Dislocation Dynamics (part 2)

Computational material science
Lecture 8

Last time

- Dislocations are lattice defects in crystalline solids that can be represented in a continuum framework by their slip plane, line direction, and Burgers vector

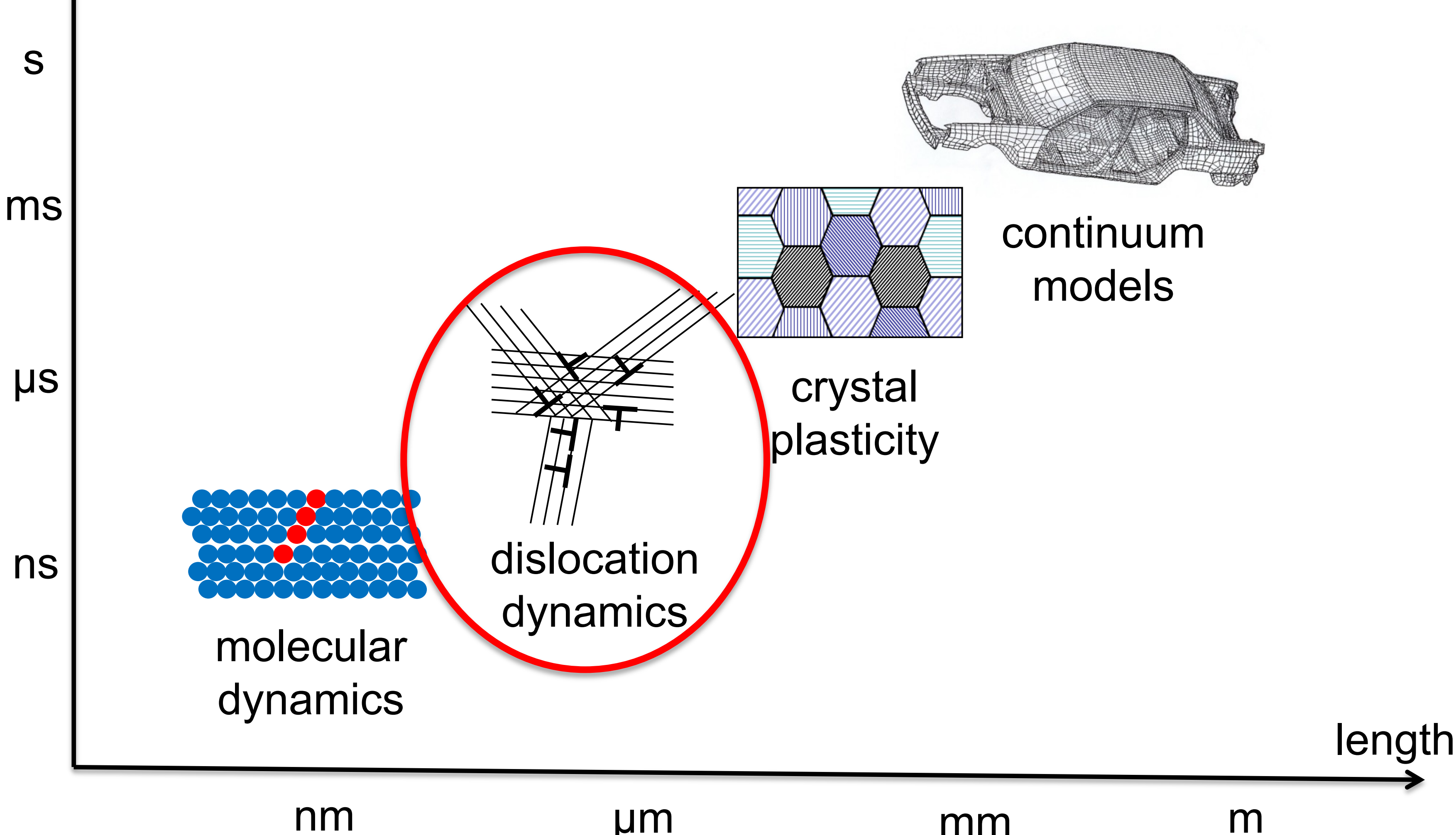
- The dislocations can be represented, outside of their core, as the elastic distortion of an elastic continuum

- Dislocations fields have a long range effect, and therefore dislocations attract or repel each other forming structures

- Dislocations glide on highly packed slip planes and directions

modeling plasticity at different scales

Essentially, all models are wrong, but some are useful.
G. Box



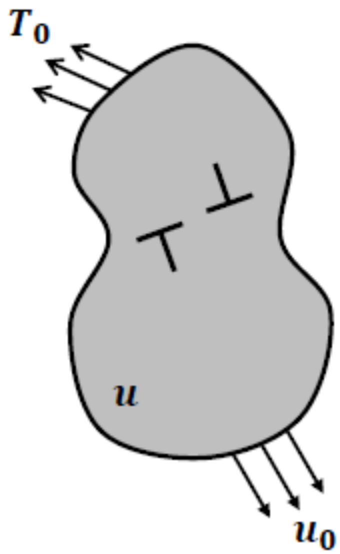
why interested in the microscale?

1. Micro-sized components: various components used for instance in the electronic industry (including micromachines) have dimensions at the microscale (films, cantilevers, interconnects, micro-motors…)

1. Micro-structures: what happens/originates at the micro-scale can affect the behavior of a large structure (see Titanic).
    - interaction dislocations/boundaries (GB, PB)
    - competition between crack propagation and plasticity

discrete dislocation plasticity

The static problem:



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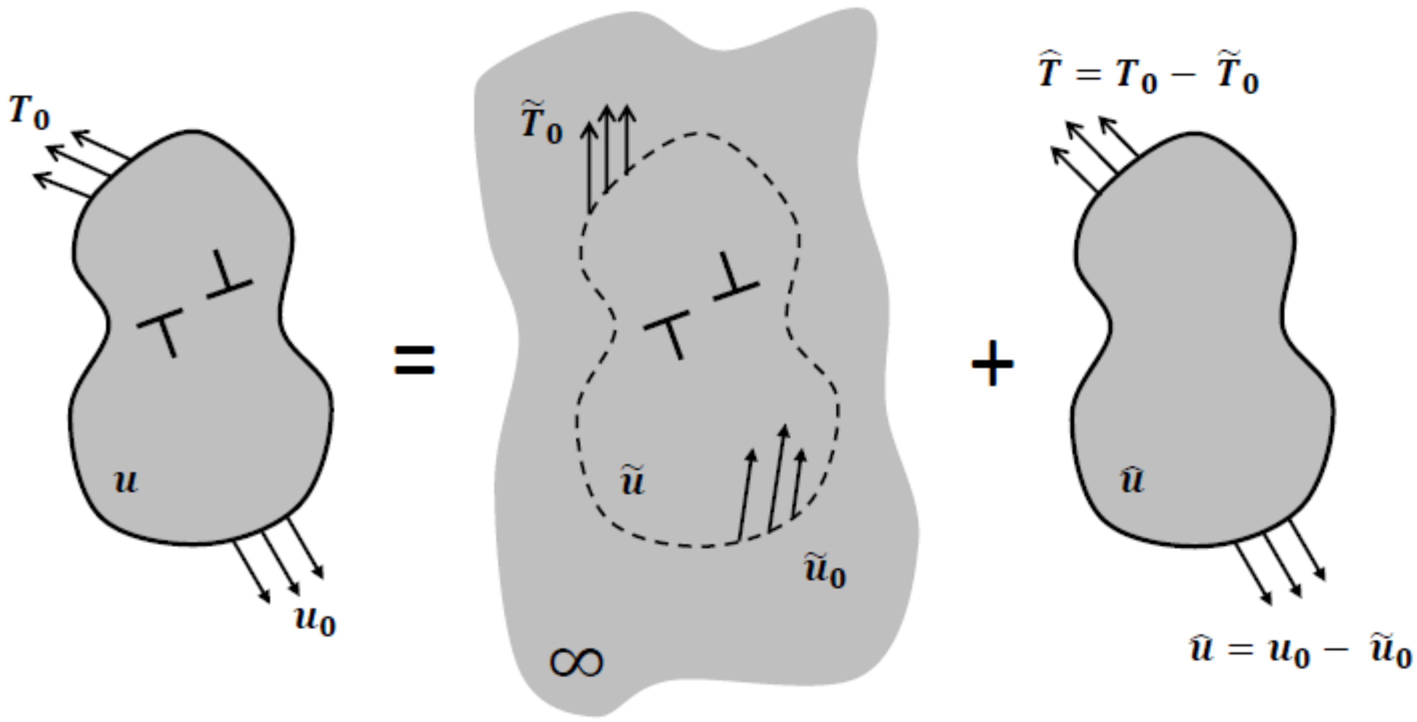
Van der Giessen and Needleman, MSMSE 1995

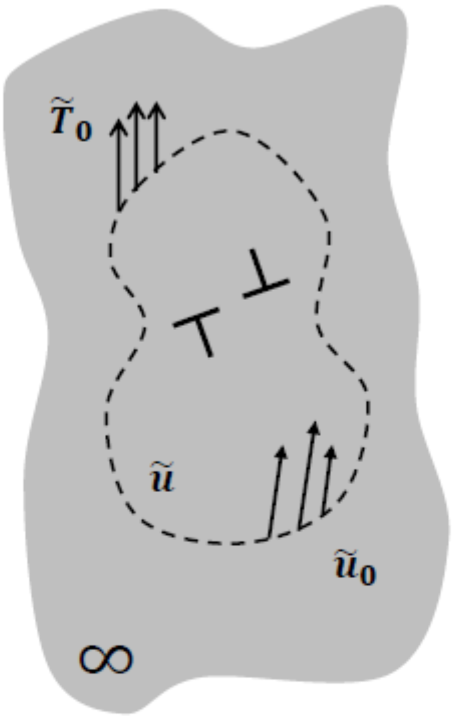
discrete dislocation plasticity

The static solution:

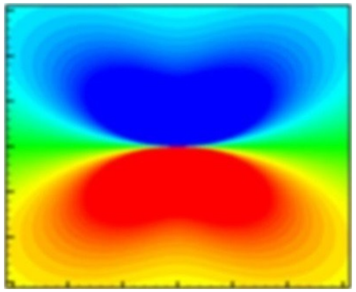


$$u = \tilde{u} + \hat{u}\,, \quad \epsilon = \tilde{\epsilon} + \hat{\epsilon}\,, \quad \sigma = \tilde{\sigma} + \hat{\sigma}$$

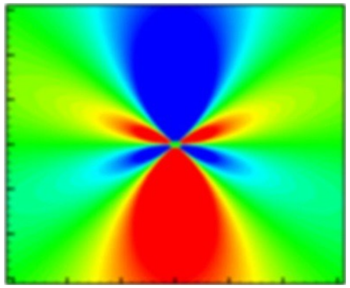
dislocation fields



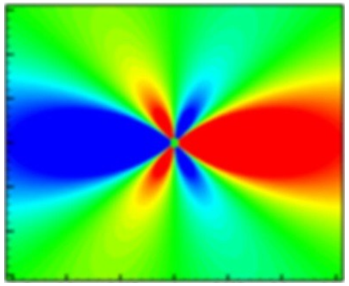
$$\sigma_{xx} = \frac{-\mu b}{2\pi(1-\upsilon)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$



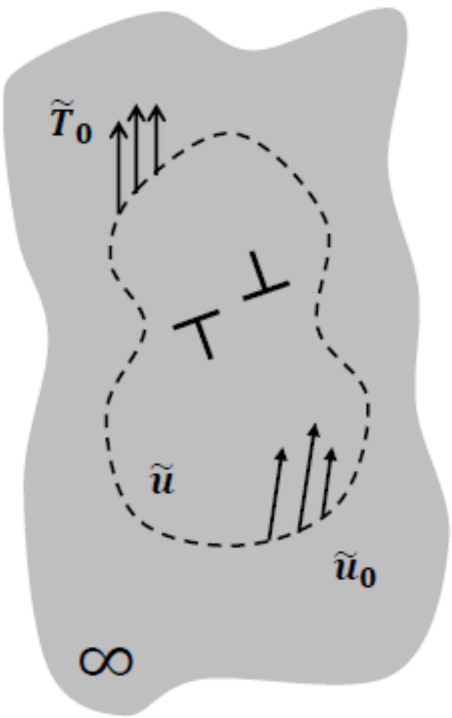
$$\sigma_{yy} = \frac{\mu b}{2\pi(1-\upsilon)} \frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

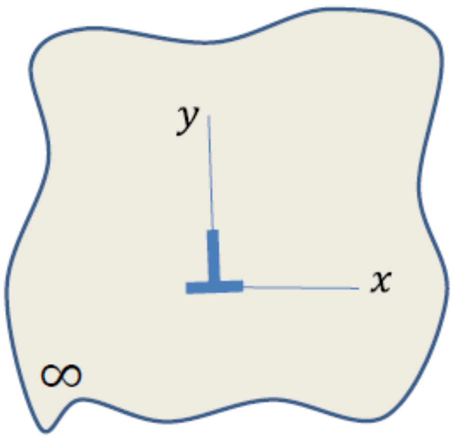


$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\upsilon)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$



dislocation fields





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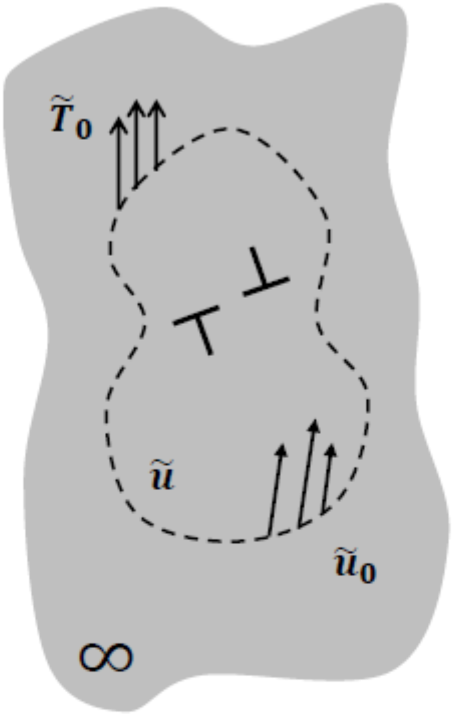
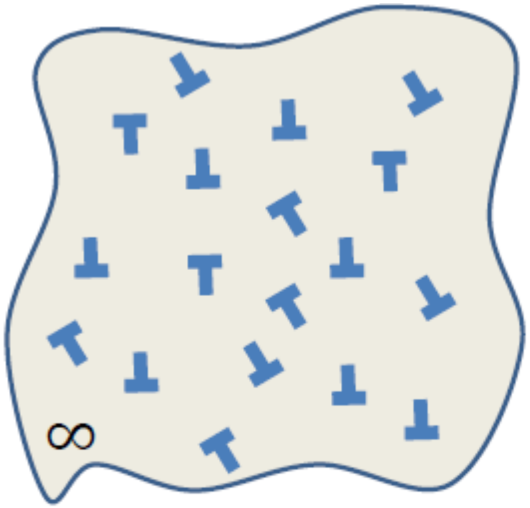
$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\upsilon)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

dislocation fields



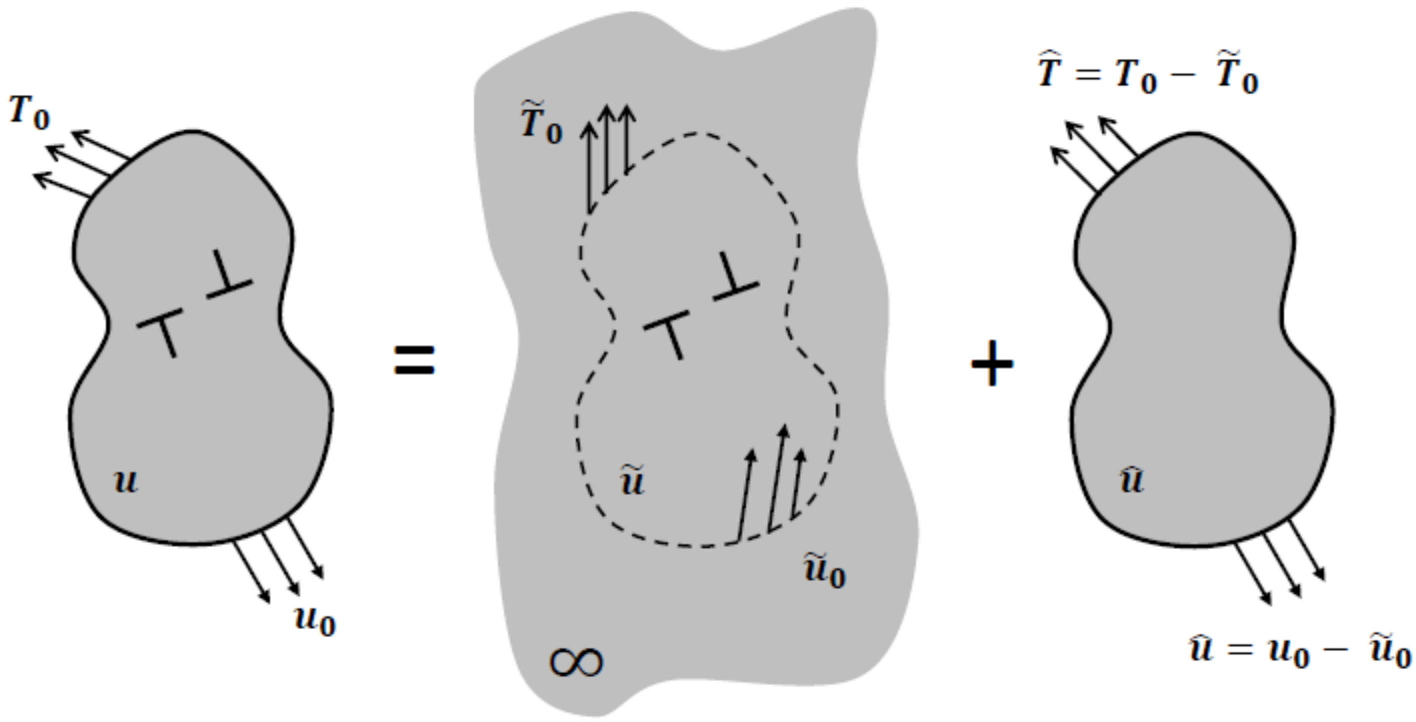


$$\sigma_{xx} = \sum_{i=1}^{N} \frac{-\mu b_i}{2\pi(1-\upsilon)} \frac{y_i\,(3x_i^2 + y_i^2)}{(x_i^2 + y_i^2)^2}$$

$$\sigma_{yy} = \sum_{i=1}^{N} \frac{\mu b_i}{2\pi(1-\upsilon)} \frac{y_i(x_i^2 - y_i^2)}{(x_i^2 + y_i^2)^2}$$

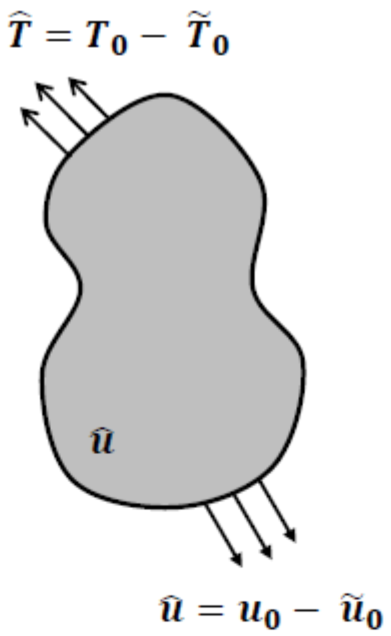
$$\sigma_{xy} = \sum_{i=1}^{N} \frac{\mu b_i}{2\pi(1-\upsilon)} \frac{x_i(x_i^2 - y_i^2)}{(x_i^2 + y_i^2)^2}$$

discrete dislocation plasticity



$$u = \tilde{u} + \hat{u}\,, \quad \epsilon = \tilde{\epsilon} + \hat{\epsilon}\,, \quad \sigma = \tilde{\sigma} + \hat{\sigma}$$

complementary solution



$$\text{div}\,\hat{\boldsymbol{\sigma}} = 0$$

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} : \hat{\boldsymbol{\epsilon}}$$

$$\hat{\boldsymbol{\epsilon}} = \tfrac{1}{2}[\text{grad}\,\hat{\boldsymbol{u}} + (\text{grad}\,\hat{\boldsymbol{u}})^T]$$

with the boundary conditions

$$\hat{\boldsymbol{T}} = \boldsymbol{T}^0 - \tilde{\boldsymbol{T}} \text{ on } S_f$$

$$\hat{\boldsymbol{u}} = \boldsymbol{u}^0 - \tilde{\boldsymbol{u}} \text{ on } S_u$$

dislocation dynamics

Dislocation dynamics are governed by constitutive rules.

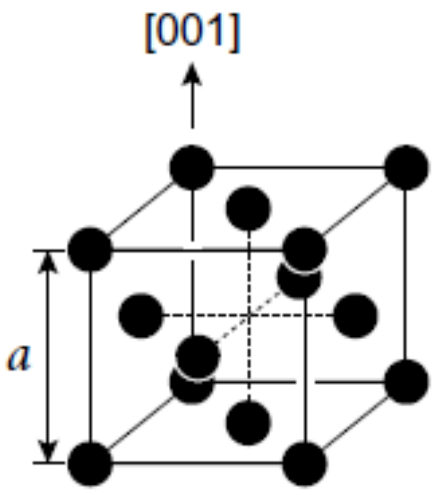
These rules are based on the Peach-Koehler force acting on a dislocation:

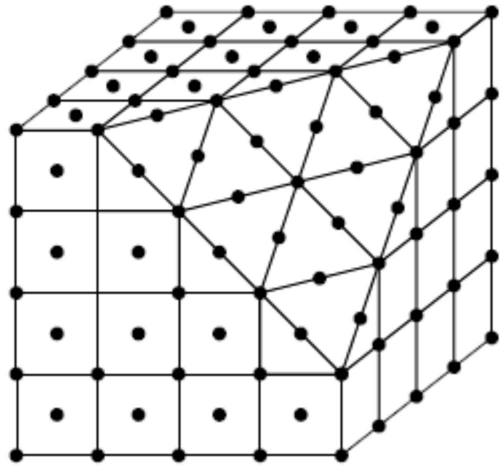
$$f^{(I)} = b_i^{(I)} \left(\hat{\sigma}_{ij} + \sum_{J \neq I} \tilde{\sigma}_{ij}^{(J)} \right) m_j^{(I)} \sim \tau^{(I)} b^{(I)}$$

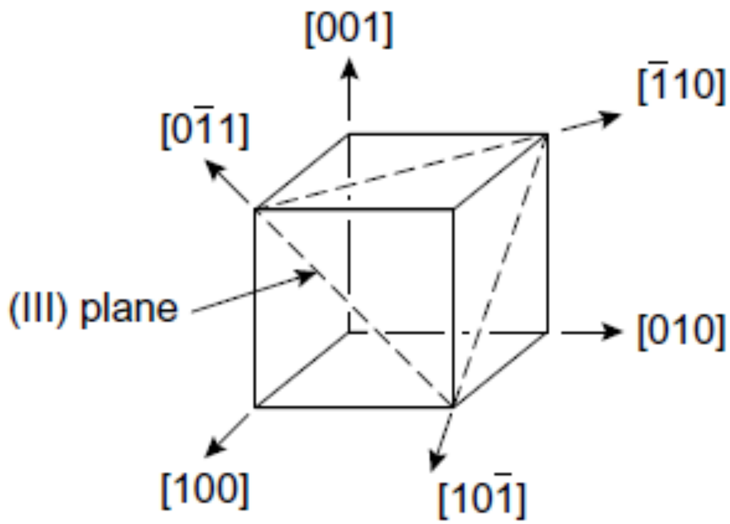
The rules control the way the dislocations

1) are generated
2) move
3) overcome obstacles
4) annihilate

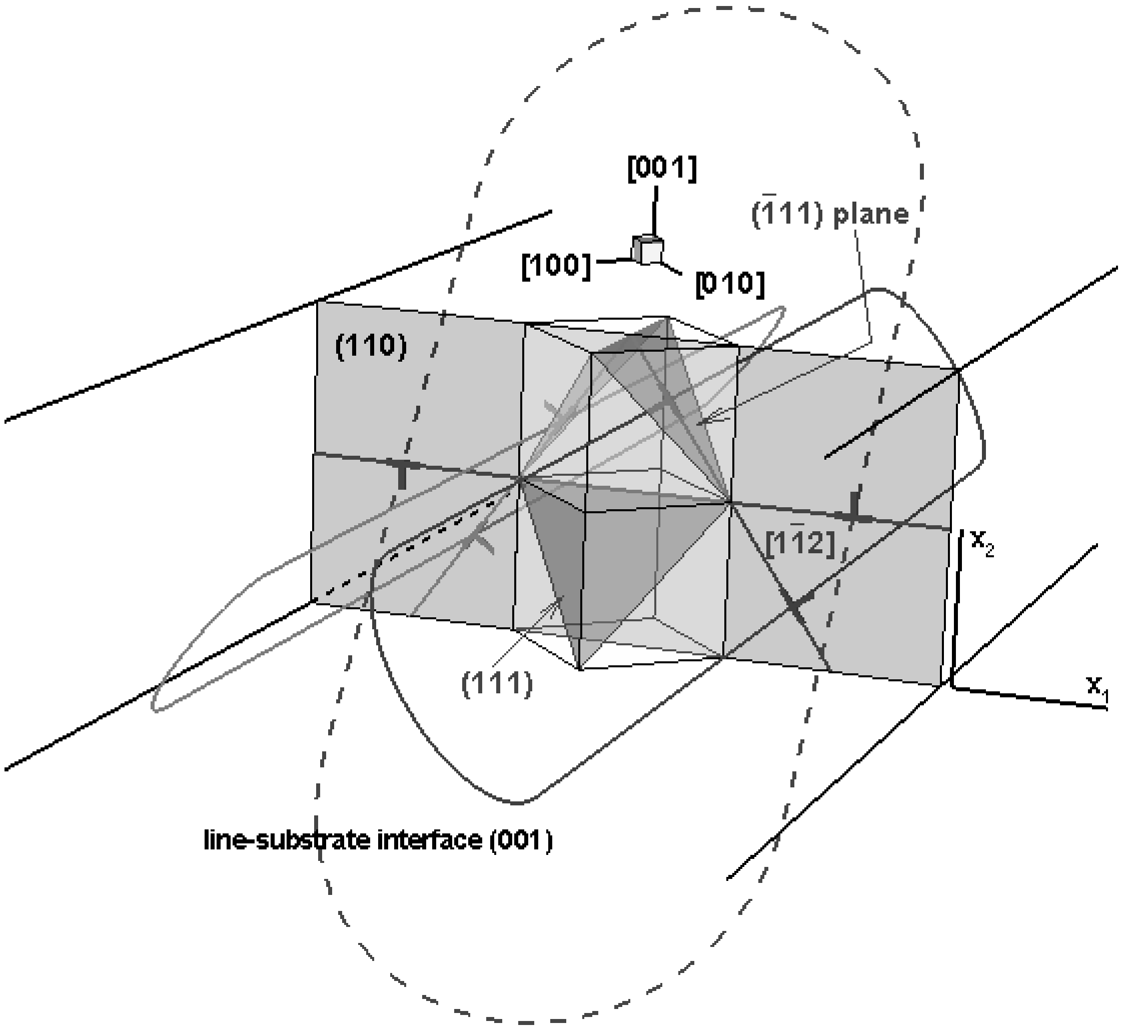
FCC structure



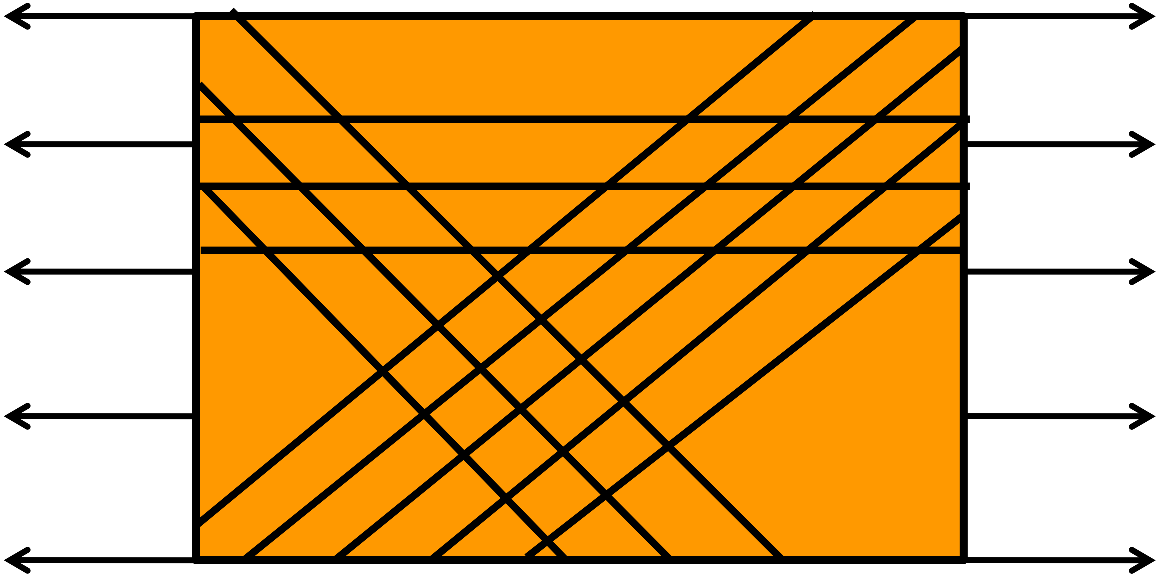




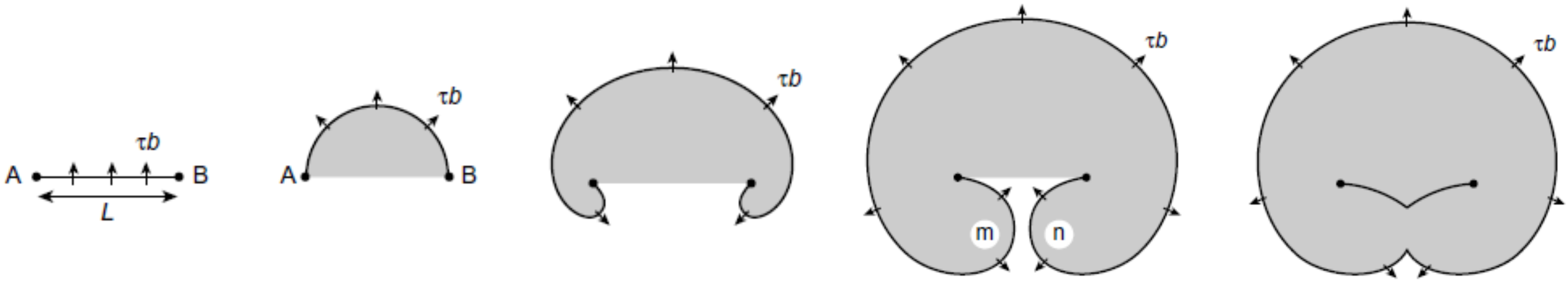
2D view


[001]
[100]
[010]
(-111) plane
(110)
[1-12]
x_2
x_1
(111)
line-substrate interface (001)

slip plane traces

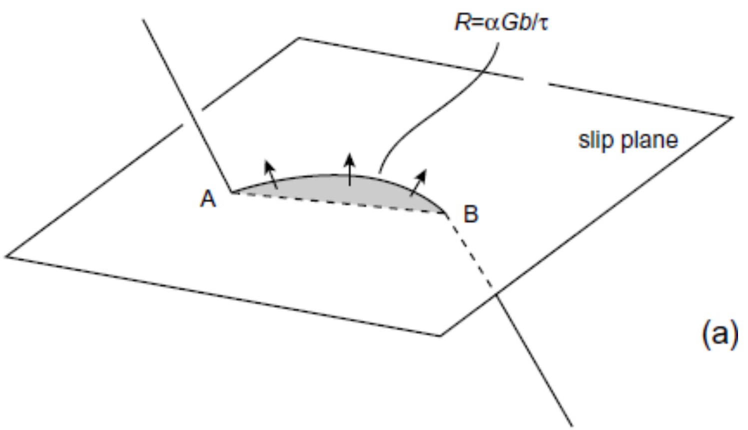


Frank-Read sources

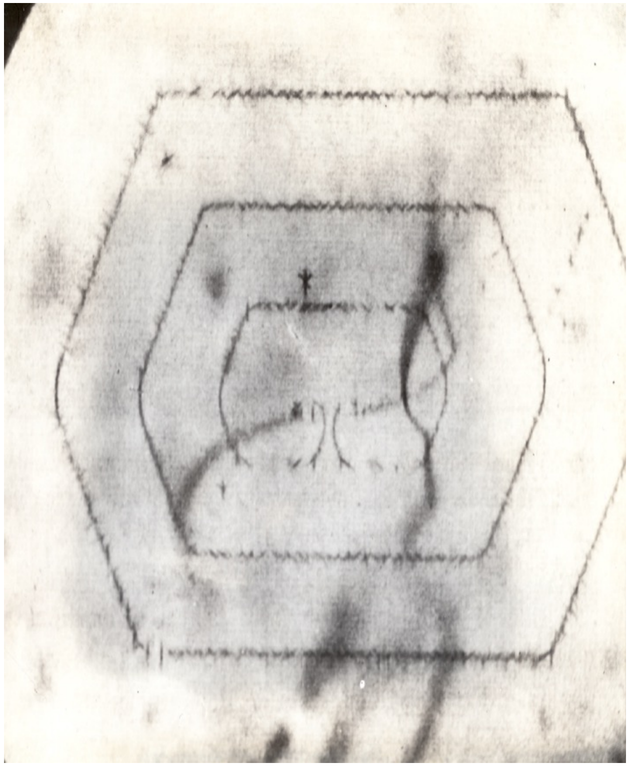


AB are the pinning points of a dislocation segment

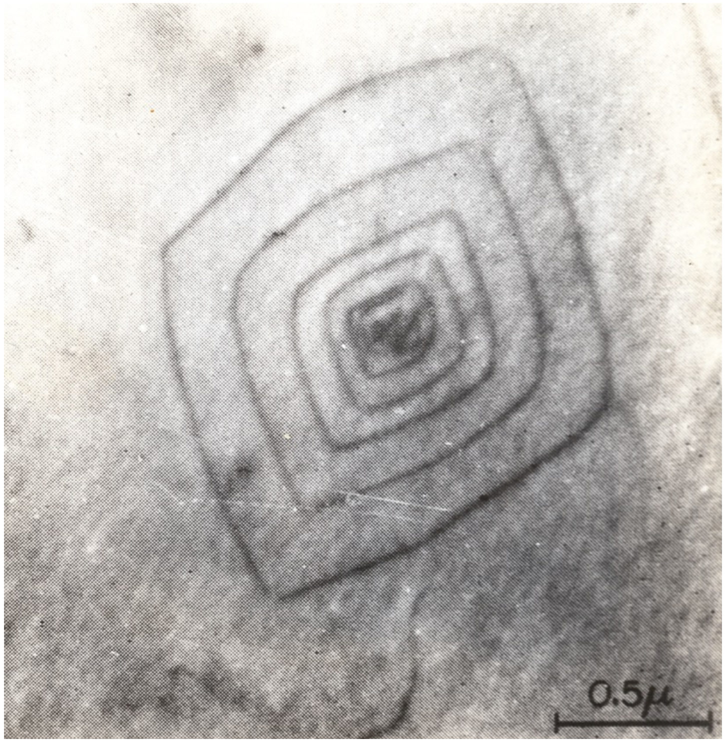
A resolved shear stress acting on the dislocation will make it bow until a full loop is formed and detaches from the original source



evidence of Frank-Read sources



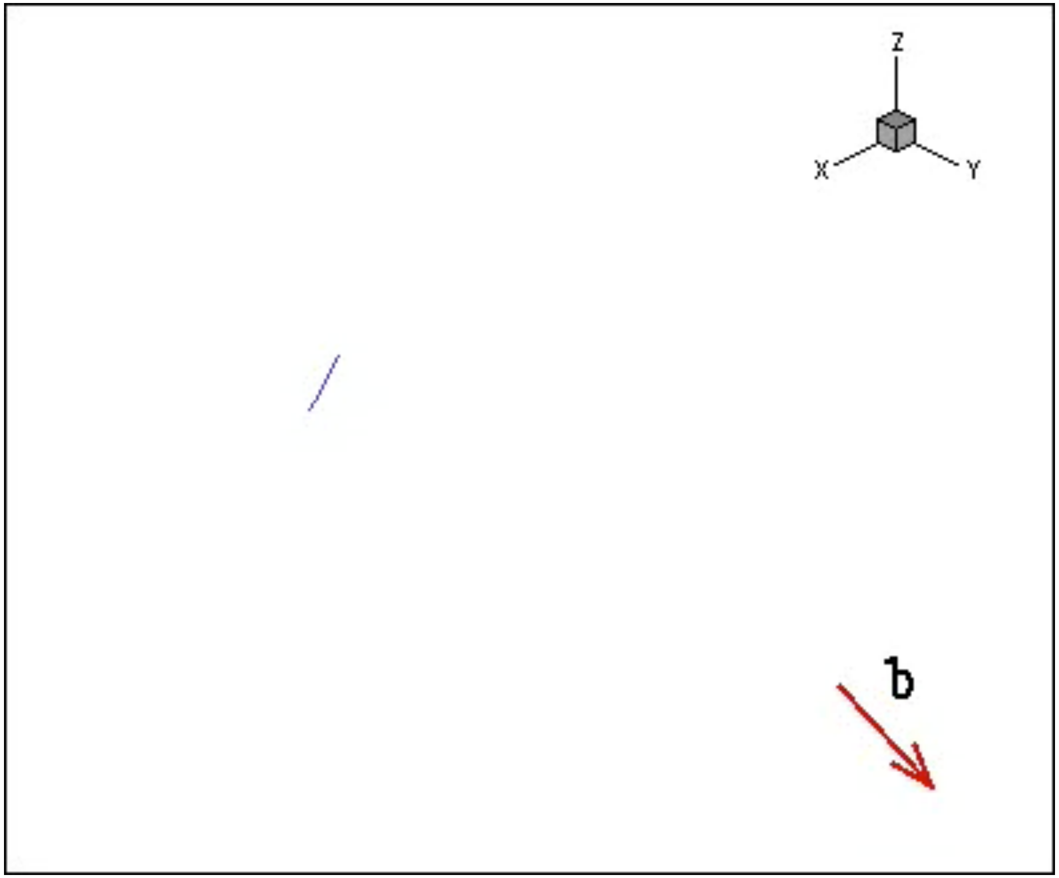
Si



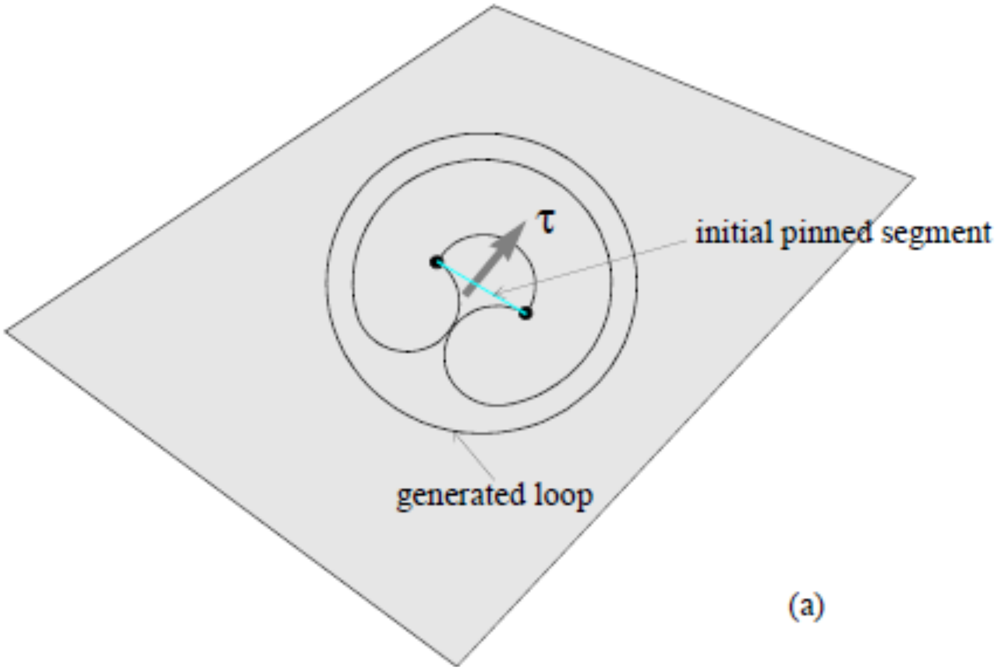
Al + 3.5 wt% Mg

Courtesy of Dr. Wim Sloof

Frank-Read source

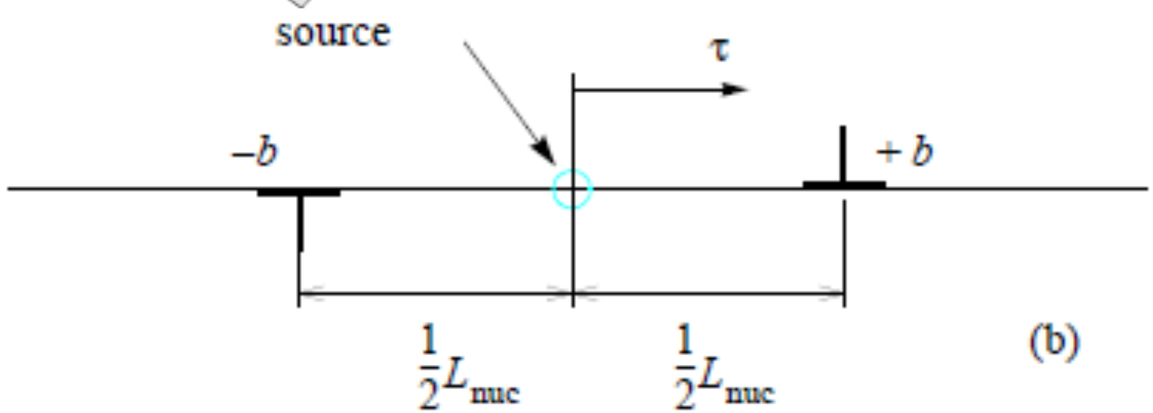


Frank-Read source



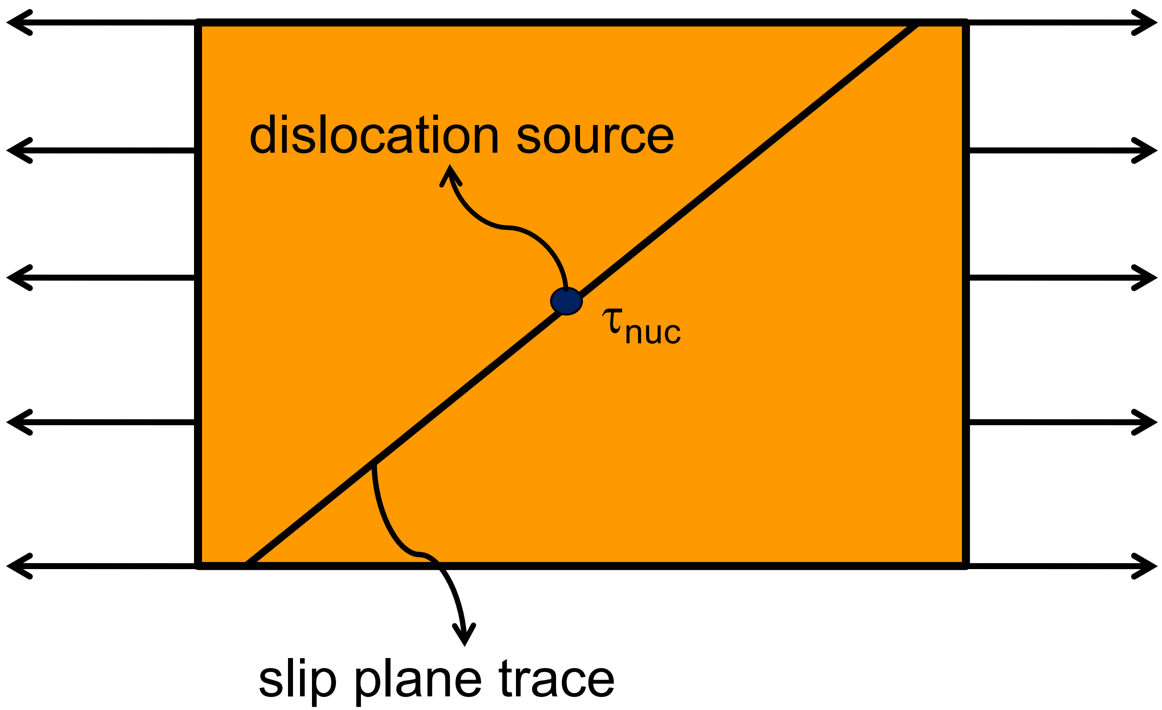
(a)

$$L_{nuc} = \frac{\mu b}{2\pi(1-\nu)\tau_{nuc}}$$

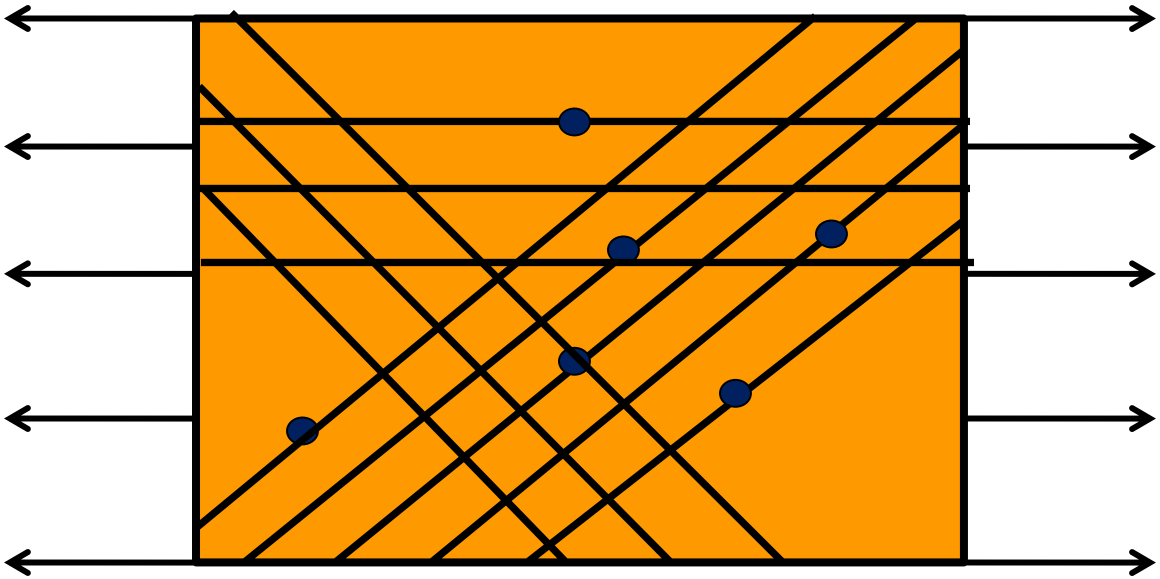


(b)

slip plane and source

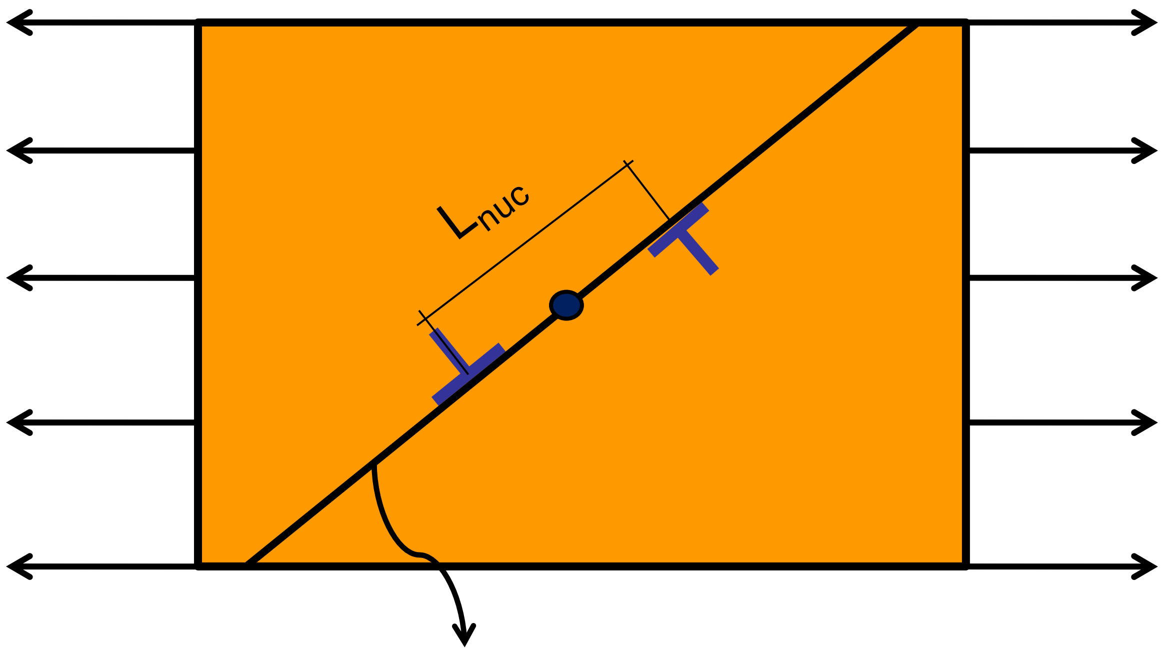


dislocation sources



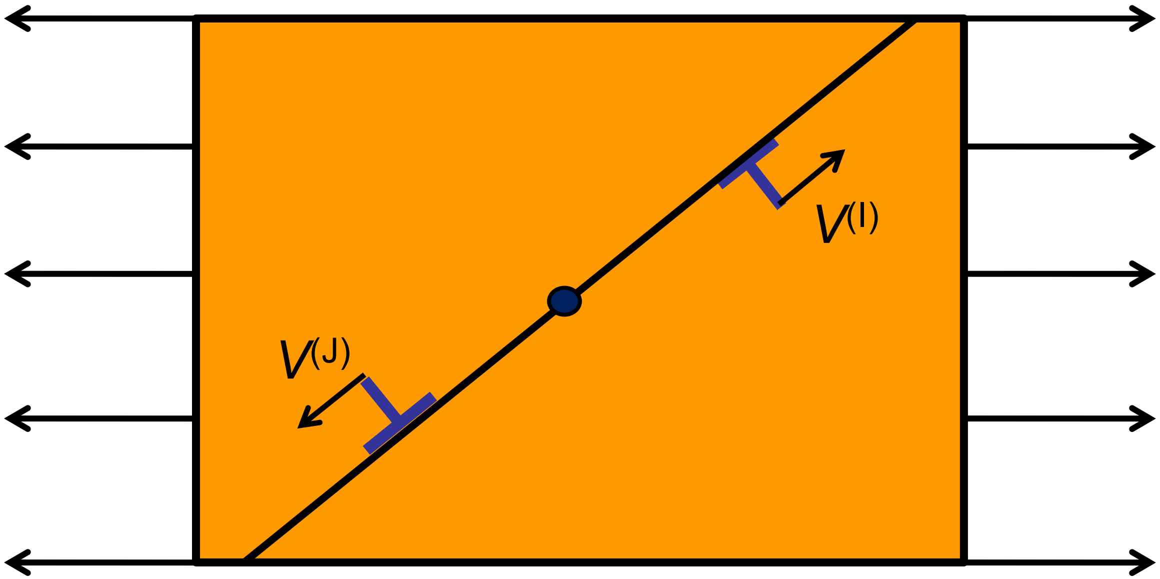
dislocation nucleation

nucleation when $\tau \geq \tau_{\mathrm{nuc}}$ for $t > t_{\mathrm{nuc}}$

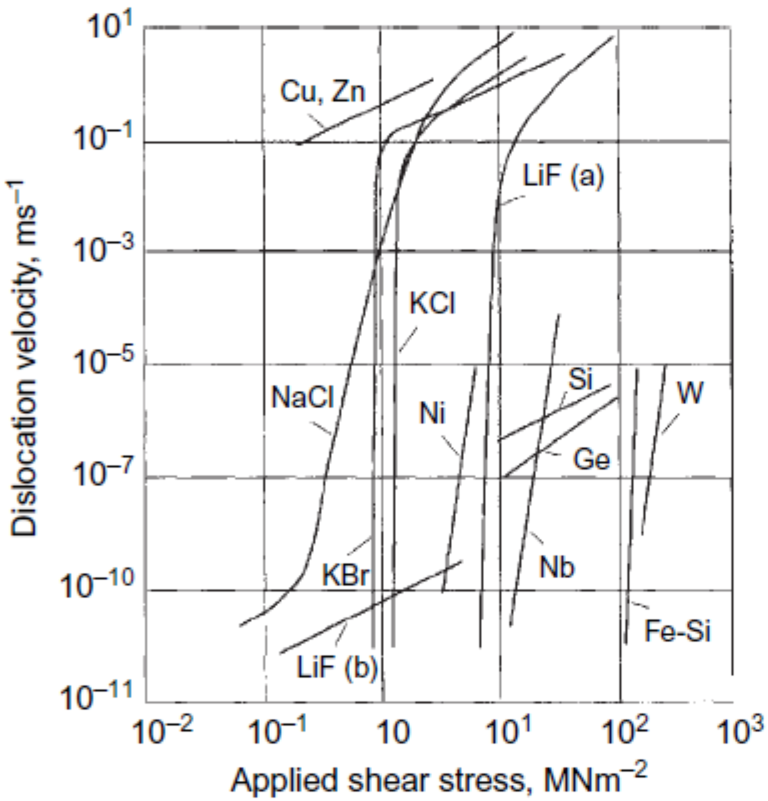


dislocation glide

glide: $v^{(I)} = f^{(I)}/B$



dislocation velocity



from Hull and Bacon, Introduction to dislocations

v=f (applied stress, temperature, type and purity of the crystal)

for FCC and HCP crystals

$$v = A\tau^{m}$$

where m~1 for pure metals at 300K

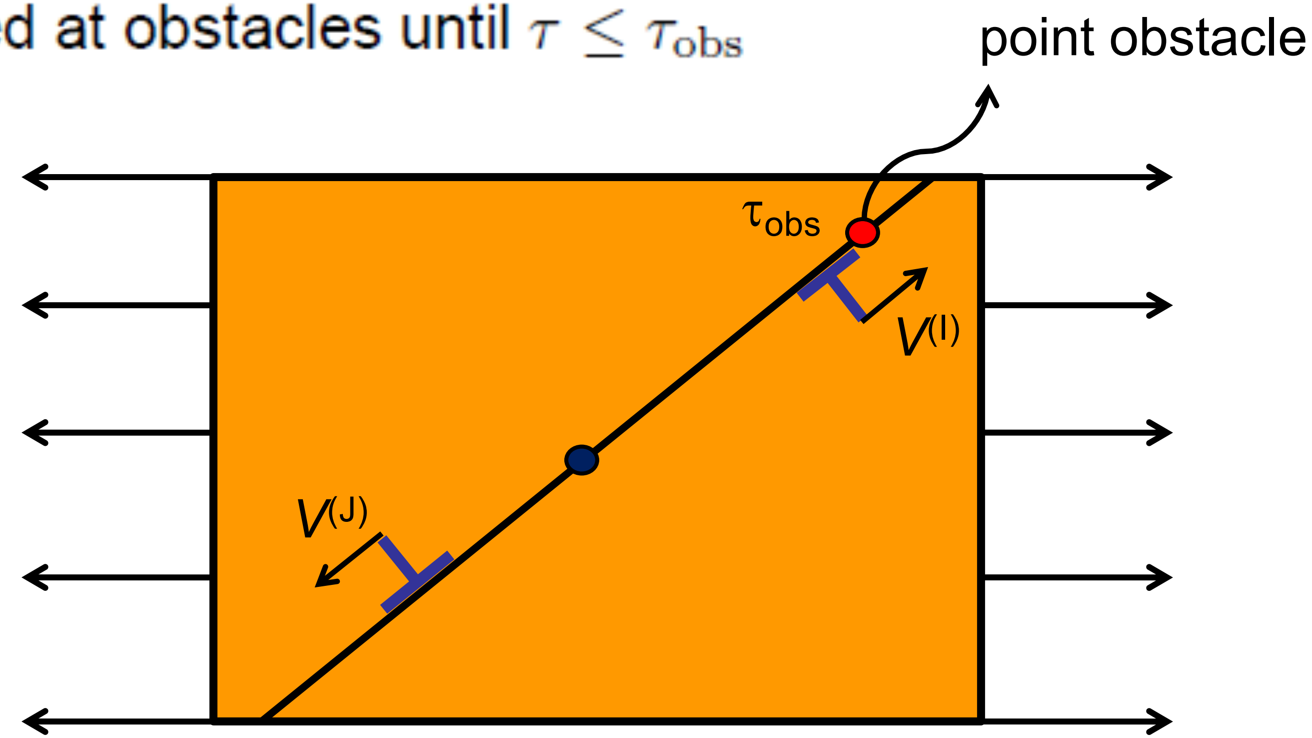
in DDP→ $v = \frac{b}{B}\tau$

where B is the drag coefficient

$$B = 10^{-4}\,\mathrm{Pa\,s}$$

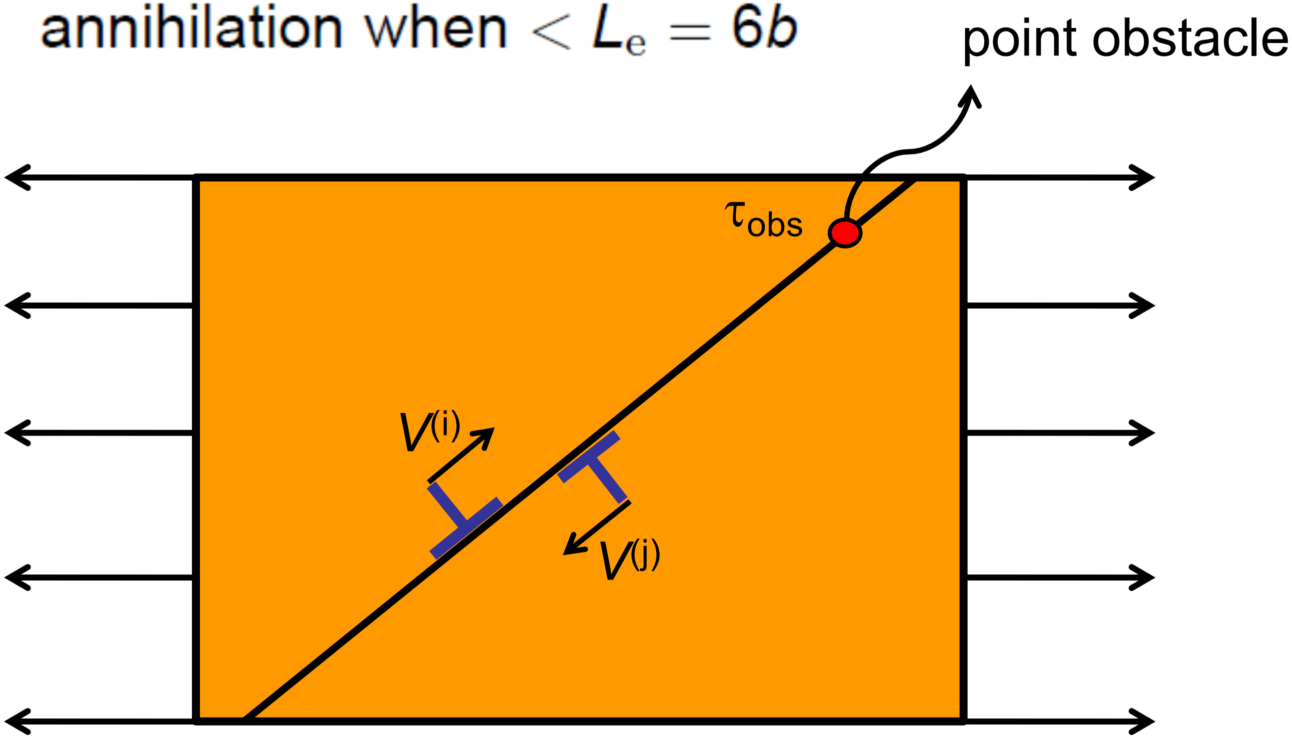
pinning at obstacles

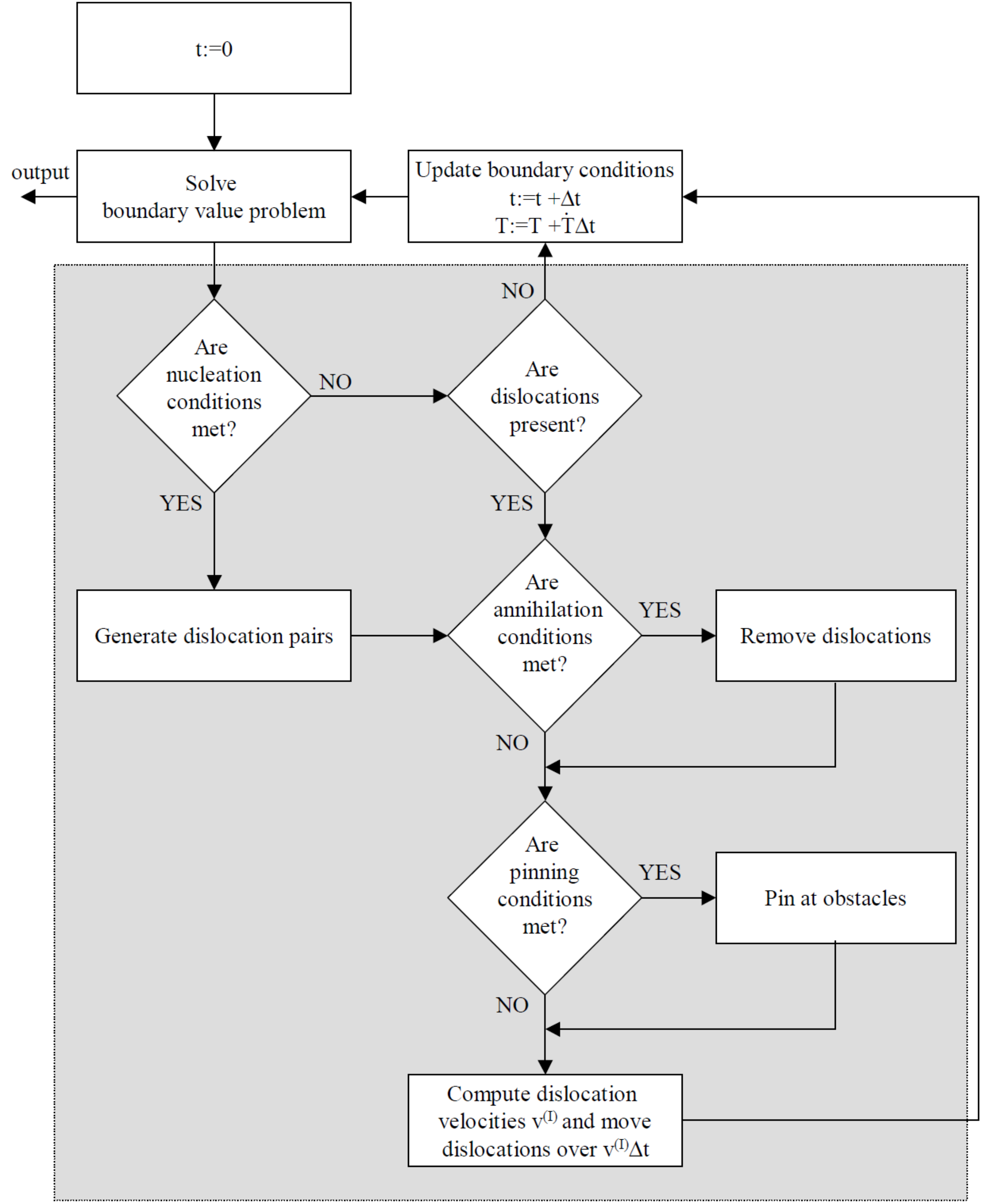
pinned at obstacles until $\tau \leq \tau_{obs}$

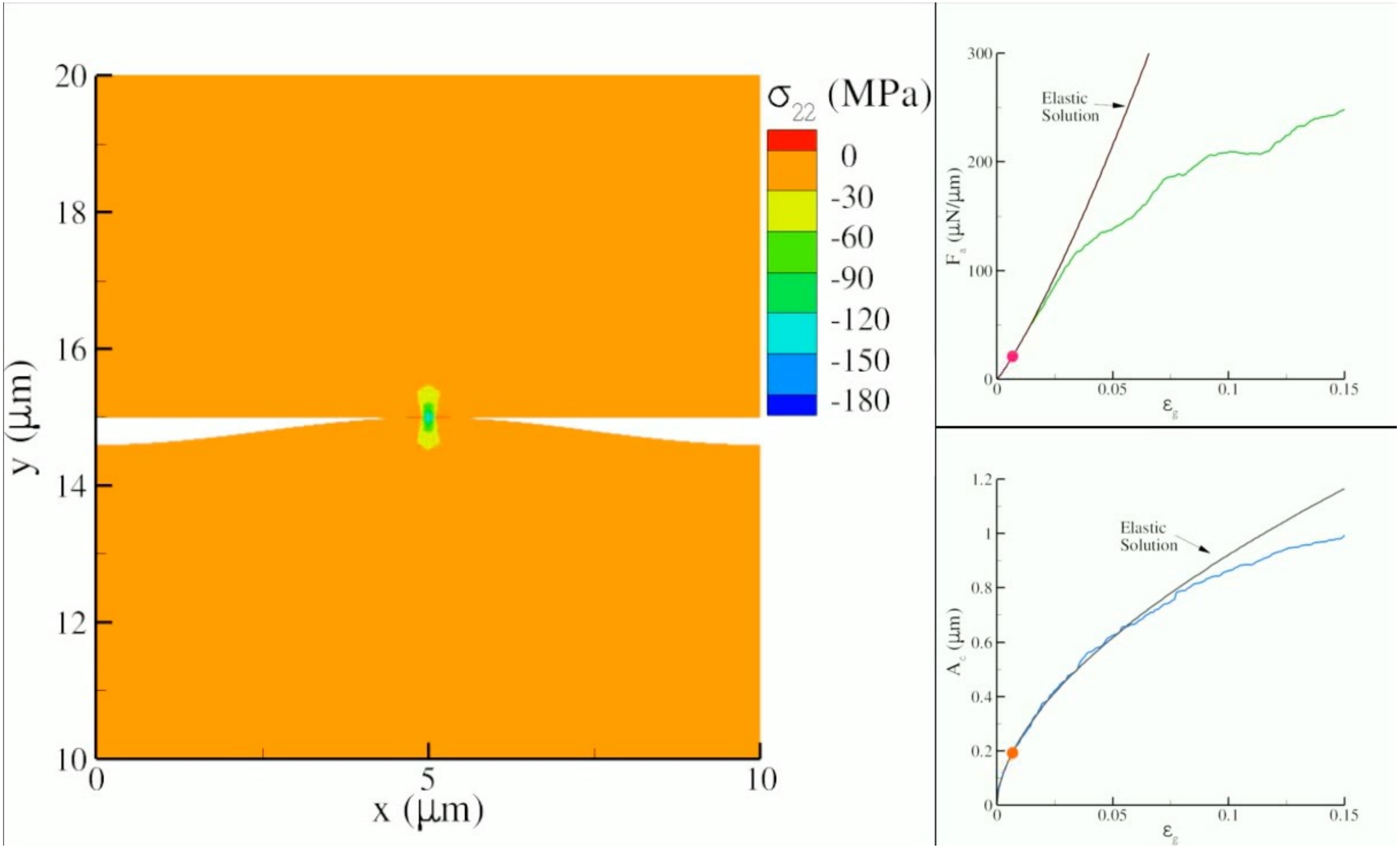


annihilation

annihilation when $< L_e = 6b$




t:=0
output
Solve boundary value problem
Update boundary conditions
t:=t +Δt
T:=T +ṪΔt
NO
Are nucleation conditions met?
NO
Are dislocations present?
YES
YES
Generate dislocation pairs
Are annihilation conditions met?
YES
Remove dislocations
NO
Are pinning conditions met?
YES
Pin at obstacles
NO
Compute dislocation velocities v(I) and move dislocations over v(I)Δt


σ22 (MPa)
0
-30
-60
-90
-120
-150
-180
y (μm)
x (μm)
Elastic Solution
Fa (μN/μm)
εg
Elastic Solution
Ac (μm)
εg

what is DDP used for?

a) Study the mechanical behavior of micro-sized objects
b) Study the behavior of the microstructure in a macro-scale object

Why not MD?

Why not continuum mechanics (FEM)?

what is DDP used for?

a) Study the mechanical behavior of micro-sized objects
b) Study the behavior of the microstructure in a macro-scale object

Why not MD? The domain that MD can tackle is too small

Why not continuum mechanics (FEM)? Because it fails to see the effect of dislocations motion, which are relevant at the micro-scale

Thin films on substrates

You deposit a thin metal film on a silicon substrate. While cooling to room temperature what happens to the system?

a) A negative stress builds up in the film

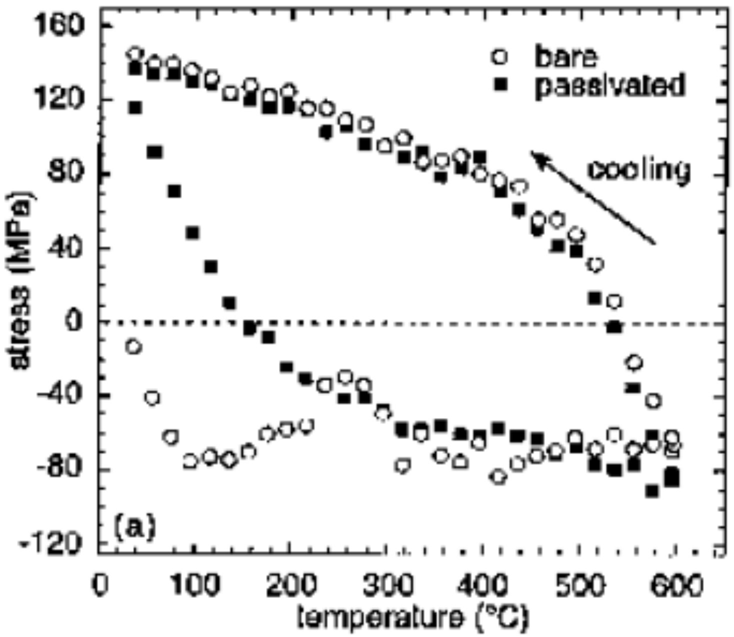
b) A positive stress builds up in the film

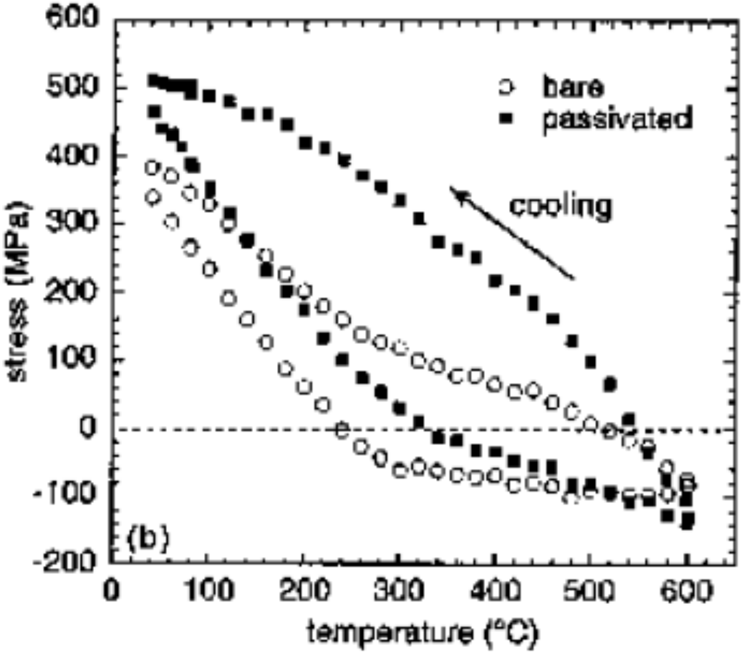
c) A negative stress builds up in the substrate

d) A positive stress builds up in the substrate

e) Both substrate and films stay stress free

Thin films on substrates



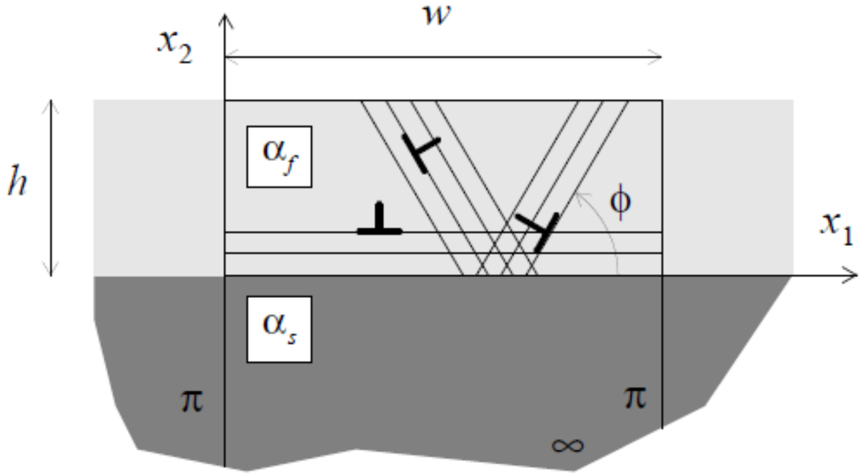


$h = 0.75\mu$m

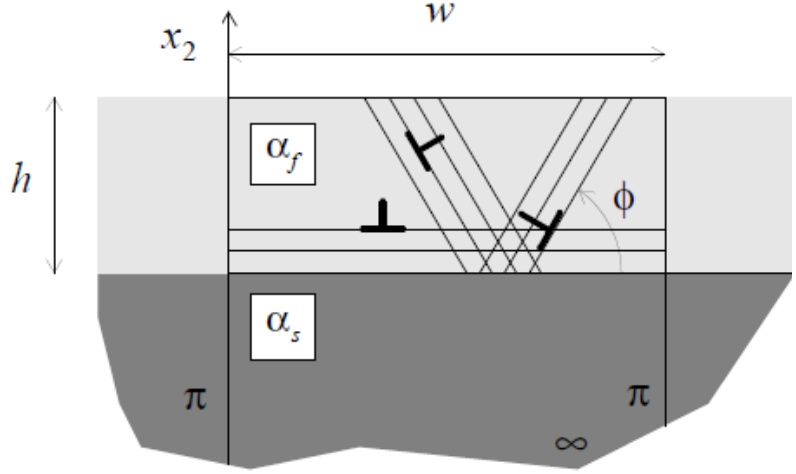
$h = 0.5\mu$m

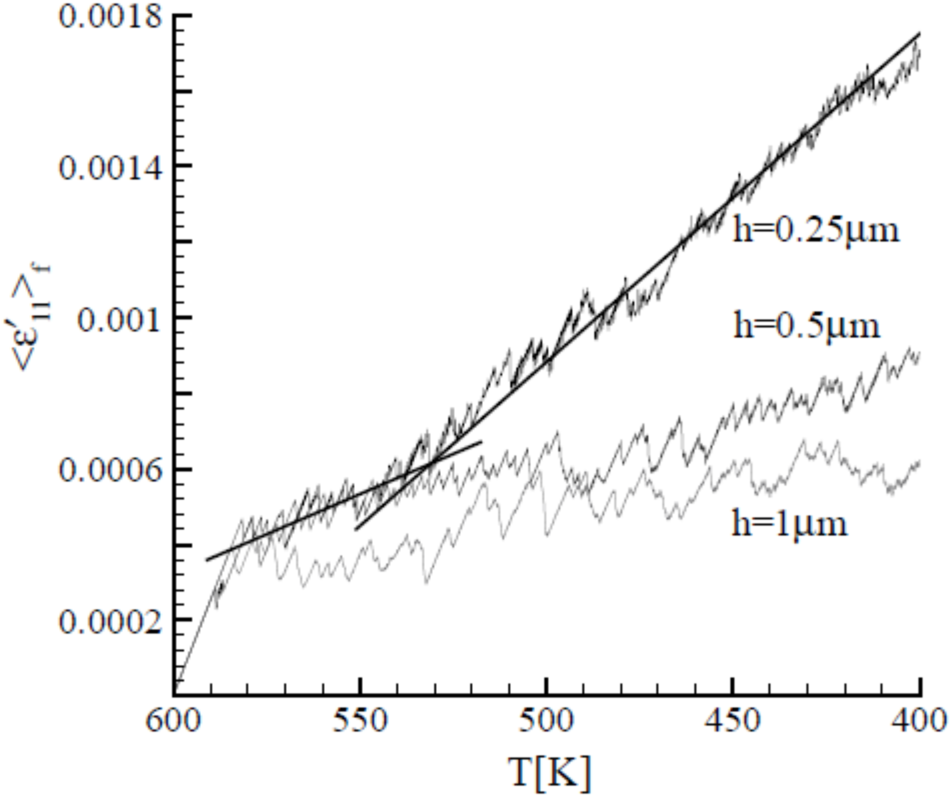
Leung, Munkholm, Brennan and Nix, J. Appl. Phys. (2000)

Thin films on substrates

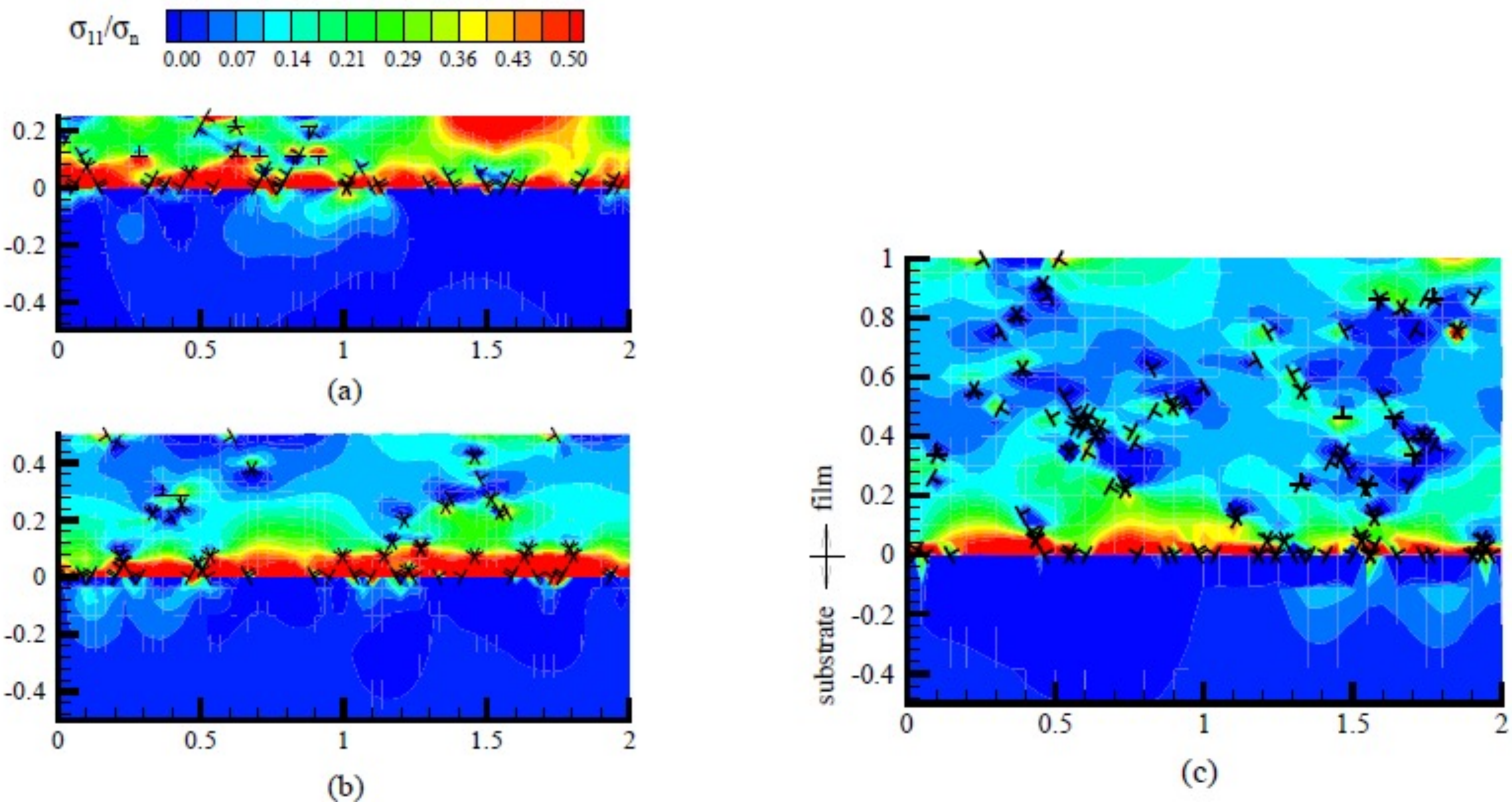


Thin films on substrates



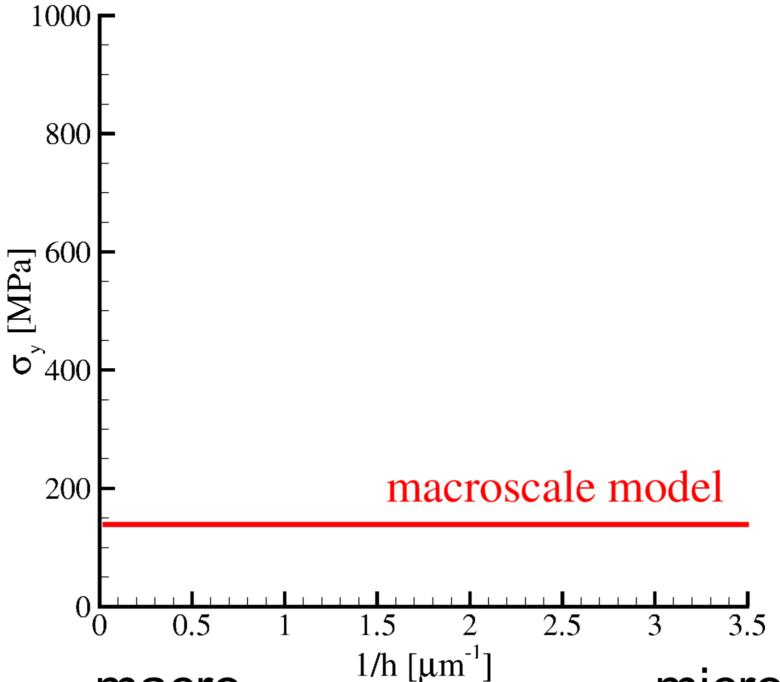


Thin films on substrates



size-dependent plasticity

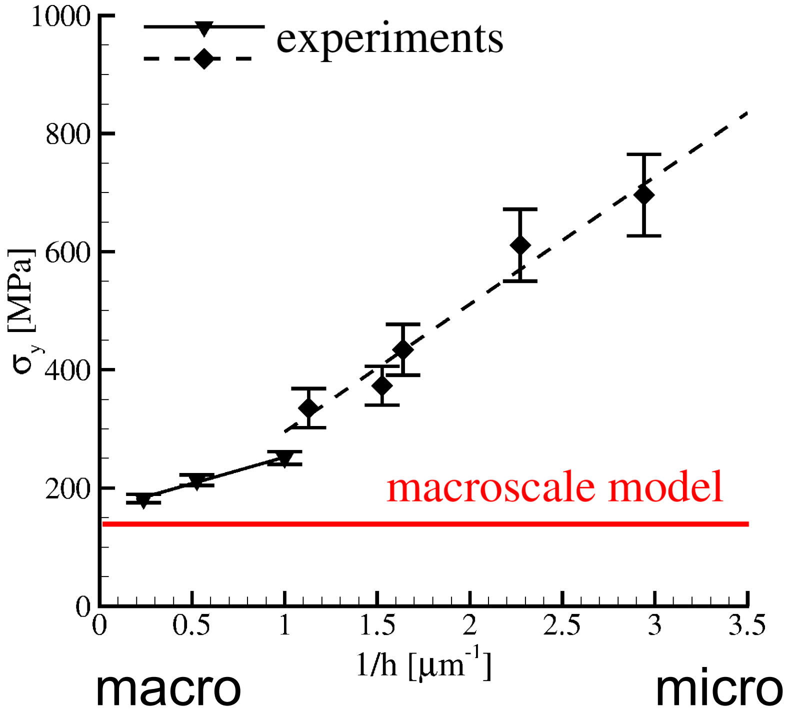
Strength=
force/ area

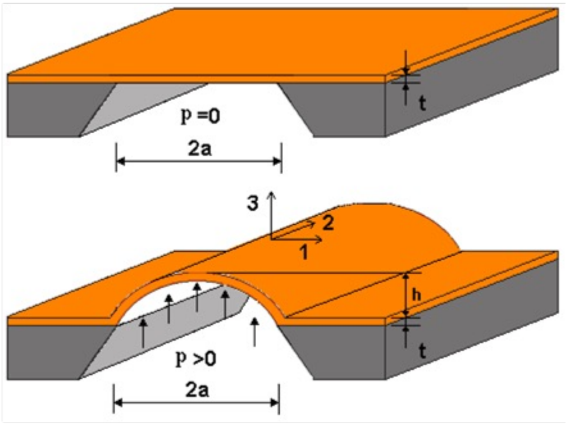


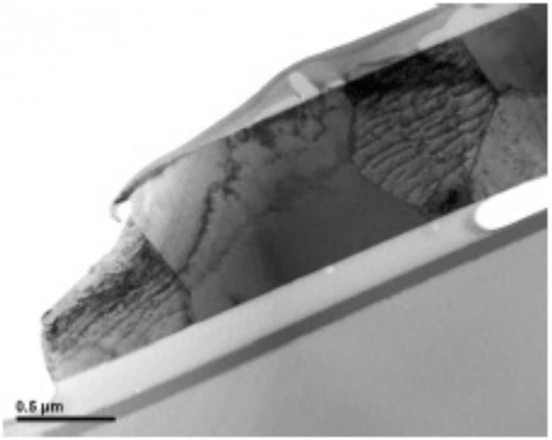
macro micro

smaller is stronger!

Strength= force/ area



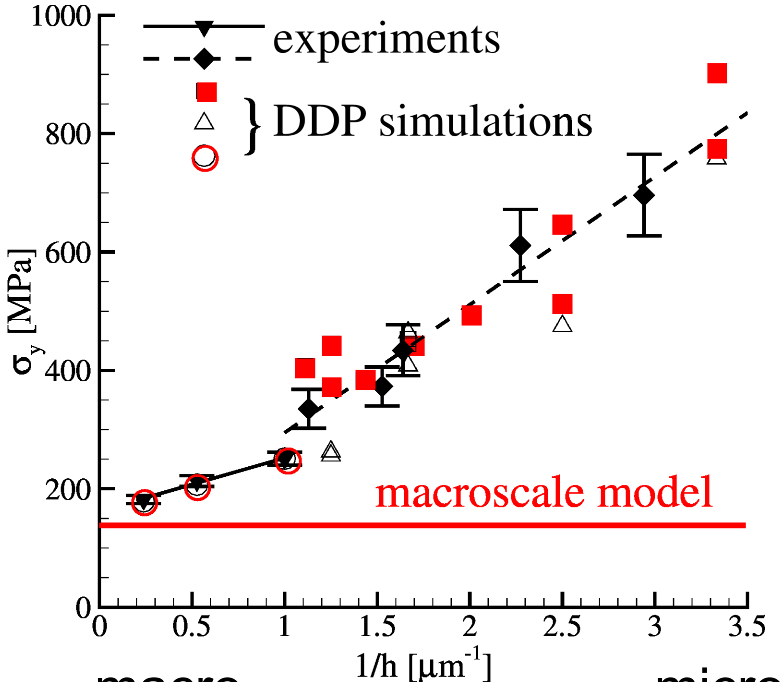




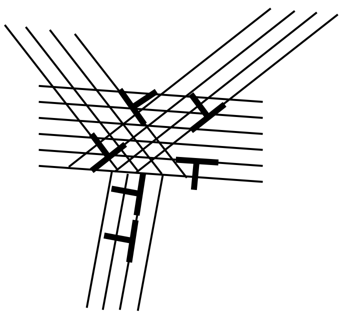
Xiang and Vlassak: Acta Mater 2005

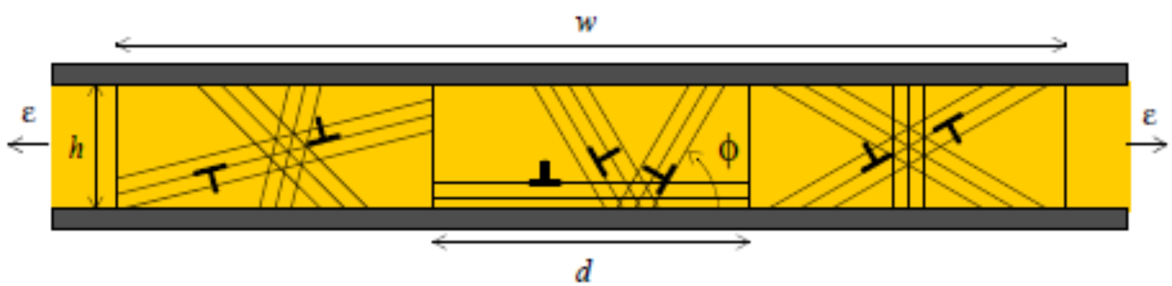
smaller is stronger!

Strength=
force/ area



macro micro





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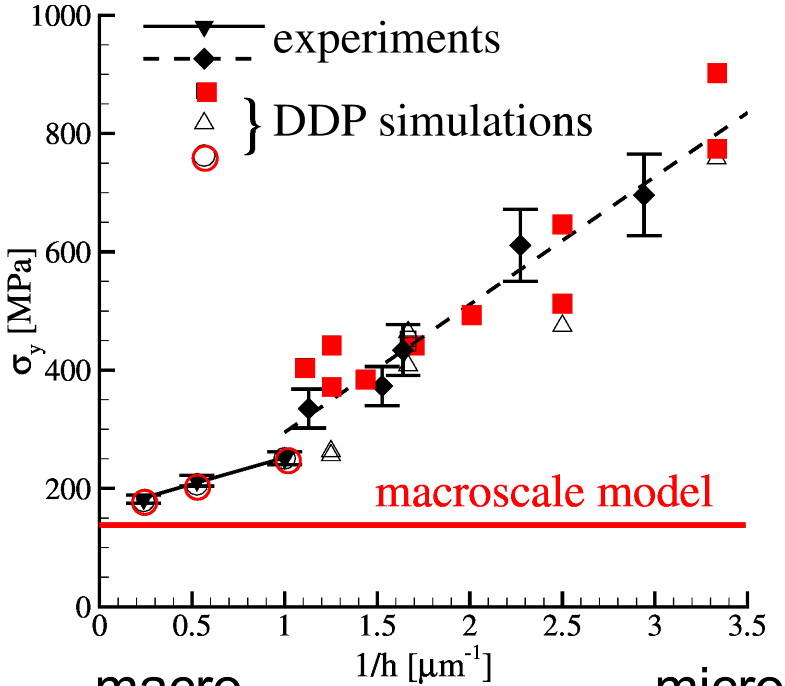
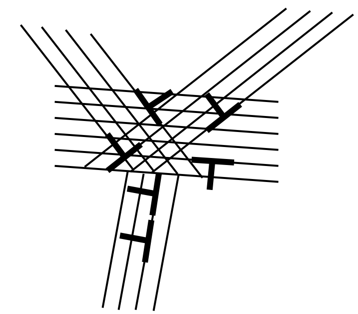
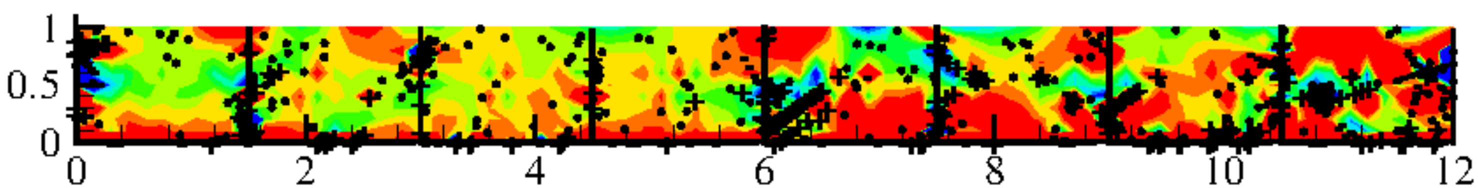


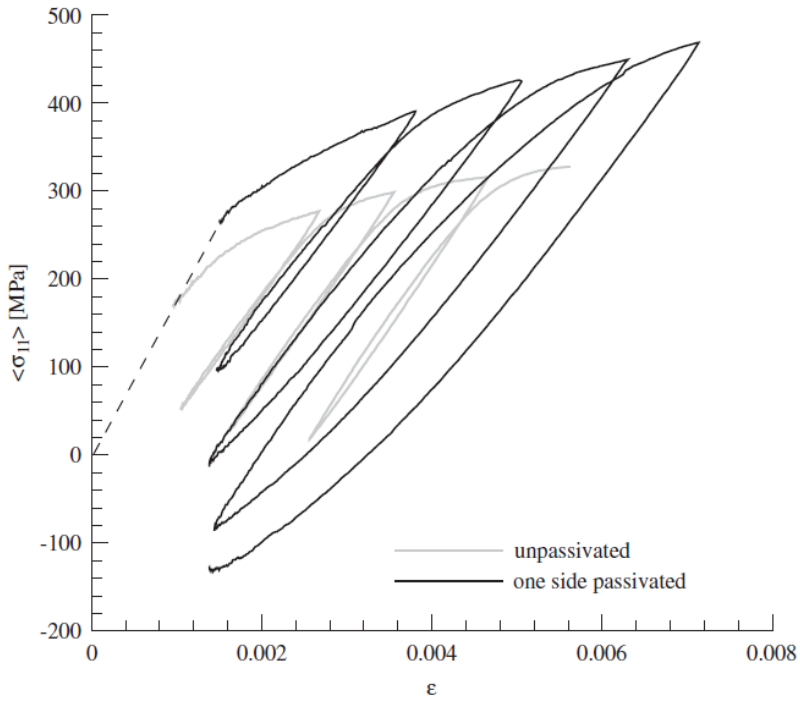
macro

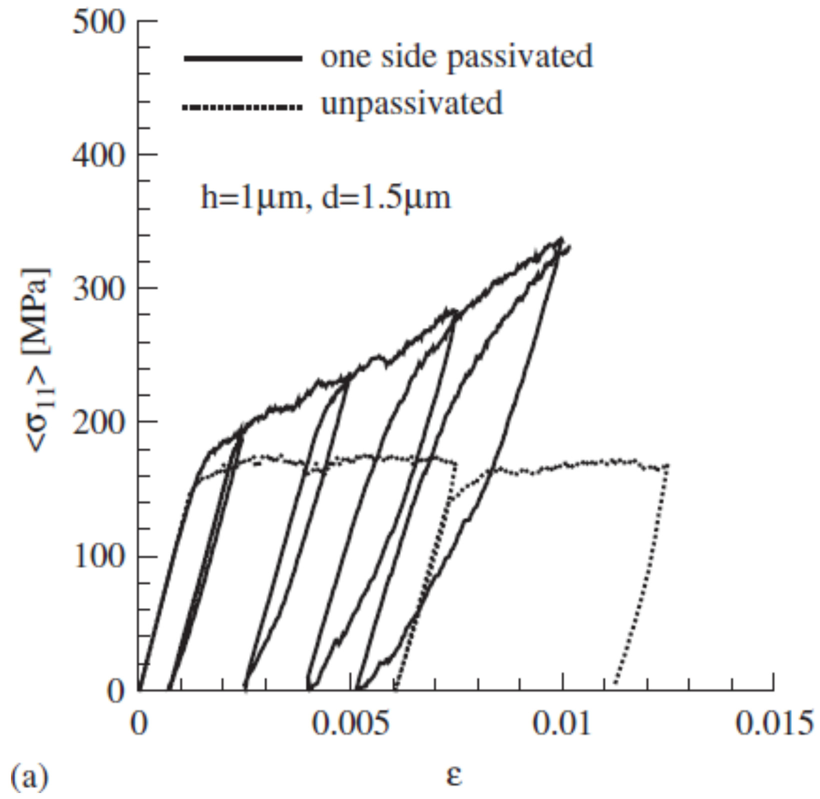
micro



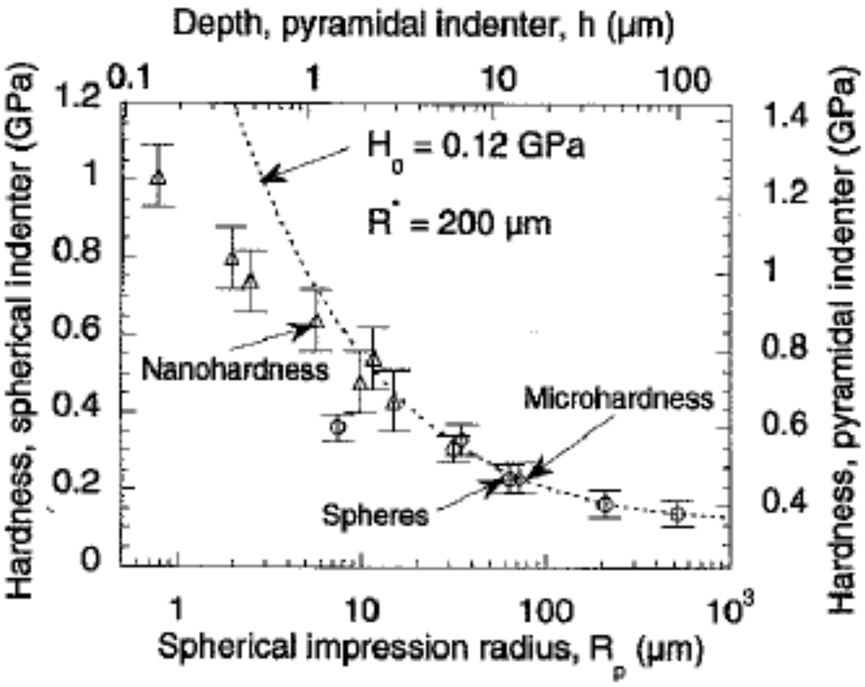


Bauschinger effect



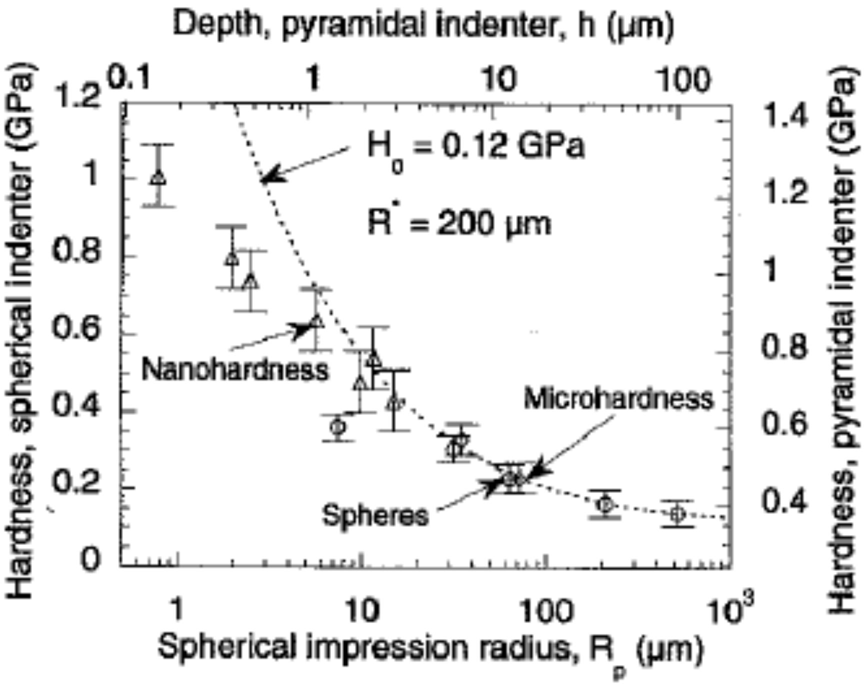


indentation size effect

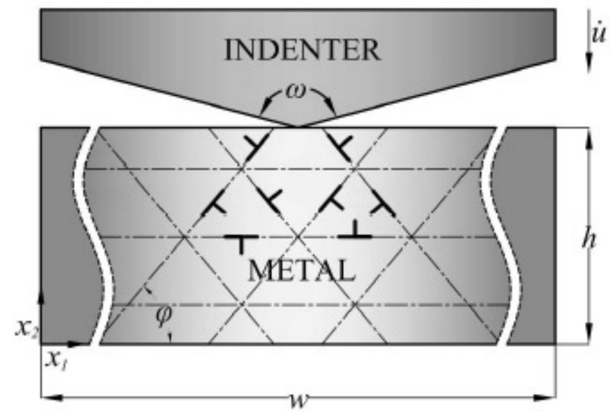


Swadener, George and
Pharr, JMPS 2002

microindentation

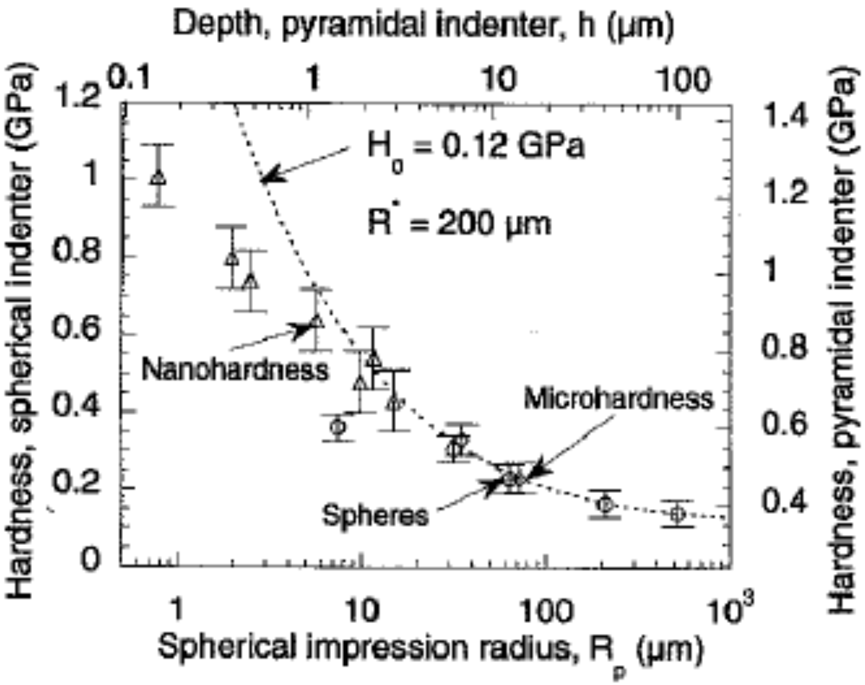


Swadener, George and Pharr, JMPS 2002

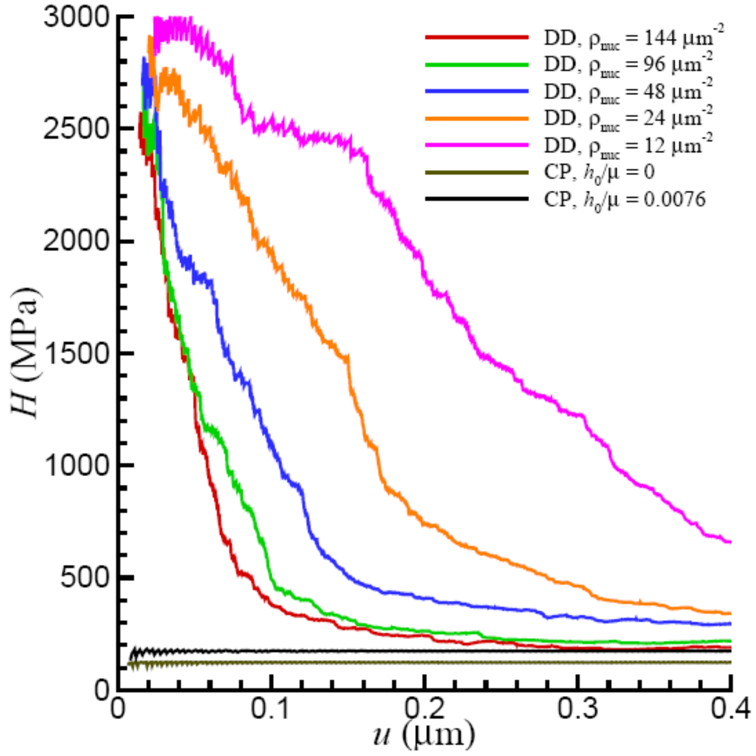


Zhang et al. JMPS 2014

indentation size effect

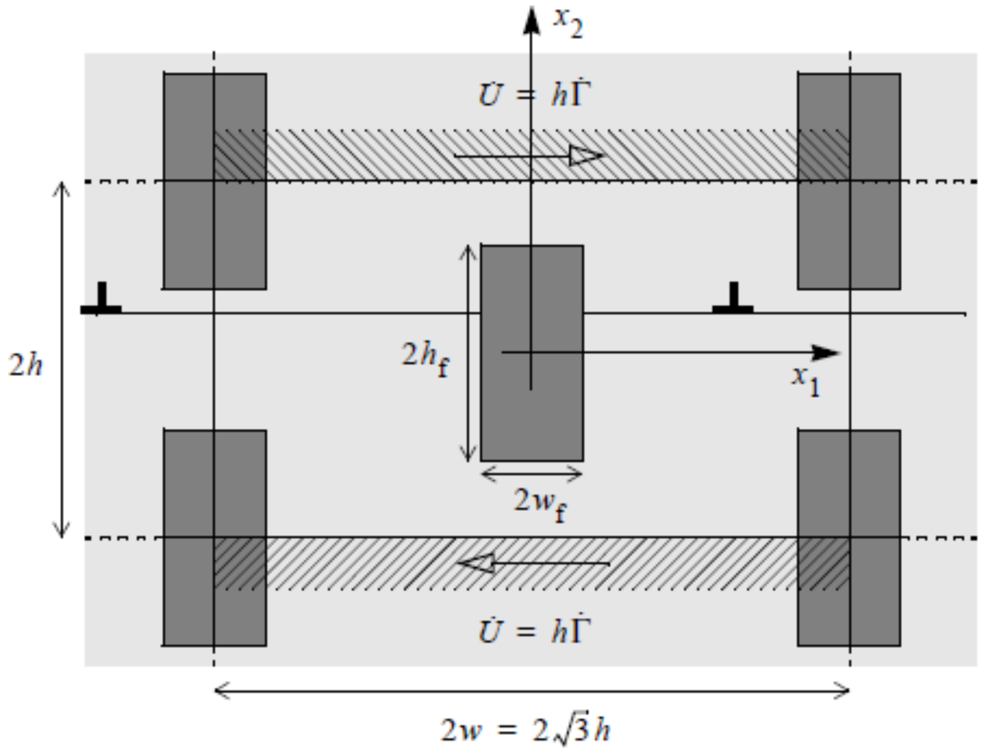


Swadener, George and Pharr, JMPS 2002



Zhang et al. JMPS 2014

shear of a composite



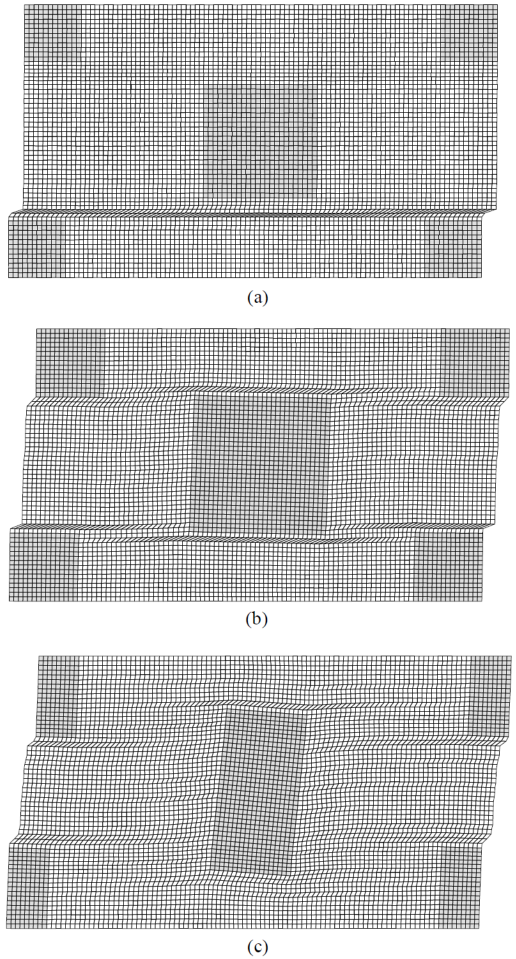
Two morphologies (both 20% of reinforcing particles):

(i) square particles $h_f = w_f$

(iii) rectangular particles $h_f = 2w_f$

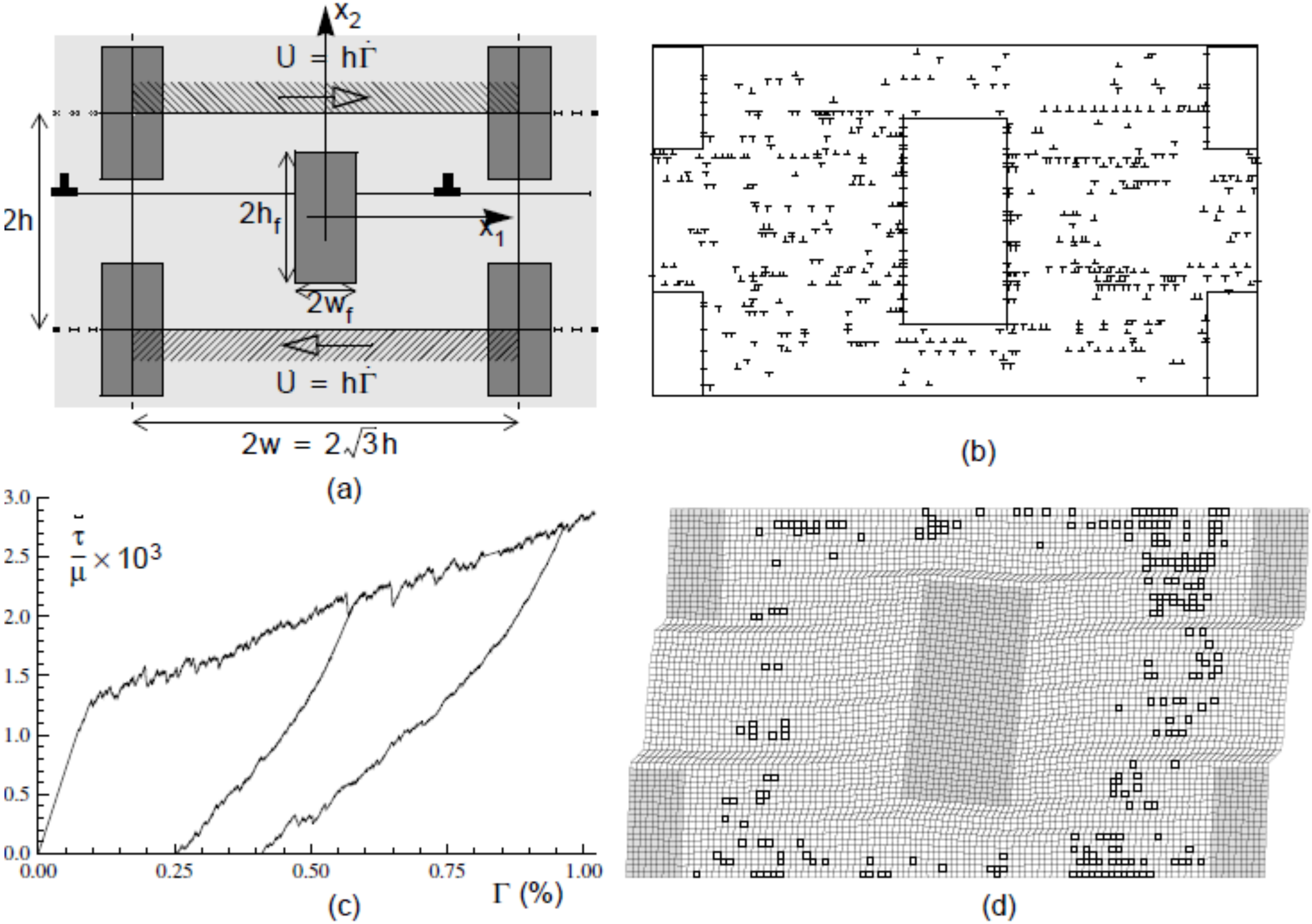
Cleveringa, Van der Giessen, Needleman, Acta Mater 45, 1997

shear of a composite

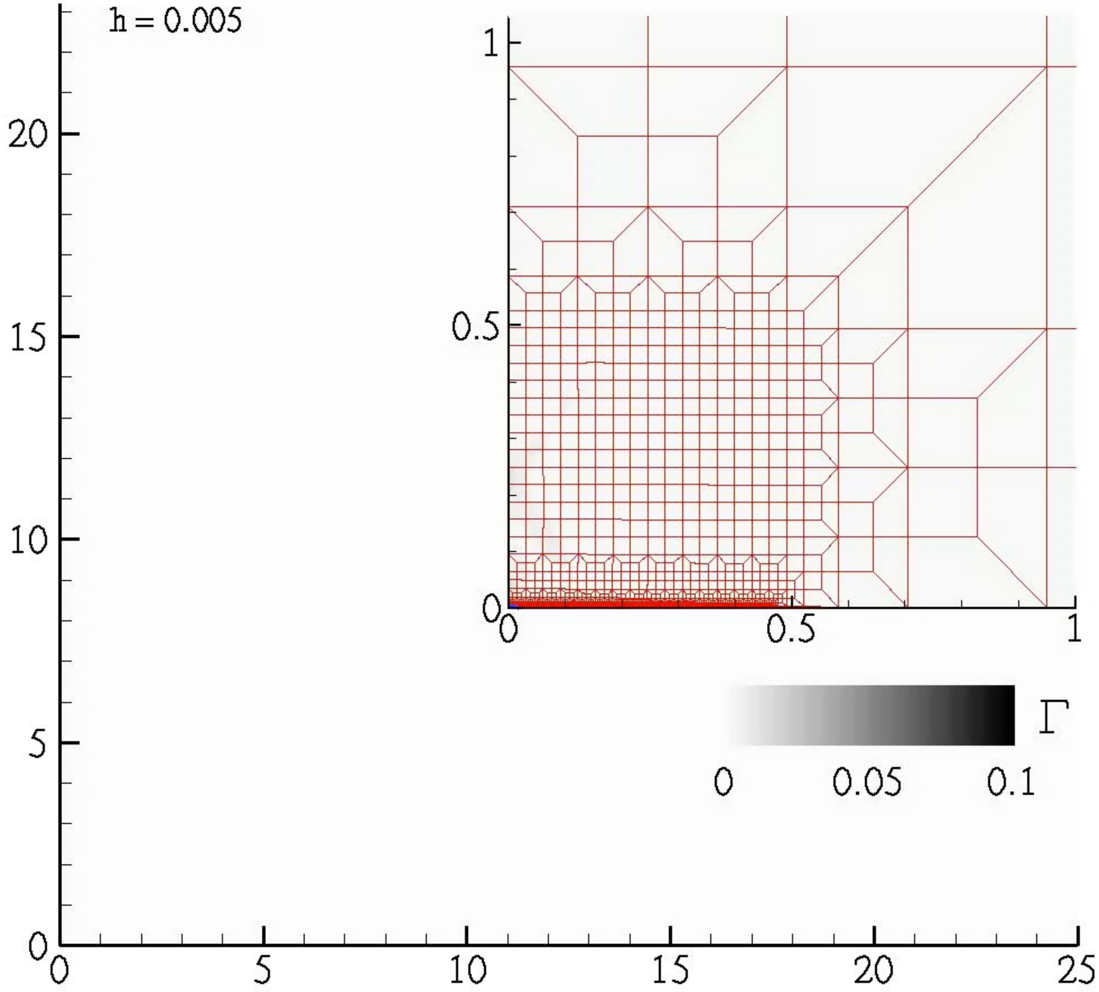


Cleveringa, Van der Giessen, Needleman, Acta Mater 45, 1997

shear of a composite

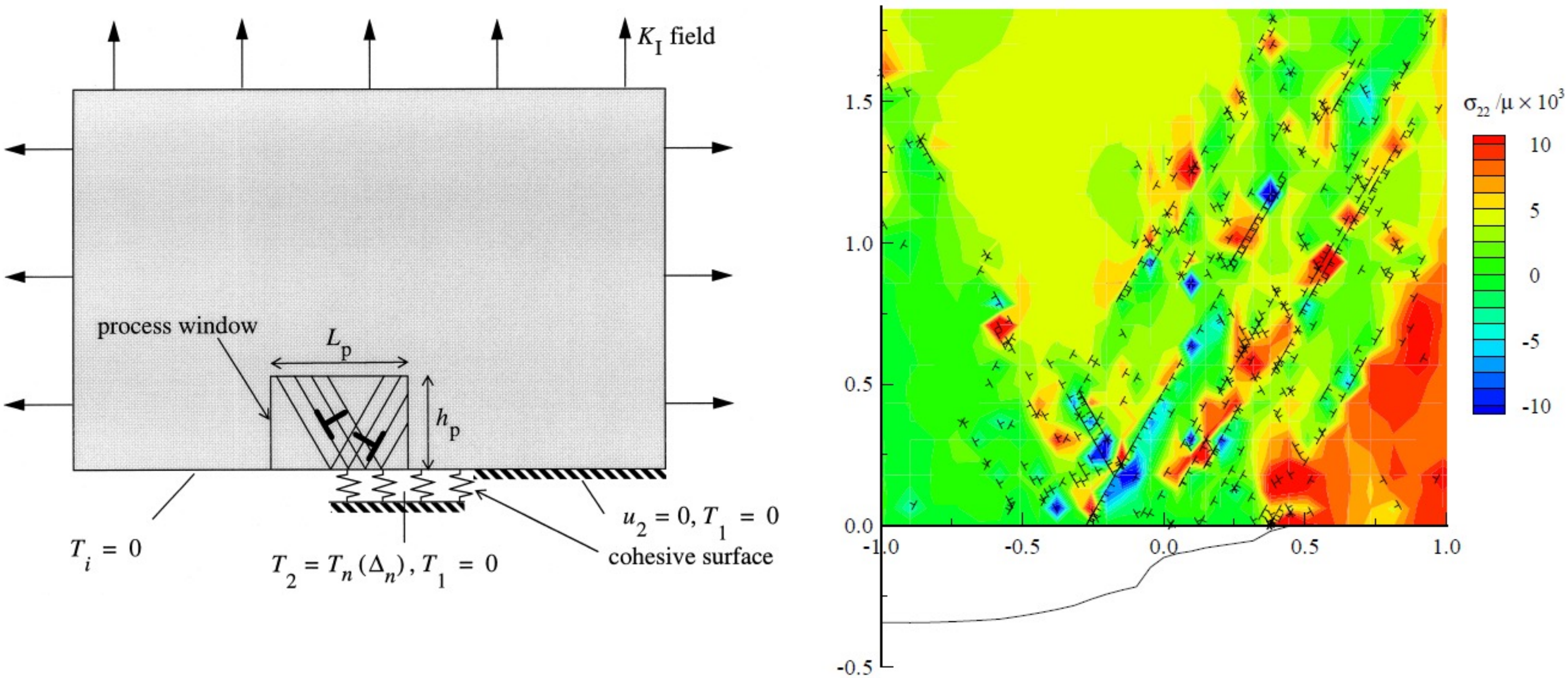


indentation and plastic slip



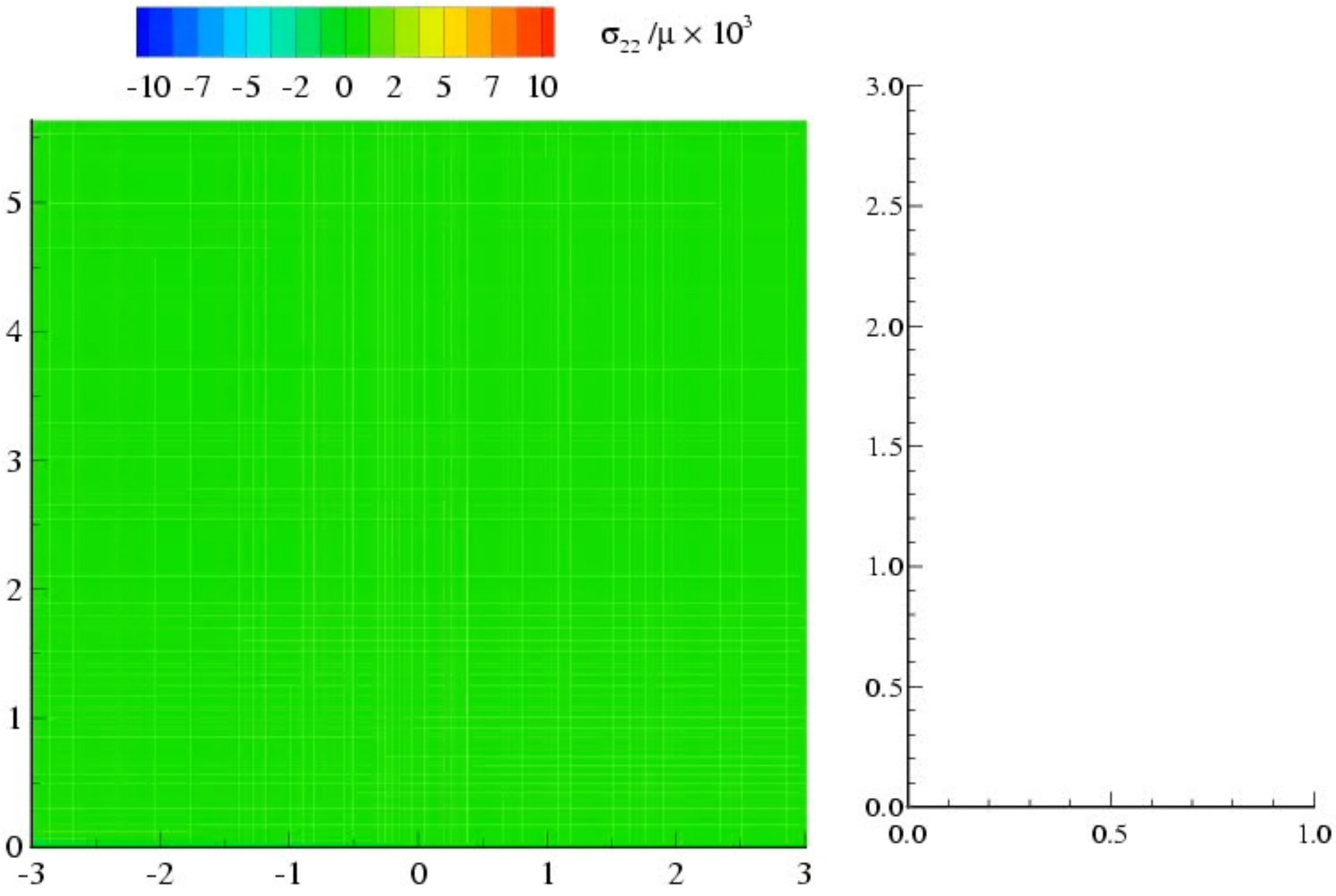
Courtesy of Andreas Widjaja & E. van der Giessen

cracks and plasticity

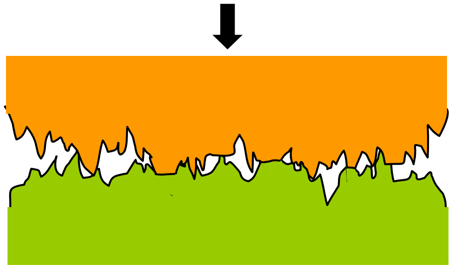


Cleveringa, Van der Giessen and Needleman, Acta Mater 2004

cracks and plasticity



contact



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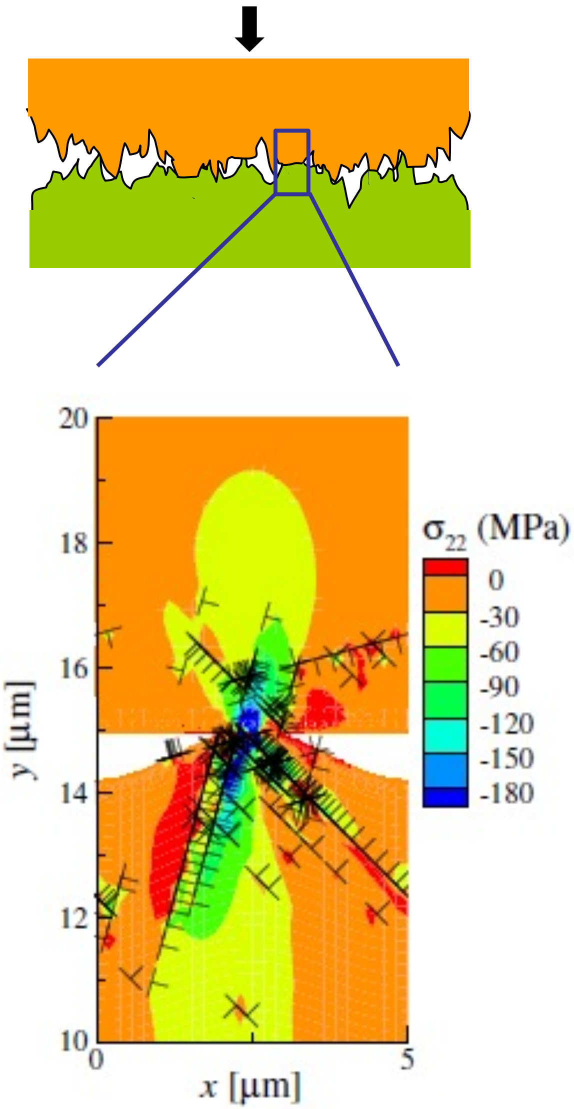

K. Ng Wei Siang et al., MSMSE 2016

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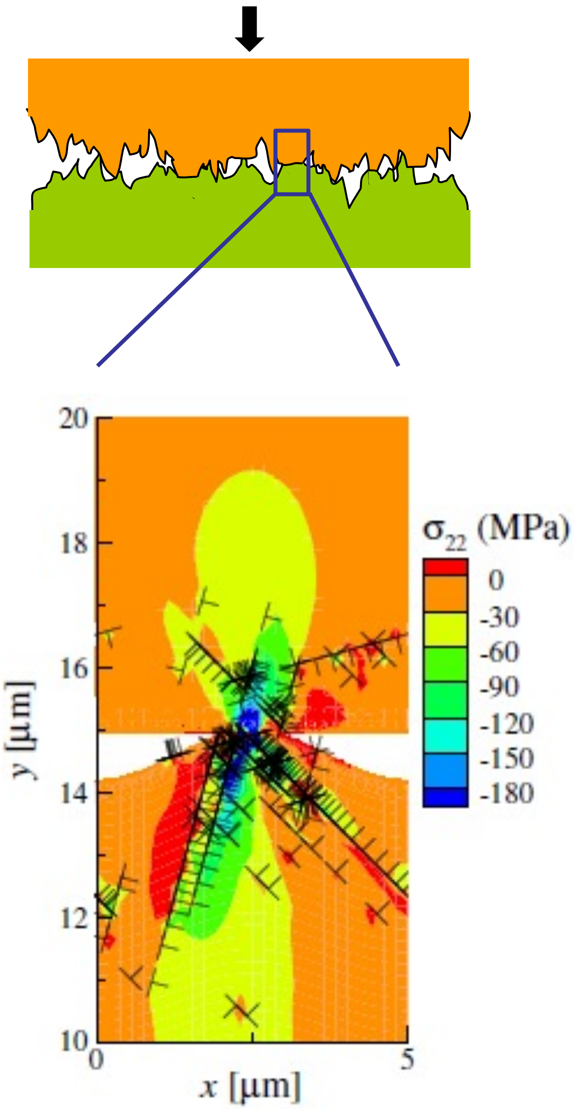
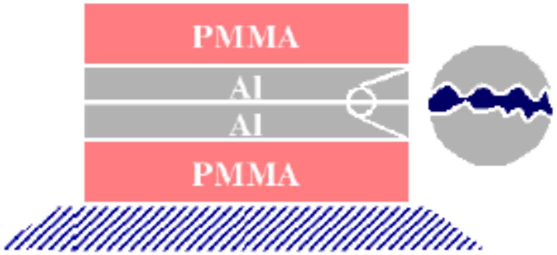
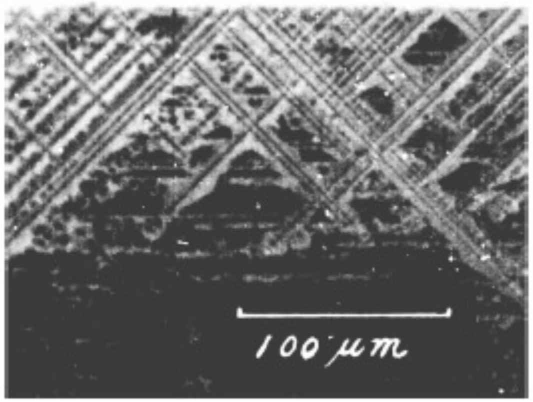
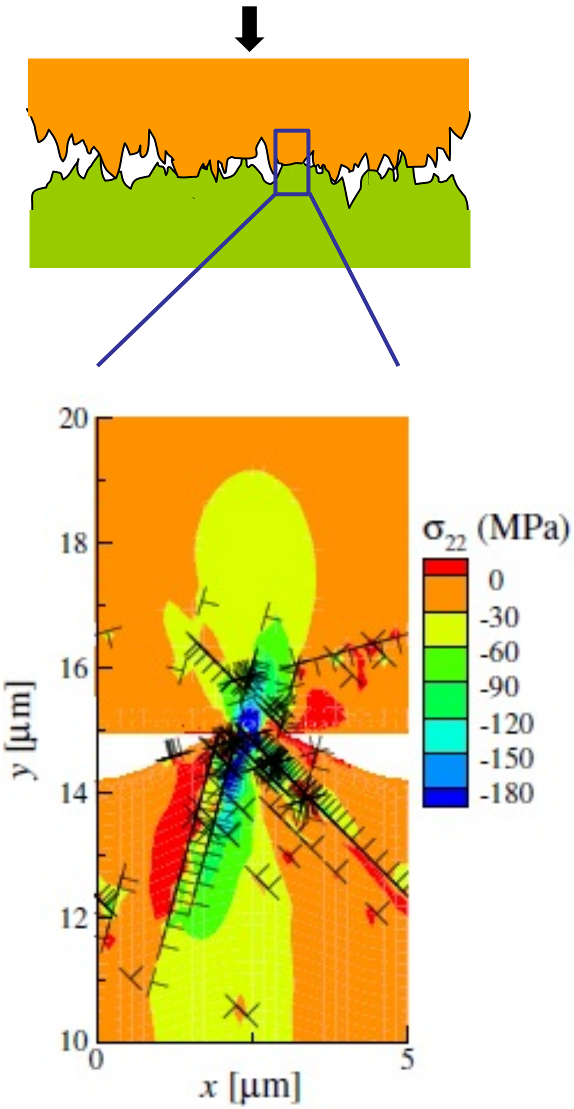


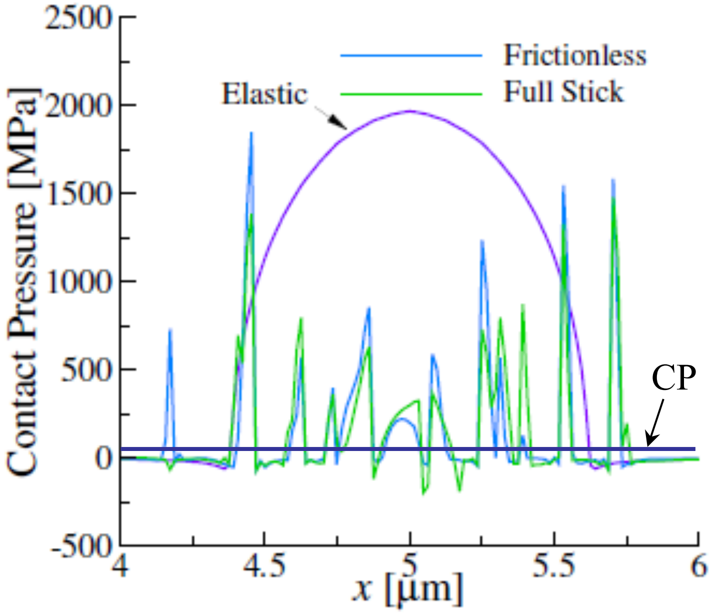




courtesy of prof K-S Kim, Brown University

contact





K. Ng Wei Siang et al, MSMSE 2016

Take home messages

- Discrete dislocation plasticity studies the micro-scale
- The method is based on a continuum description of the body and a discrete description of dislocations, sources, slip planes, obstacles and grain boundaries
- The solution is given as the sum of the elastic solution of dislocations in an infinite medium and the complementary boundary value problem
- Solution to a LEBVP can be obtained by FEM (next two classes) , BEM, GFMD

Dislocation books

Introduction to Dislocations, 4th Edition, D. Hull and D. J. Bacon (Butterworth Heinemann, Oxford, UK, 2001).

Theory of Dislocations , J. P. Hirth and J. Lothe, (Kreiger Publishing, Malabar, Florida, 1992).

Graded assignment 3

Carry out a dislocation dynamics simulation considering at least 500 edge dislocations gliding on parallel slip planes.

1) Check what is the effect of the time step on the convergence: at convergence forces between dislocations should become very small with exception to few dipoles that are very close and might still exchange large forces.

2) Compare results for a program including periodicity using the minimum image convention to one that uses the sums over dislocation walls. What are the main differences you observe?

3) Include an external stress field sigma; f(i) will become f(i)=f(i)+sigma*b
What is the effect of the applied stress field on the simulation results?

Dislocation dynamics

Let's write a very simple DD code in 2 dimensions. Edge dislocations can glide only along horizontal planes. A density of randomly positioned dislocations are the starting point of the simulations.
There are no external fields, so that the dislocations move only due to interaction between their stress fields.

Start as usual with initializing the system

```
% create initial positions
%
% input: n = number of dislocations  (assumed to be even)
%        a = size of dislocation cell
%
% output: (x,y) coordinates and Burgers vector b for each dislocation
%
%
function[x,y,b] = initDD(n,a)
```

initDD.m

```
% create initial positions
%
% input: n = number of dislocations  (assumed to be even)
%        a = size of dislocation cell
%
% output: (x,y) coordinates and Burgers vector b for each dislocation
%
%
function[x,y,b] = initDD(n,a)
%  created scaled coordinates in an fcc lattice
x = rand(n,1)*a;
y = rand(n,1)*a;
% assign b
b = zeros(n,1);

for i=1:n/2
   b(i) = 1;
end

for i=n/2+1:n
   b(i) =-1;
end
scatter(x,y,50,b,'d'); axis square;
```

sumDD.m

Now sum over the forces that dislocations exchange with each other.
This is similar to the force calculation we did for the atoms in the MD code.

In the absence of external loading the dislocations glide due to the Peach-Koehler force induced by the other dislocations.
The force that one dislocation exerts on the other is:

$$F_x(i) = bb_i\sigma_{xy}(j)$$

$$F_x(i) = \frac{Gb^2 b_j b_i}{2\pi(1-\nu)} \frac{x_{ji}\left(x_{ji}^2 - y_{ji}^2\right)}{\left(x_{ji}^2 + y_{ji}^2\right)^2} \quad \Rightarrow \quad F_x(i) = b_j b_i \frac{x_{ji}\left(x_{ji}^2 - y_{ji}^2\right)}{\left(x_{ji}^2 + y_{ji}^2\right)^2}$$

```
function[fx,fmax]= sumDD(n,a,rc,x,y,b)
```

sumDD.m

```
function[fx,fmax]= sumDD(n,a,rc,x,y,b)

%  set force component to 0
fx=zeros(n,1);

for i = 1:n-1  % note limits
    for j=i+1:n  %  note limits
% mimimum image convention
        dx = x(j) - x(i);
        dy = y(j) - y(i);
        dx = dx - a*round(dx/a);
        dy = dy - a*round(dy/a);
        dsq = dx^2 + dy^2;
        dist = sqrt(dsq);
        if dist <= rc
            ffx = -b(i)*b(j)*dx*(dx^2-dy^2)/dsq^2;
            fx(i) = fx(i) + ffx
%  add -f to sum of force on j
            fx(j) = fx(j) - ffx
        end
    end
end
```

sumDD.m

Now calculate the maximum force in the time step to be used in the adaptive time stepping

$$F_{\max} = \max\left(\left|F_x(i)\right|\right) \qquad \Delta t = \Delta x_{\max} / F_{\max}$$

sumDD.m

Now calculate the maximum force in the time step to be used in the adaptive time stepping

$$v_i = \frac{F_x(i)}{B} = MF_x(i)$$

$$F_{max} = \max\left(\left|F_x(i)\right|\right)$$

$$\Delta t = \Delta x_{max} / F_{max}$$

```
% calculate maximum value of force for time step determination
fmax=0;
for i=1:n
  afx = abs(fx(i));
  if afx > fmax
        fmax = afx;
  end
end
```

Main code: DD2D.m

Now move the dislocations according to the Peach-Koehler force acting on them. Plot original and final positions. How did dislocations move? Assume that the acceleration can be ignored, then the velocity is just:

$$v_i = \frac{F_x(i)}{B} = MF_x(i)$$

$$x_i(t+\Delta t) = x_i(t) + v_i(t)\Delta t$$

```
function[xi,x,y,b,fx,xdm] = DD2D(ndis,nsteps,dxmax)
```

Main code: DD2D.m

Move the dislocations according to the Peach-Koehler force acting on them

```
function[xi,x,y,b,fx,xdm] = DD2D(ndis,nsteps,dxmax)
% set size of system (arbitrary)
a = 1000;
% set curoff to be 1/2 the box length
rc = a/2;
% initial positions
[x,y,b] = initDD(ndis,a);
% store initial position
xi = x

 % start the time steps
 for j=1:nsteps
   [fx,fmax] = sumDD(ndis,a,rc,x,y,b);
   dt = dxmax/fmax;
   for i=1:ndis
    x(i) = x(i) + fx(i)*dt

  end
 end
 scatter(x,y,50,b,'s','fill'); axis square;
 xd=x-xi;
 xdm= max(abs(xd));
```

Run the simulation and see where the dislocations ended up

Main code: DD2D.m

Keep all dislocations in the simulation cell!

Main code: DD2D.m

Keep all dislocations in the simulation cell!

```
% start the time steps
for j=1:nsteps
  [fx,fmax] = sumDD(ndis,a,rc,x,y,b);
  dt = dxmax/fmax;
  for i=1:ndis
   x(i) = x(i) + fx(i)*dt

% keep all dislocations in the simulation cell
    if x(i) > a
        x(i) = x(i) - a;
    end
    if x(i) < 0
        x(i) = x(i) + a;
    end

  end
end
scatter(x,y,50,b,'s','fill'); axis square;
xd=x-xi;
xdm= max(abs(xd));
```