 83, No. 5, 539–567 — Taylor & Francis, Taylor & Francis Group

Periodic image effects in dislocation modelling

Wei Cai†‡§, Vasily V. Bulatob†, Jinpeng Chang‡, Ju Li‡, and Sidney Yip‡

- **atomic** scale for dislocation-obstacle interaction mechanisms, strength parameters, etc. (not obvious *a priori*)

VOLUME 82, NUMBER 16 PHYSICAL REVIEW LETTERS 19 APRIL 1999

Dislocation Pinning by Small Interstitial Loops: A Molecular Dynamics Study

D. Rodney and G. Martin

PHYSICAL REVIEW B VOLUME 61, NUMBER 13 1 APRIL 2000-I

Dislocation pinning by glissile interstitial loops in a nickel crystal: A molecular-dynamics study

D. Rodney and G. Martin

Preprint
UCRL-JC-152885

Atomistic Simulations of Dislocations and Defects

John A. Moriarty, Vaclav Vitek, Vasily V. Bulatov and Sidney Yip

This article has been submitted to the Journal of Computer-Aided Materials Design

April 28, 2003

PHILOSOPHICAL MAGAZINE, 1 Nov–1 Dec 2003
VOL. 83, NOS. 31–34, 3623–3641
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Atomic modelling of strengthening mechanisms due to voids and copper precipitates in α-iron

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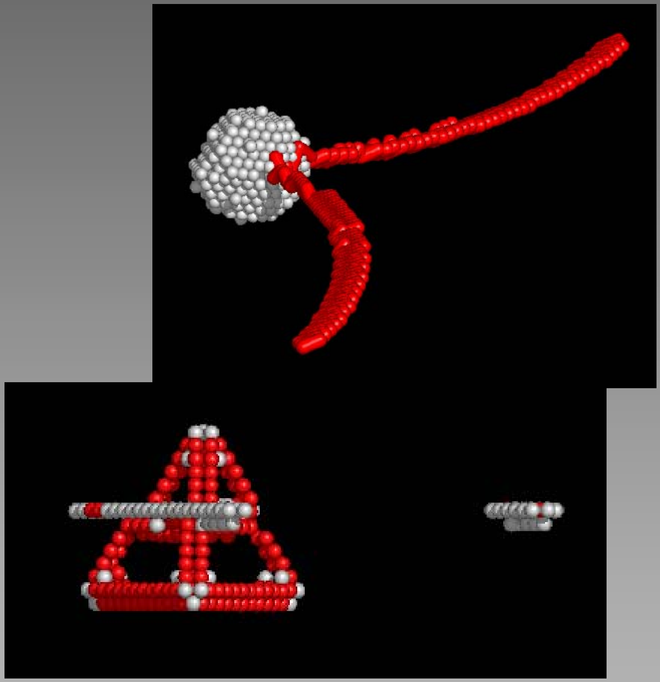
Pergamon
Available online at www.sciencedirect.com
SCIENCE DIRECT
Acta Materialia 51 (2003) 5711–5742
Acta MATERIALIA
www.actamat-journals.com

Atomistic modeling of mechanical behavior☆

Ju Li [a,*], Alfonso H.W. Ngan [b], Peter Gumbsch [c,d]

Atomic-scale

- Requirements
  - long-distance motion of dislocation
  - extraction of stress/strain and stress/strain-rate characteristics
  - T = 0K and T > 0K
  - atomic structure of obstacle and dislocation after interaction

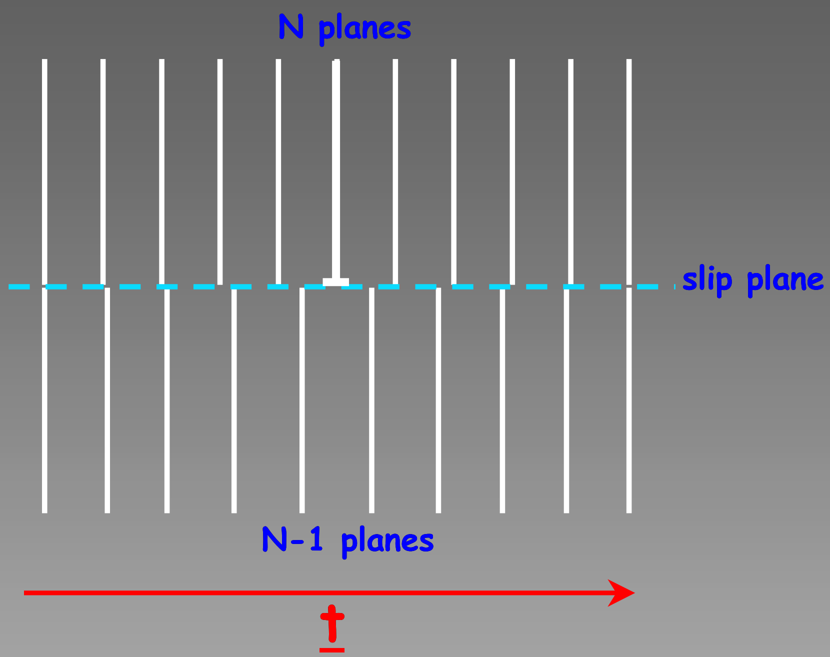


Issue: models able to give quantitative information?

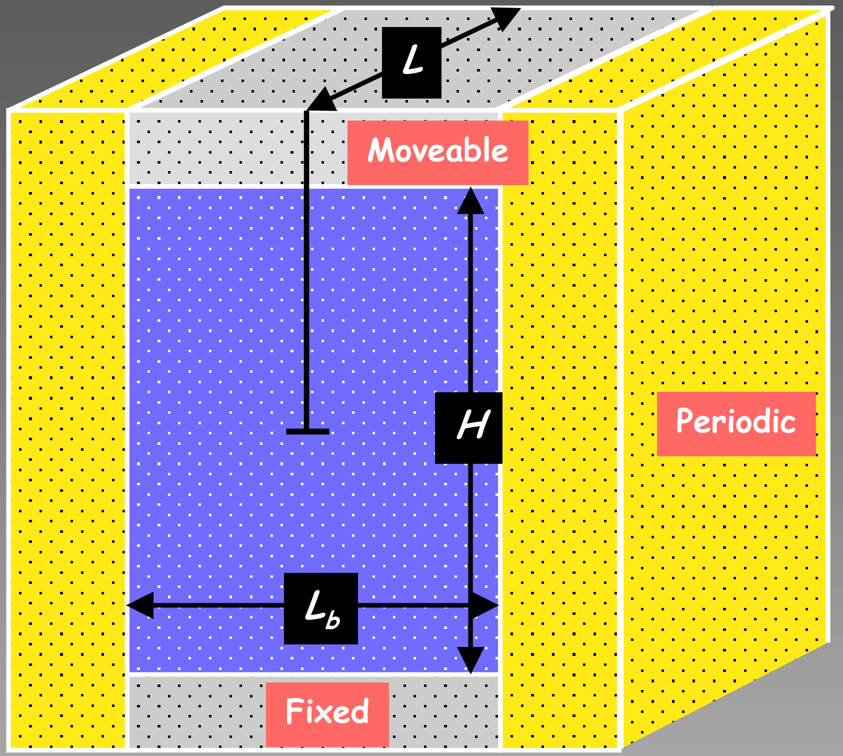
  - ~1-10M atoms
  - simple, short-range potentials

Issue: models able to describe candidate materials?

Model - edge dislocation:

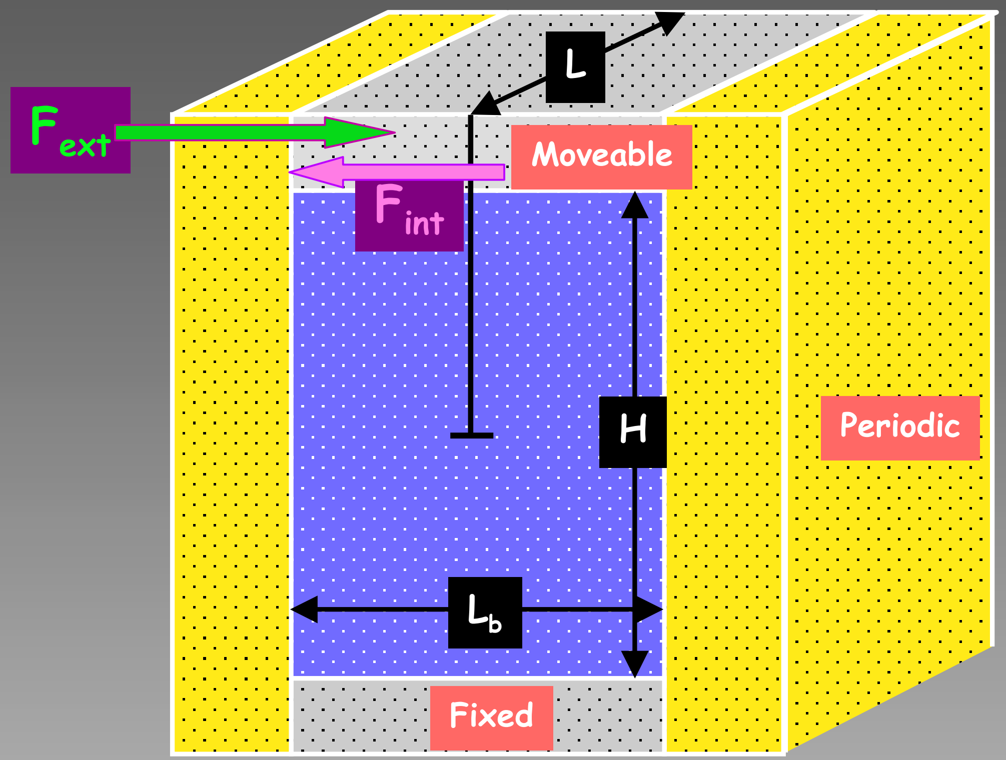


translation vector of two half crystals
= translation vector of MD cell



MD cell
(periodic boundaries along line
and glide direction)

$\sigma_{appl} = F_{ext} /(L_b L)$ $\sigma_{gen} = F_{int} /(L_b L)$



Issue: dislocation density?

e.g. $L_b = 120b$
$H = 80b$
$L = 120b$

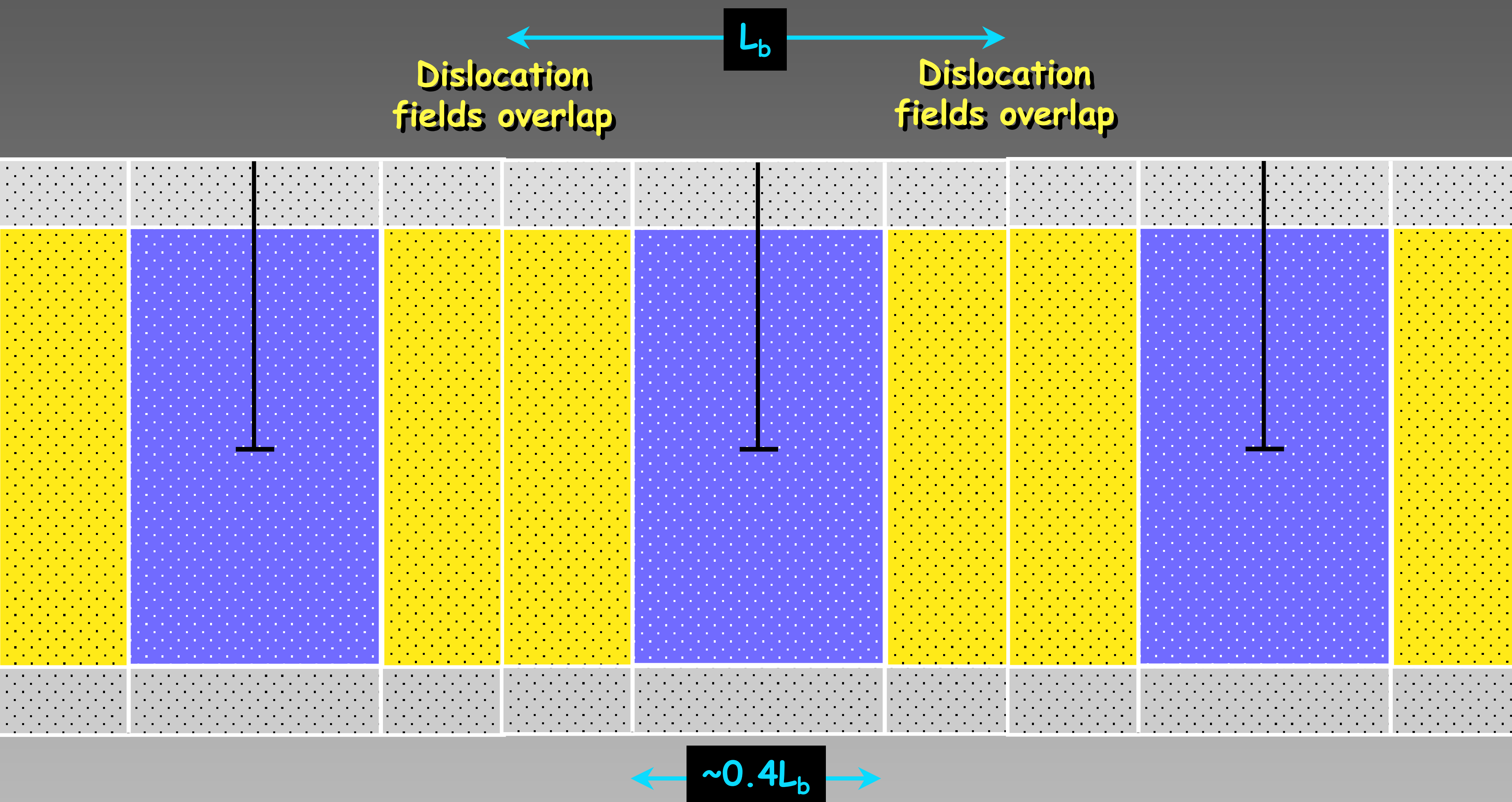
$\rho_D = 1/(L_b \times H)$
$\sim 1/(10^4 b^2)$
$\sim 1.6 \times 10^{15} m^{-2}$

$N_{atoms} \sim 1.5M$

Issue: statics or dynamics?

- T=0K (statics) simulations - apply shear strain
- T>0K (dynamics) simulations - apply shear stress or strain rate

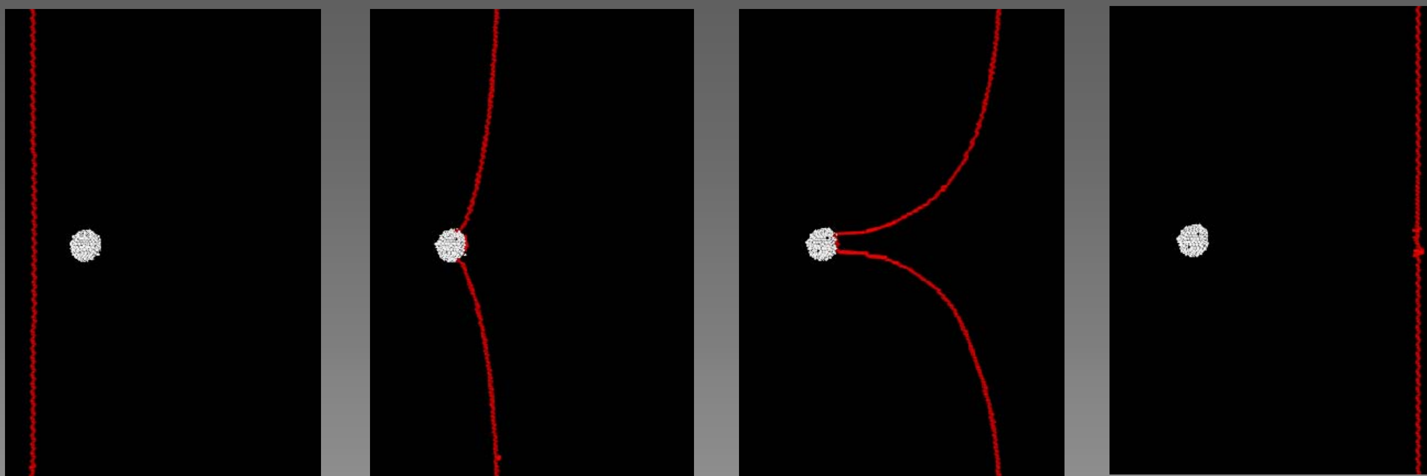
Issue: periodic boundary conditions?



'true' region

⇒ good match to infinite-body stress field

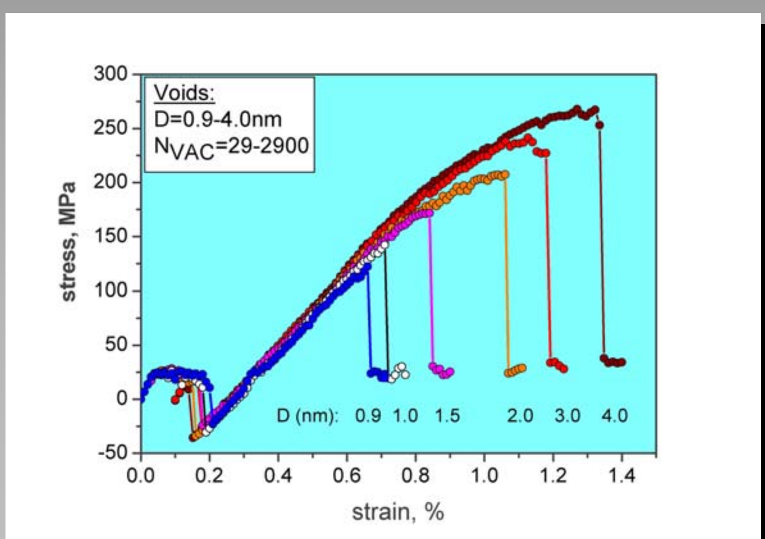
Static simulation (T = 0K)
Ex. edge dislocation ⇒ row of voids in α-Fe at T = 0K



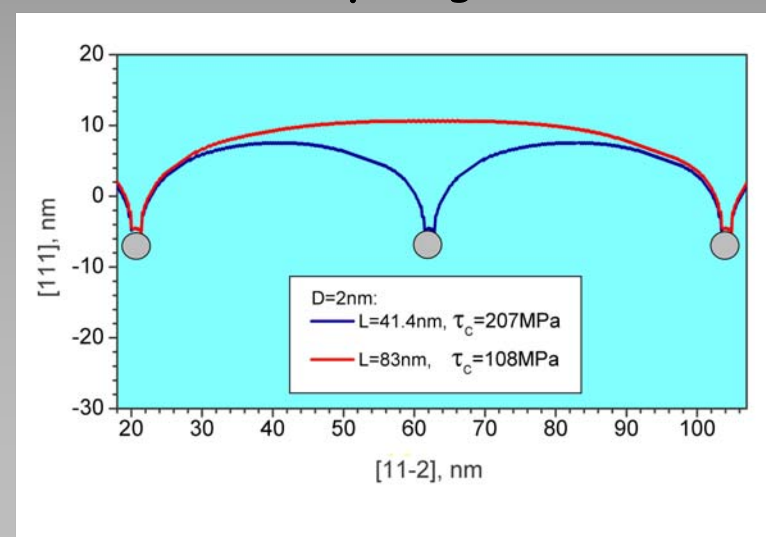
increasing strain →

2nm (339v) void in Fe
L=42nm, T=0K. C1 xtal

void size D



void spacing L

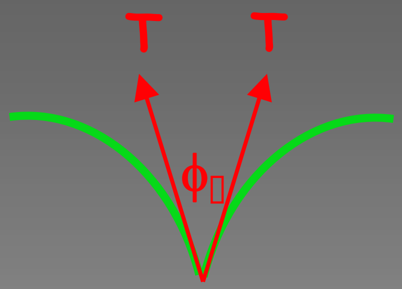


Issue: are results for dislocation shape and critical stress comparable with elasticity theory?

Line Tension

$T = Gb^2/2$ - approximation

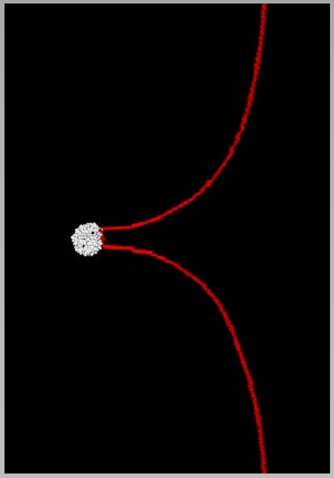
$\cos\phi_c$ characterises obstacle strength



$\tau_c bL = 2T\cos(\phi_c/2)$ (for strong obstacles)

$\therefore\ \tau_c = \alpha Gb/L$ (or $\tau \simeq \alpha Gb/L$)

$\alpha = \cos(\phi_c/2)$

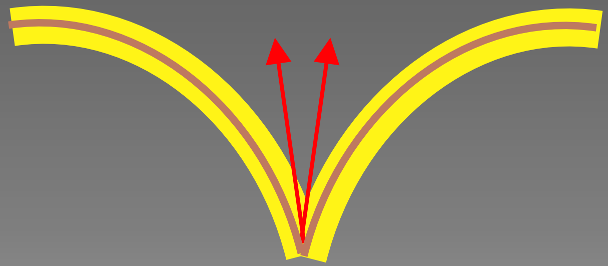


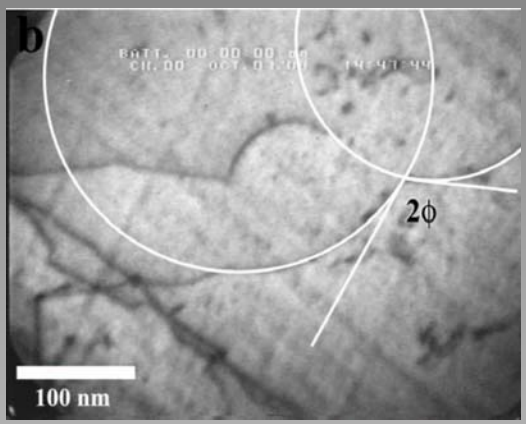
ϕ_c(line tension) should not to be equated to ϕ_c(atomic modelling)

Issue: what shape should be taken from MD or experiment for DD?

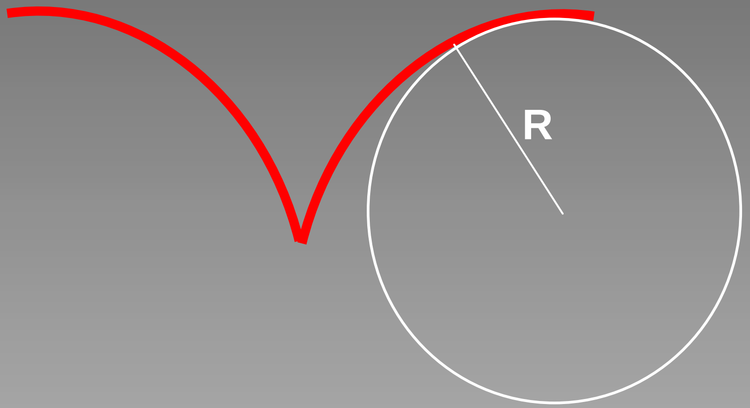
- TEM

resolution?





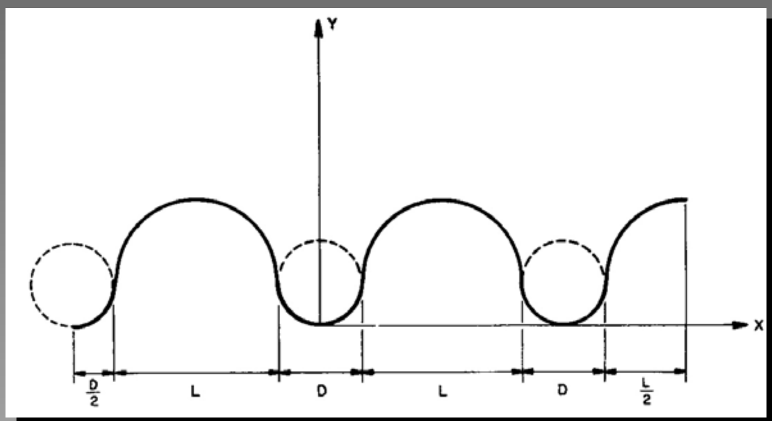
Angle?

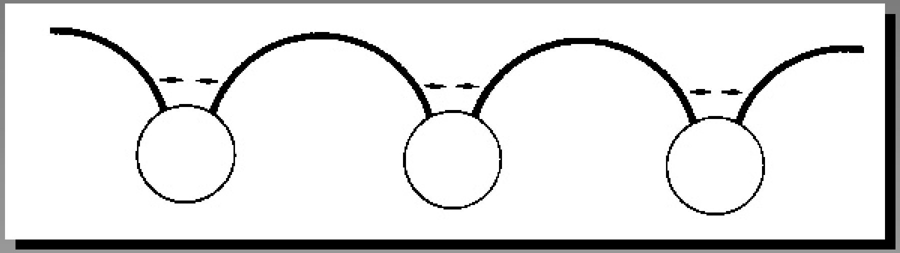


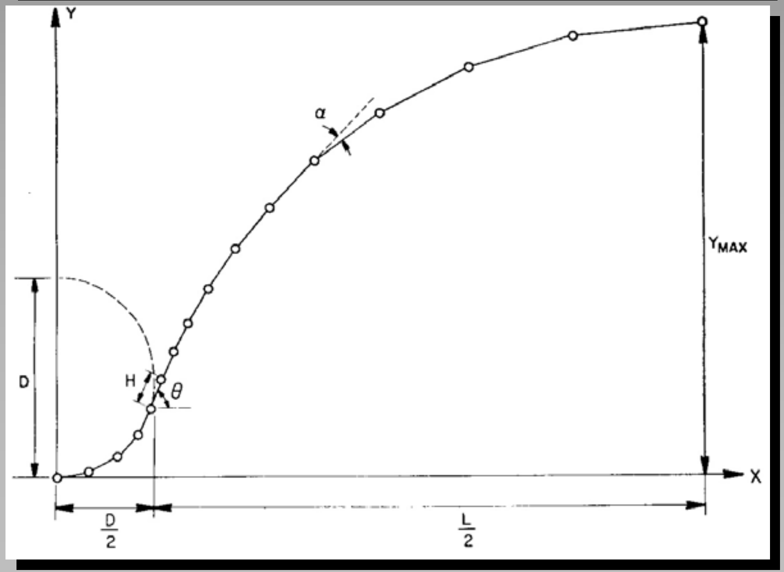
τ = T/bR in line tension, but what is T? (ln(R/r_0) and r_0 unknown)

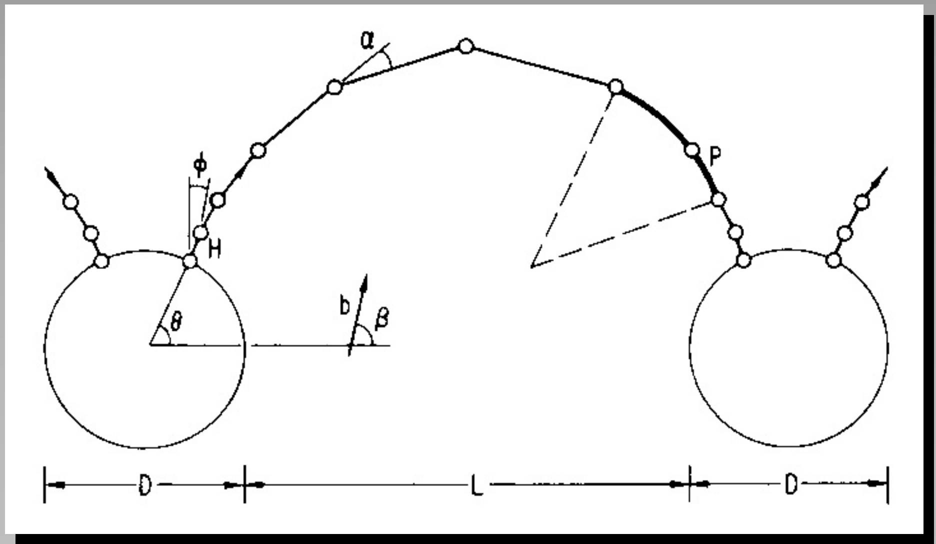
Issue: how good is simulation based on elasticity theory?

- Bacon, Scattergood, Kocks (1973-)
  - the effect of self-interaction on the critical stress $\tau_c(L, D, \underline{b})$





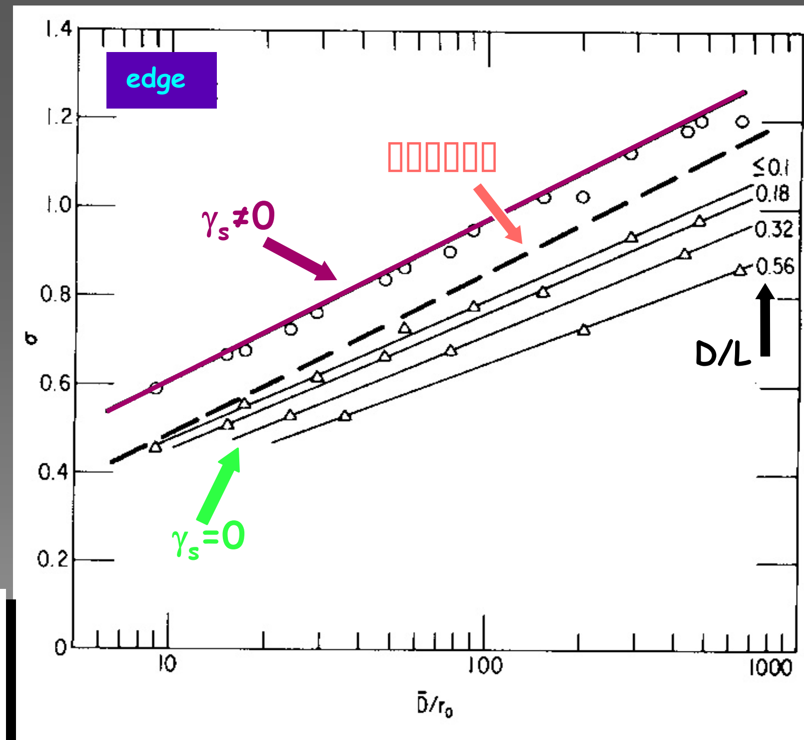


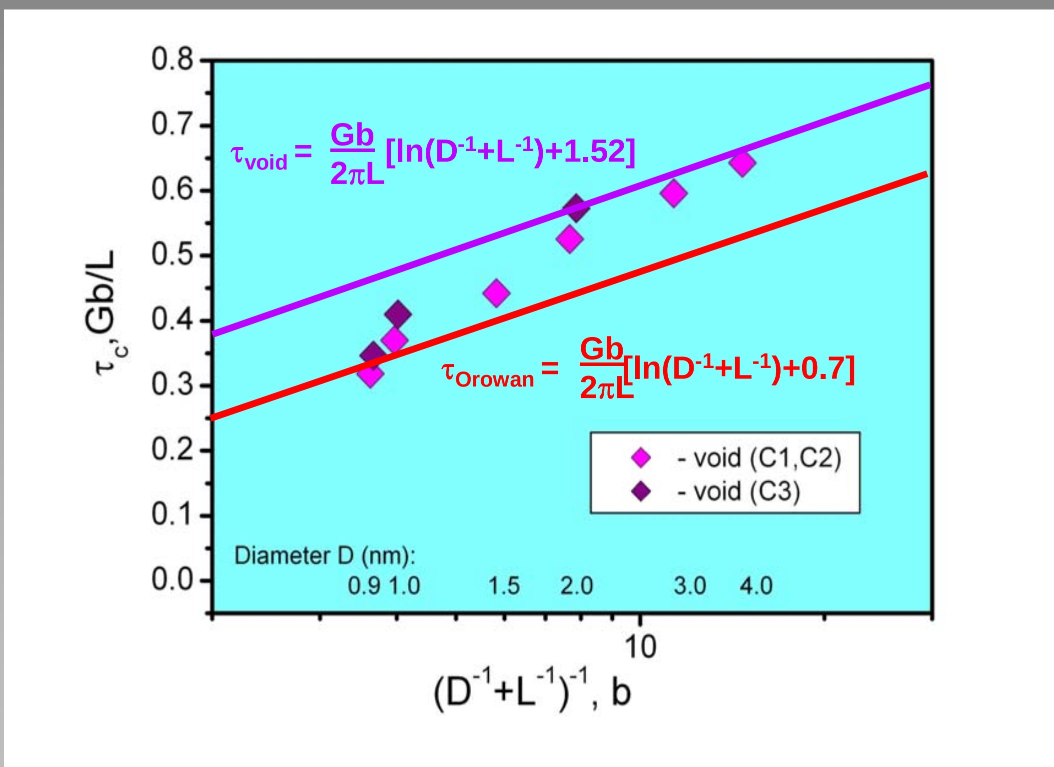


- data fits

  $\tau_{□} = (\mu b/2\pi L)[\ln(D^*) + B]$

  where $D^* = (1/D+1/L)^{-1} \approx D$

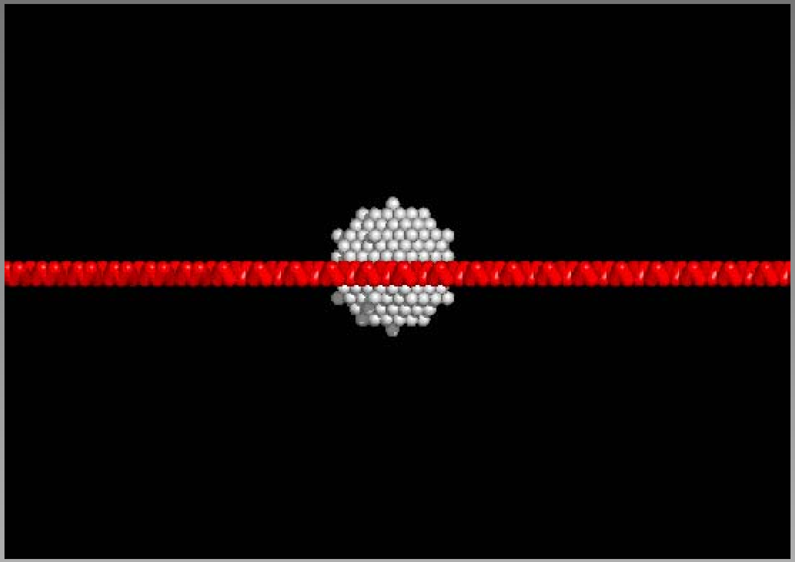


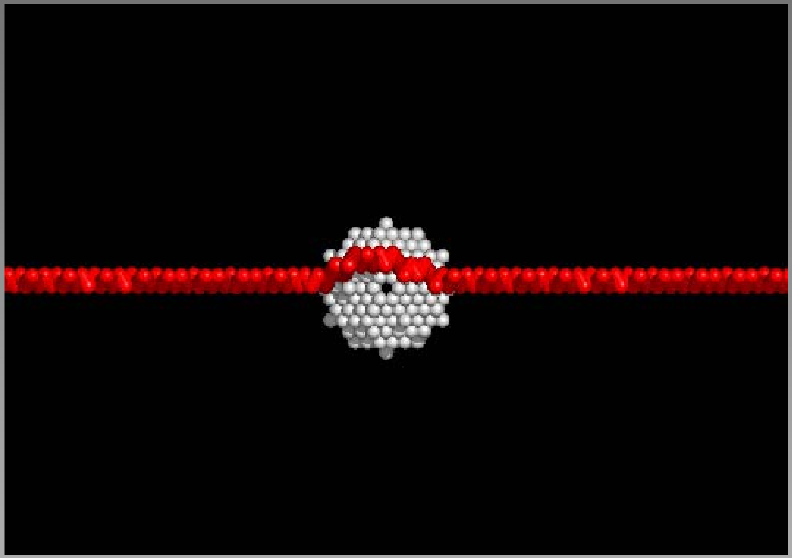


- the atomic simulation stress values are similar
- so are the line shapes

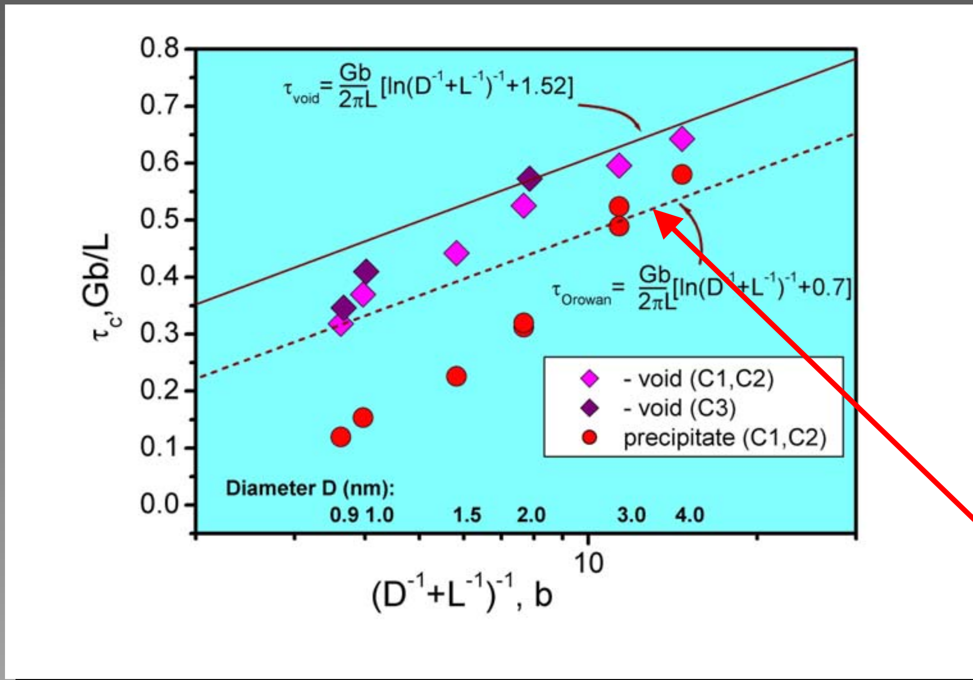
Issue: incorporation of atomic-scale mechanisms into models based on elasticity theory?

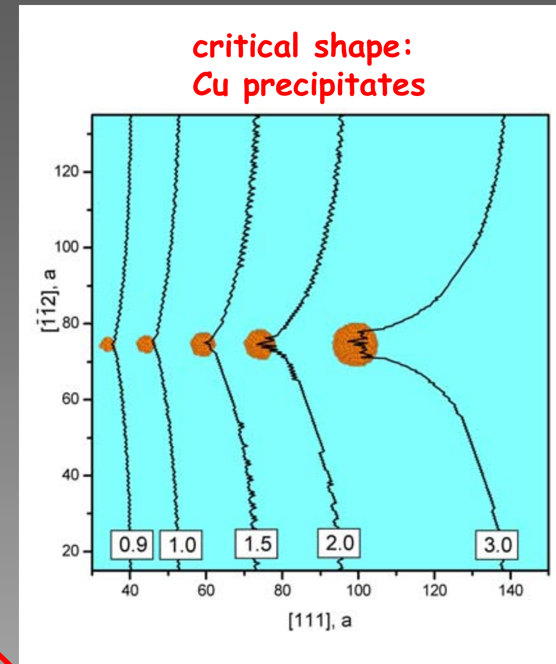
Ex 1 - Dislocation climb due to vacancy absorption from voids

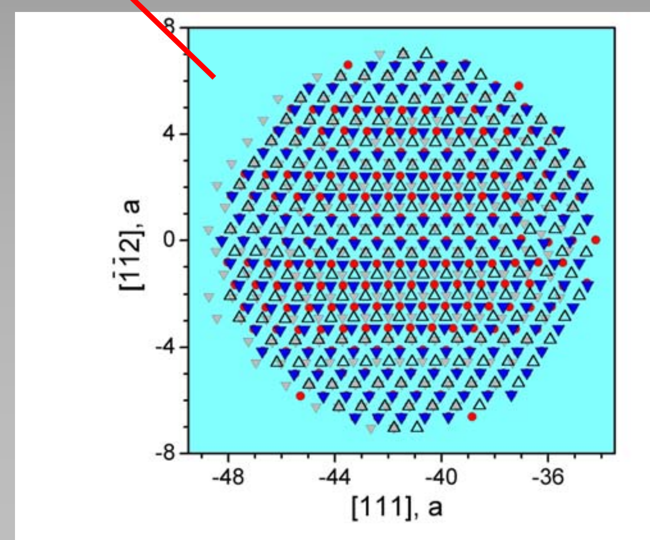




Ex 2 - Dislocation-induced transformation of Cu precipitates in Fe







Dynamics simulation (T > 0K)

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

e.g.

$SR = 5 \times 10^6 s^{-1}$, $L_b = 120b$, $\rho_D = 1.6 \times 10^{15} m^{-2}$:

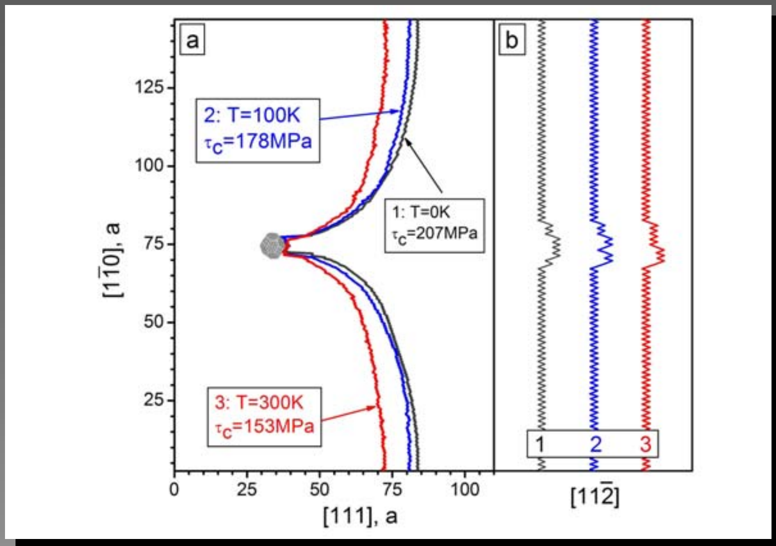
$v = 12 ms^{-1}$, $t = 2.4 ns$

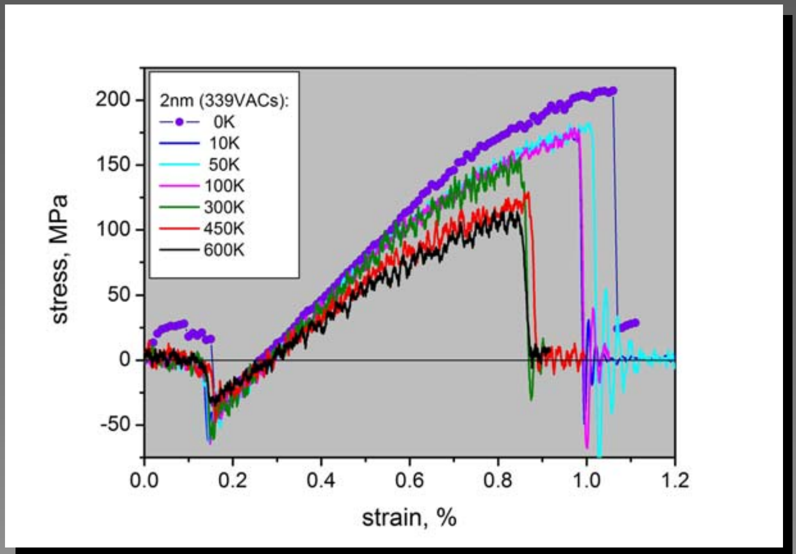
If $\Delta t = 2fs$, $N_{atom} = 1.5M$, computational speed = $10^{-5} s/atom/\Delta t$:

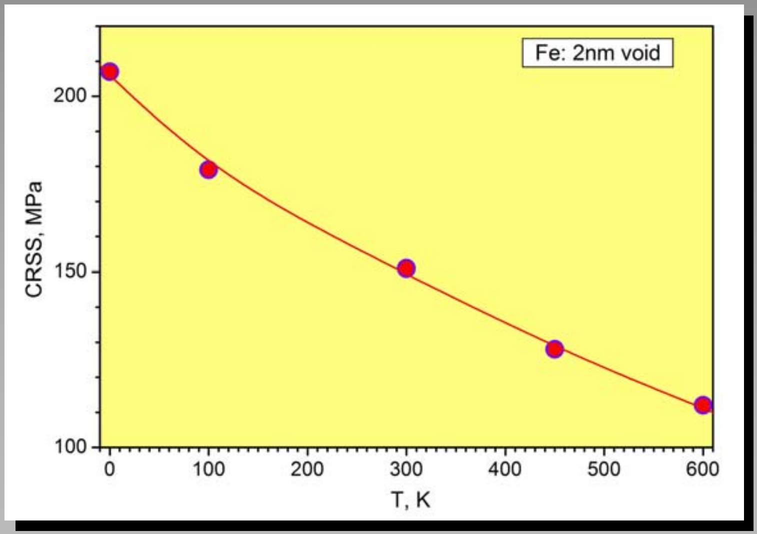
time = 170 days

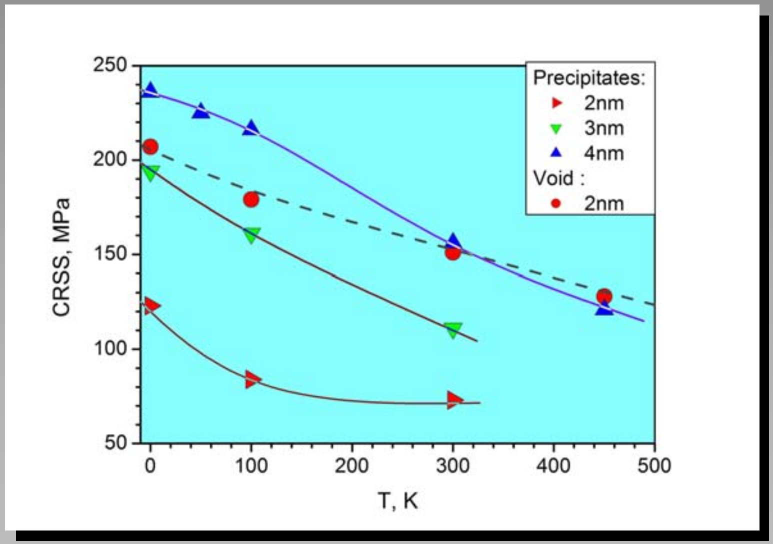
Issue: is high strain rate unavoidable? - is it realistic?

Ex 1. 2nm voids in Fe - strain rate $5 \times 10^6 s^{-1}$



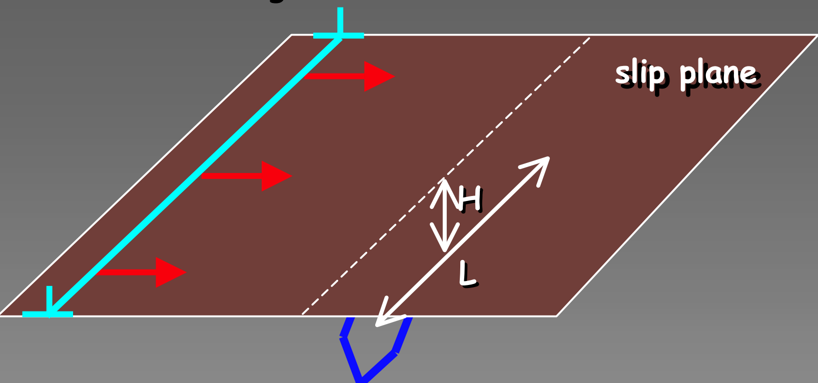




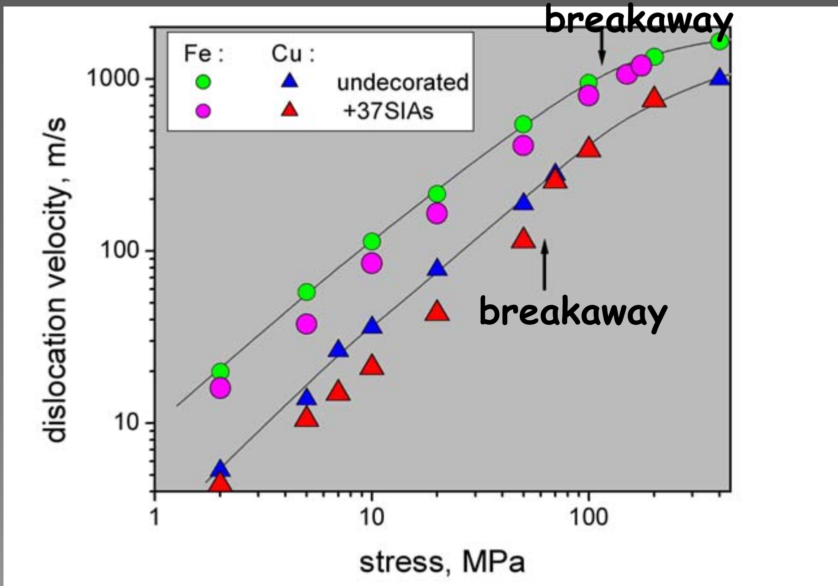


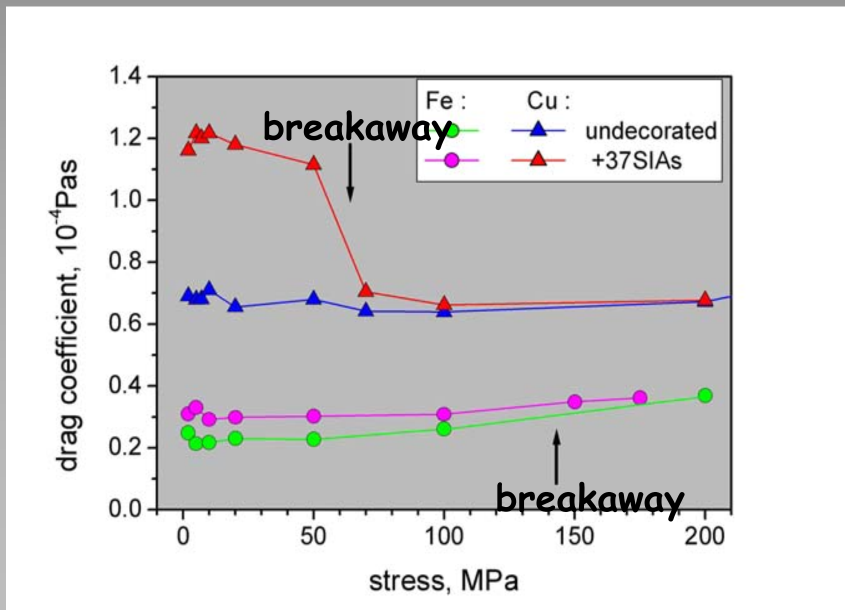
- mechanisms of T-dependence?

Ex 2. Interaction of dislocation with row of glissile interstitial loops - constant applied stress



edge+loop drag glide_1
Fe 100MPa, 300K





- drag coefficient $\tau b = (B_{disl}+B_{loop})v$:
  - drag due to moveable pinning points spacing L, mobility m:

$$B_{loop} = \frac{1}{mL} \quad \text{where} \quad m = \frac{D}{kT}$$

and for loops:

$$D = f\frac{1}{2}b^2\upsilon$$

Issue: incorporation of atomic-scale mechanisms from dynamics into models based on elasticity theory?

General Issue: incorporation of information from atomic-scale simulations into models based on elasticity theory?

- obstacle forces
- dislocation dynamics
- obstacle dynamics

Other areas:

- effects of solutes
- dislocations near cracks

<u>Issues</u>:

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- models able to describe candidate materials?
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- dislocation density?
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- are results for dislocation shape and critical stress comparable with elasticity theory?
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- <u>other areas</u>: solutes, cracks