Stochastic Dislocation Dynamics:

Dislocation-Defect Interaction

- WSU-CMM: Zbib, Hiratani
- LLNL: Diaz de la Rubia, Bulatov, Wirth

Defects of Interest

- SFTs
- Frank/ Perfect Loops
- Glissile dislocation loops
- He void

Elements Involved

1.Defects & Materials

2.Sample Conditions

- Creep
- Quasi-static Strain Rate
- High Strain Rate
- $r_{defect} = 10^{22} \sim 10^{24}/m^3$
- T = RT ~ 0.5 Tmelt

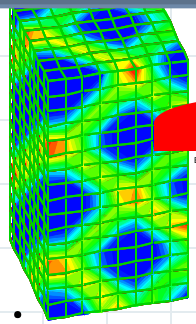
3.Simulation/ Coding

- DD with Finite Element

Objectives

- Homogeneous deformation and flow localization (Phase diagram over parameter space: σ, γ', ρ_{dis}, ρ_{defect}, T….).
- Identification of defect absorption mechanism, and formation of defect free channels.
- Dislocation- Elastic wave interaction.

Continuum Viscoplasticity



Momentum $$\mathbf{div}\,\mathbf{S} = r\,\dot{\mathbf{v}}$$

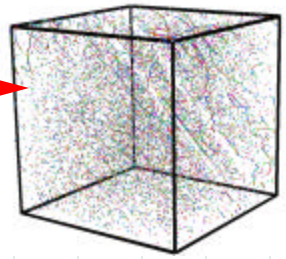
Energy: $$r\,c_v\dot{T} = k\,\nabla^2 T + \mathbf{S}.\dot{\mathbf{e}}^{\mathbf{p}}$$

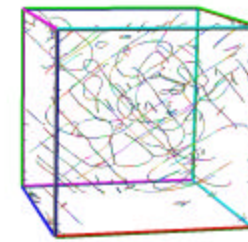
Hooke's Law: $$\overset{o}{S} = \left[C^e\right]\left[\dot{\mathbf{e}} - \dot{\mathbf{e}}^p\right]$$

$$\mathbf{S}^T = \mathbf{S} + \mathbf{S}^D$$

$$\overset{o}{\mathbf{S}} = \dot{\mathbf{S}} - w\,\mathbf{S} + \mathbf{S}\,w \qquad \mathbf{w} = \mathbf{W} - \mathbf{W}^{\mathbf{p}}$$

Discrete Dislocation Dynamics





Equation of Motion

$$\mathbf{F}_i - \sum_{\mathbf{electron,\,phonon}} B\,\mathbf{v}_i = \mathbf{m}_i^*\dot{\mathbf{v}}_i$$

$$\dot{e}^p = \sum_{i=1}^{N} \frac{\mathbf{l}_i\mathbf{v}_{gi}}{2\mathbf{V}}(n_i \otimes b_i + b_i \otimes n_i)$$

$$W^p = \sum_{i=1}^{N} \frac{\mathbf{l}_i\mathbf{v}_{gi}}{2\mathbf{V}}(n_i \otimes b_i - b_i \otimes n_i)$$

Material parameters

Elastic properties
Dislocation Mobility
Core size = 1b
Stacking-fault energy, and activation energy for cross-slip

Numerical Parameters:

DD Cell size (= FE mesh size)
Dislocation segment length (min (3b) and max) (variable), number of integration points (10)
Number of cells (infinite domain; 3x3x3)
Number of sub-cells (elements for FE)
time step for DD; Max flight distance (variable time step)
Time step for FE (dynamics) ~ (smallest dimension/shear speed)

Double-Kink Theory
(bcc: Low mobility)

$$M_g = \frac{2bh^2}{a}\frac{D_k}{kT}\exp\left(\frac{-F_k}{kT}\right)$$

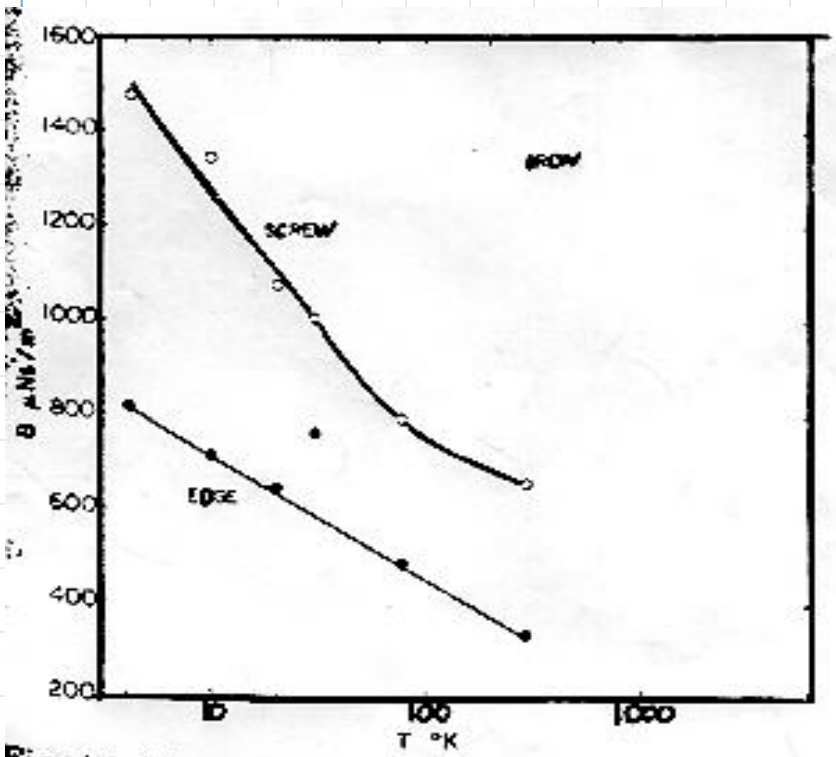


Fig. 14. Plot of damping constant B vs. log of temperature for dislocations in iron.

Urabe and Weertman (1975)

Viscous Phonon and Electron damping

$$M_g = \frac{1}{B(T)}$$

fcc: High mobility

e.g AL: $\approx 10^4 (\boldsymbol{Pa.s})^{-1}$

$$F_i = F_{Peirels} + F_{Disl-Disl} + F_{Self} + F_{External} + F_{Obstacle} + F_{Image} + F_{Osmotic} + F_{Thermal}$$

Osmotic Force: Due to non-conservative motion of edge dislocation (climb) that results in the production of intrinsic point defects

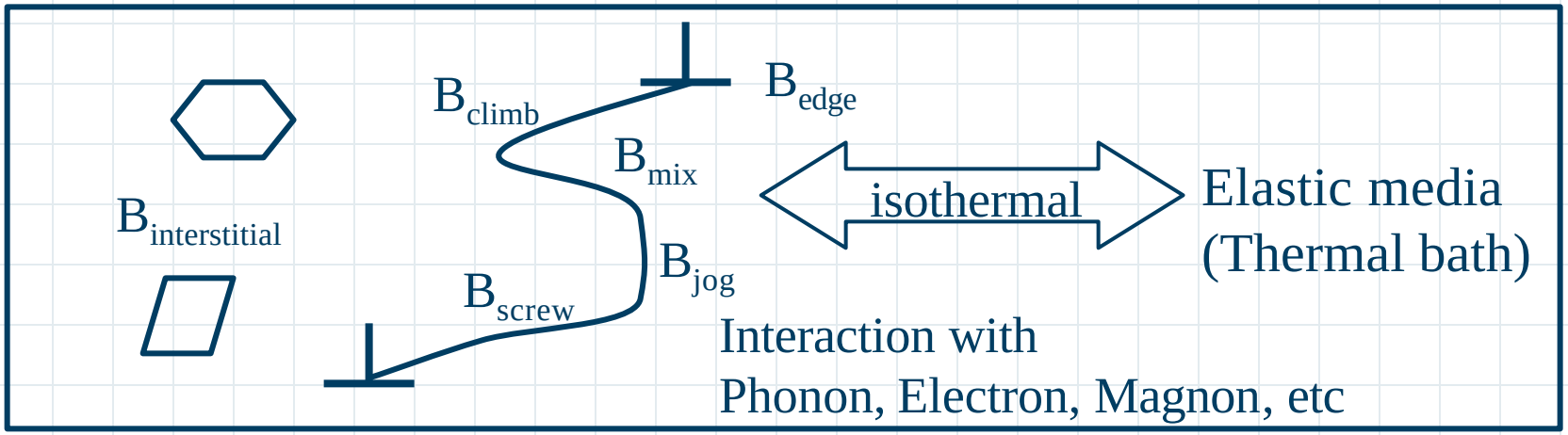
$$F_{Osmotic} = -\frac{|b|}{\Omega}\frac{b \times x}{|b \times x|}[k_b T \ln(\frac{c}{c_o})]$$

Stochastic Dislocation Dynamics (SDD)

International Journal of Plasticity, 2002 , Phi. Mag , 2002, ASME J. Eng. Mater. And Tech, 2002.

Assumptions

1. Generated heat dissipates *immediately* into heat bath (thermal equilibrium).
2. Properties in dissipation process are known in advance based on quantum mechanical calculation/ atomistic simulations.
3. Dislocation motion is Markov process
4. Stochastic thermal agitation is added self-consistently and treat SDD as Brownian dynamics
5. Under constant pressure (stress) or constant volume



SDD: Stochastic Dislocation Dynamics

- Equation of motion of a dislocation segment of length Δl with an effective mass density m^*

$$m_i^* \dot{\mathbf{v}}_i = -\sum_{electron,phonon} \mathrm{B}\ \mathbf{v}_i + \left(\sum_{j \neq i} \mathbf{s}_{i,j}^{D} + \sum_{k} \mathbf{s}_{i,k}^{S} + \mathbf{s}^{A} + \mathbf{t} \right) \mathbf{b}_i \times \mathbf{?}_i$$

- the stochastic stress component t satisfies the conditions of ensemble averages:

$$\langle \mathbf{t}(t) \rangle = 0 \quad \langle \mathbf{t}(t)\mathbf{t}(t') \rangle = \left\{ 2\left(B_e + B_{ph}\right) kT \Big/ \left(m_i^{*2} b^2 \Delta l\right) \right\} d\left(t - t'\right)$$

- The strength of t is chosen from a a bivariate Gaussian distribution we generate stress pulses with two random numbers (r_1 and r_2) between zero and unity

$$t = s_t \sqrt{-2 \ln r_1} \cos\left(2 p r_2\right)$$

$$s_t = \sqrt{2kT \sum B \Big/ \left(b^2 \Delta l_i \Delta t\right)}$$

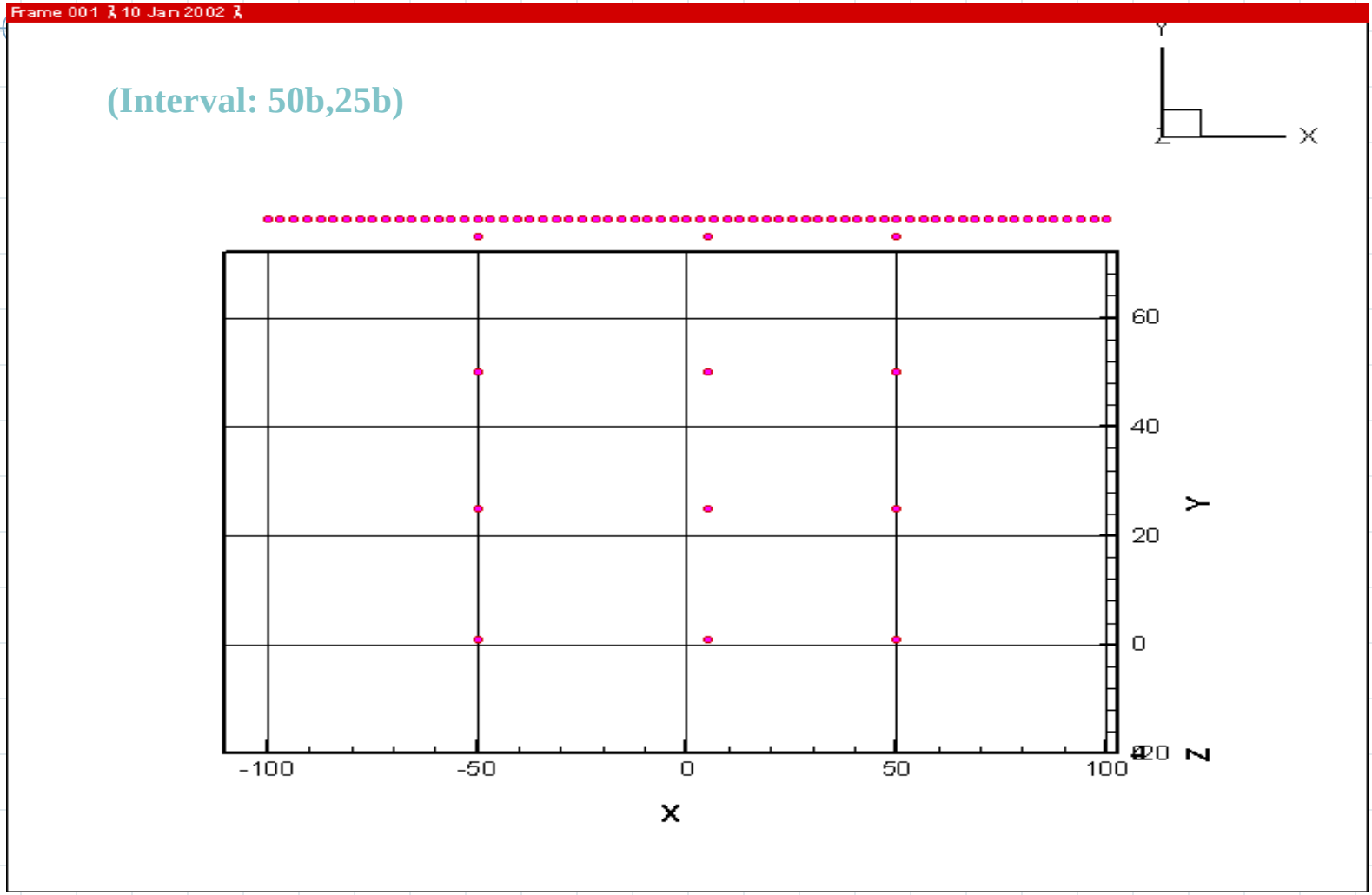
T (K)	σ (MPa) at 10b	σ (MPa) at 5b
10	8.11	11.47
50	28.68	40.56
100	57.36	81.12
300	181.4	256.5

SDD: Dislocation Percolation among Obstacle Arrays

Random SFT grids

T = 300 K, s =20 MPa

(Interval: 50b,25b)



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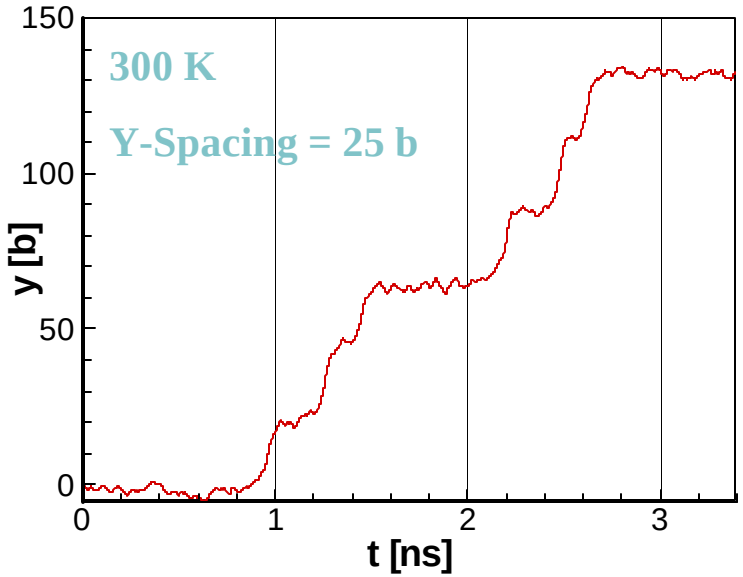
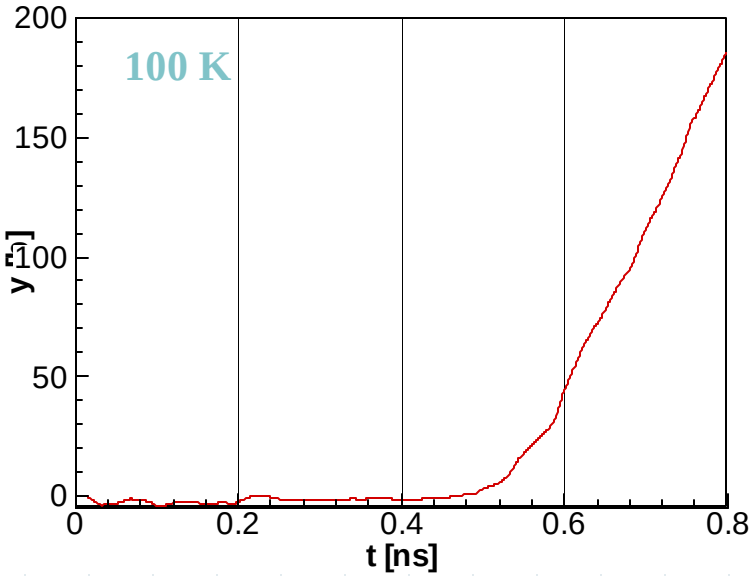
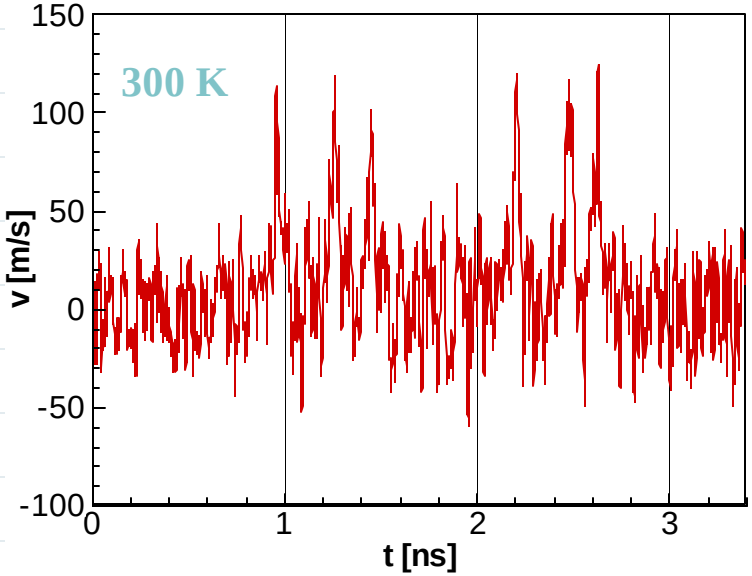
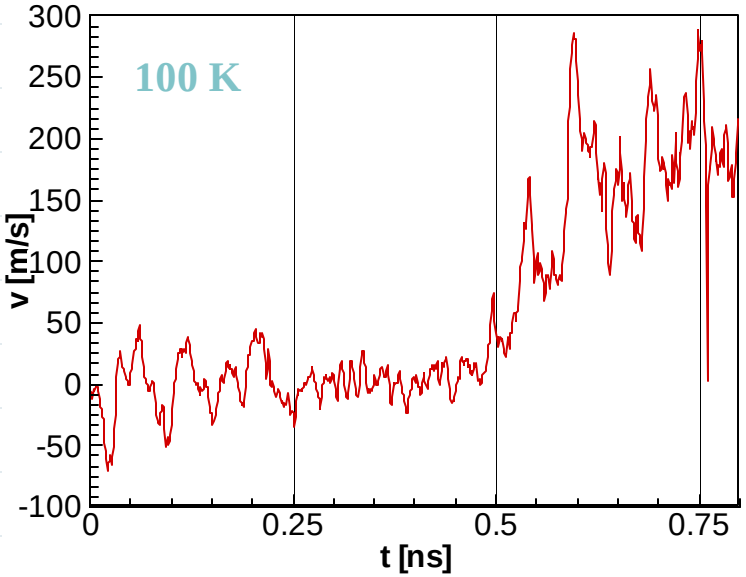
SDD: Dislocation Percolation among Periodic Obstacle Arrays

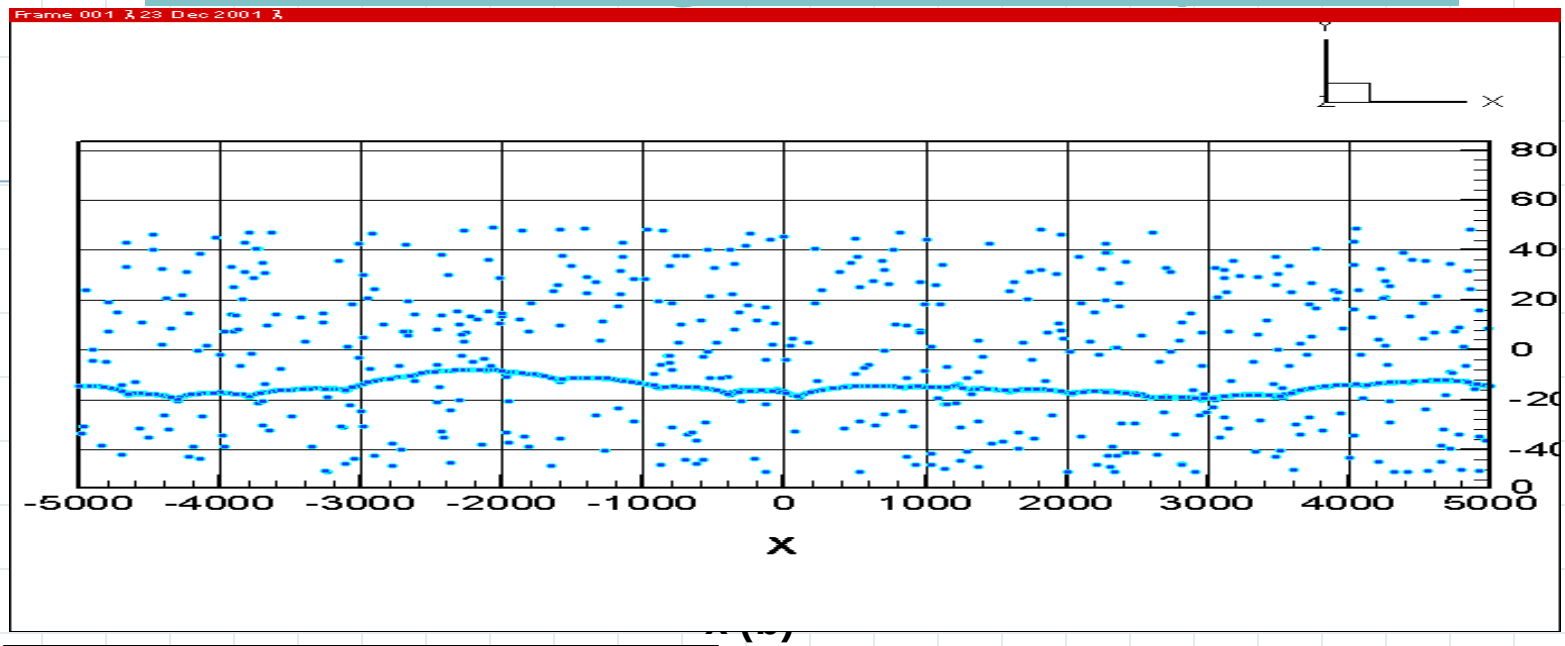


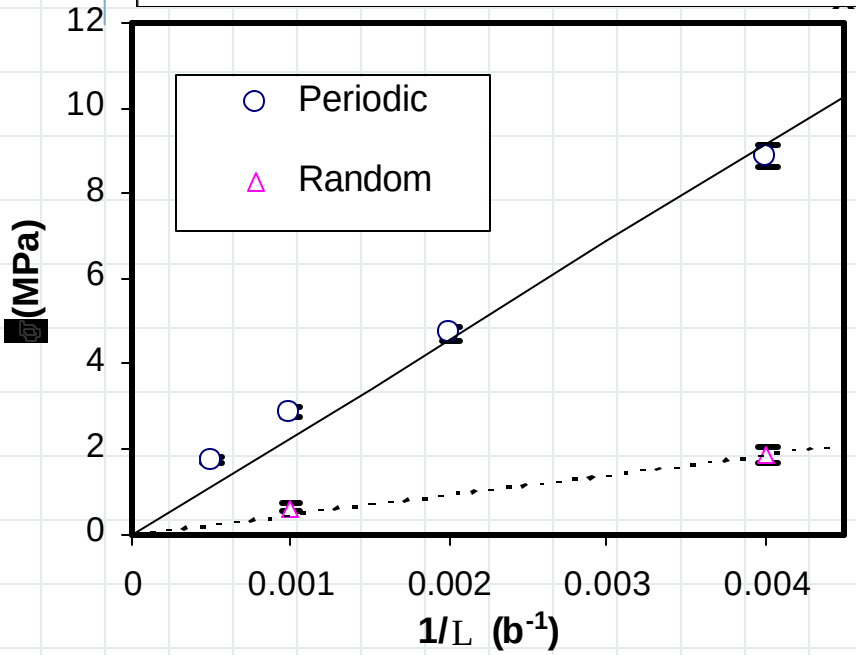






Percolation through Random Array of SFTs

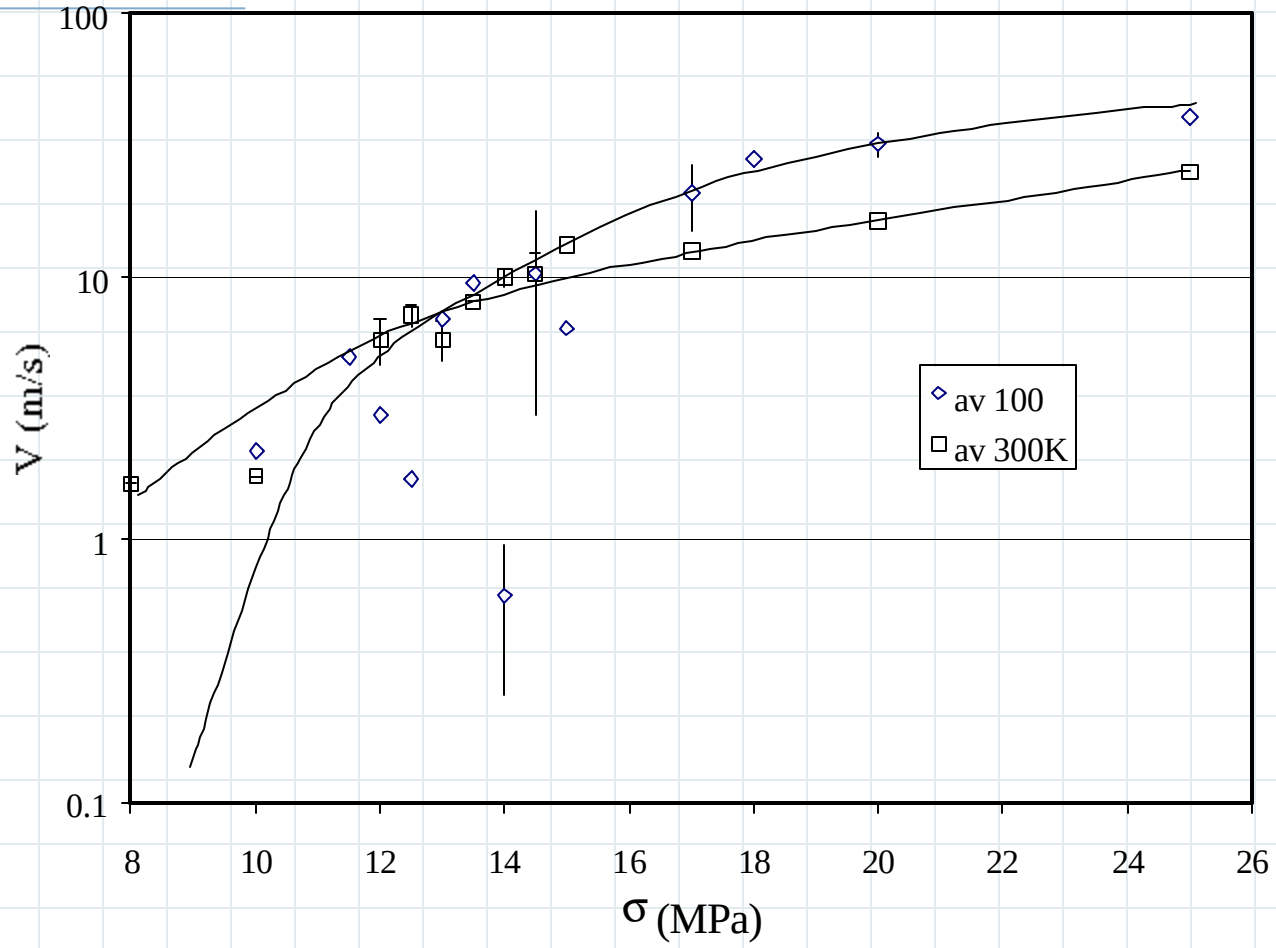




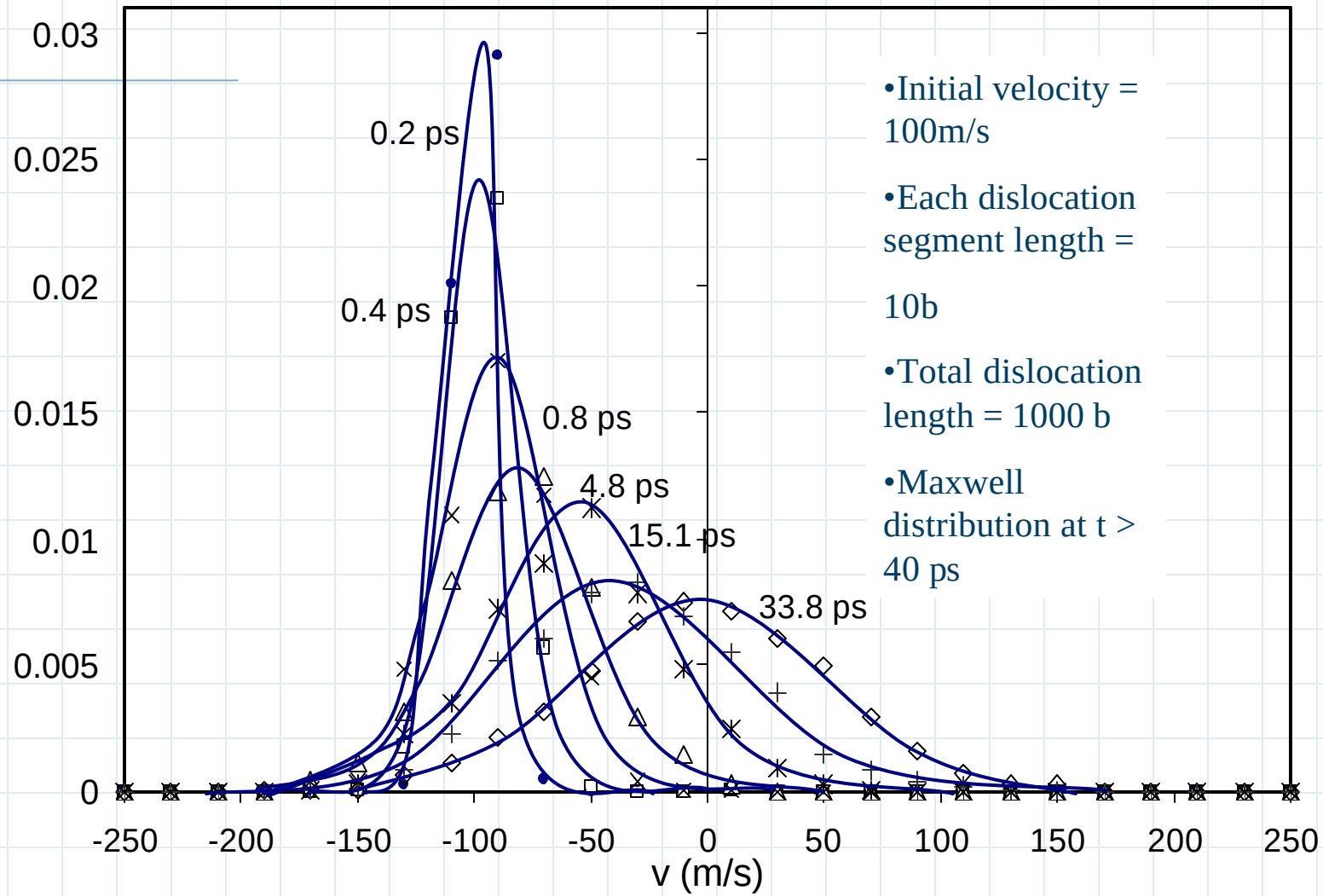
CRSS vs Obstacle Spacing

CRSS inversely proportional to the average obstacle spacing Λ

SDD: Dislocation Percolation among Random Obstacle Arrays

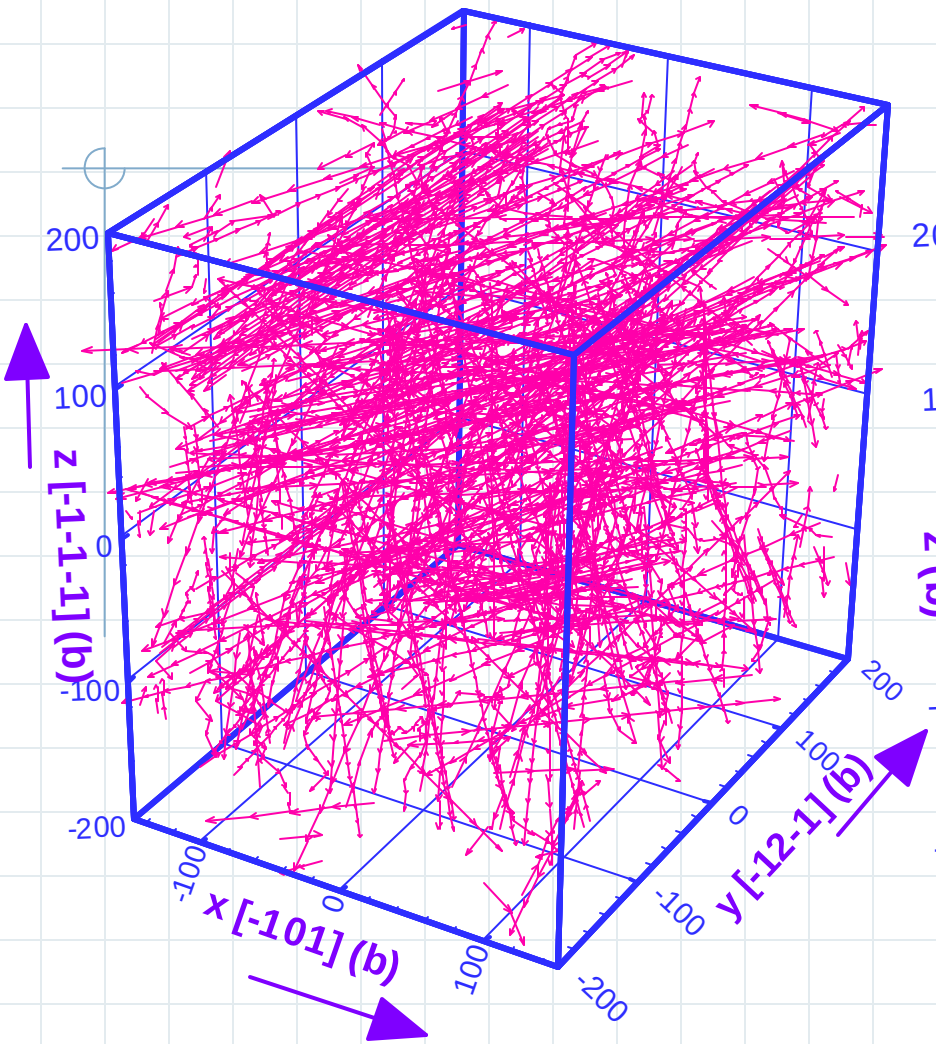


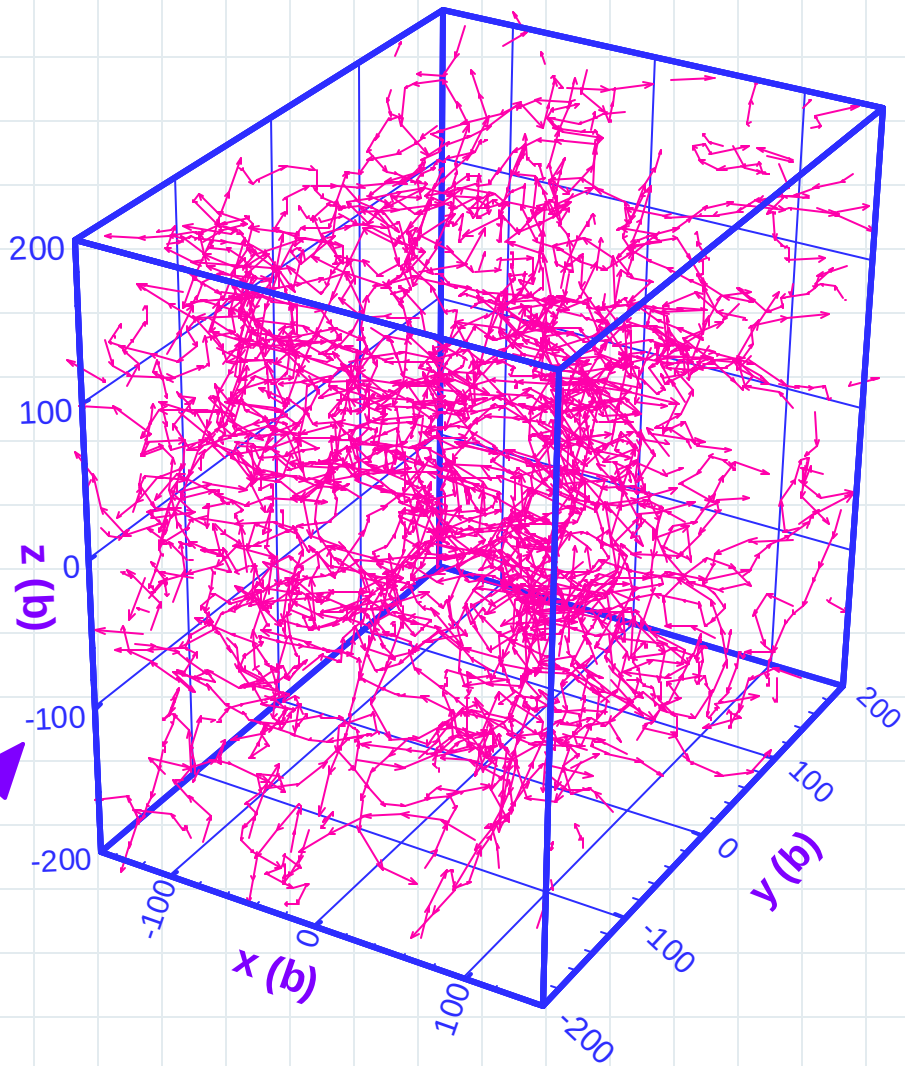
SDD:Thermalization of segment velocity at T = 300K



- Initial velocity = 100m/s
- Each dislocation segment length = 10b
- Total dislocation length = 1000 b
- Maxwell distribution at t > 40 ps

SDD: Relaxation





Right After Deformation

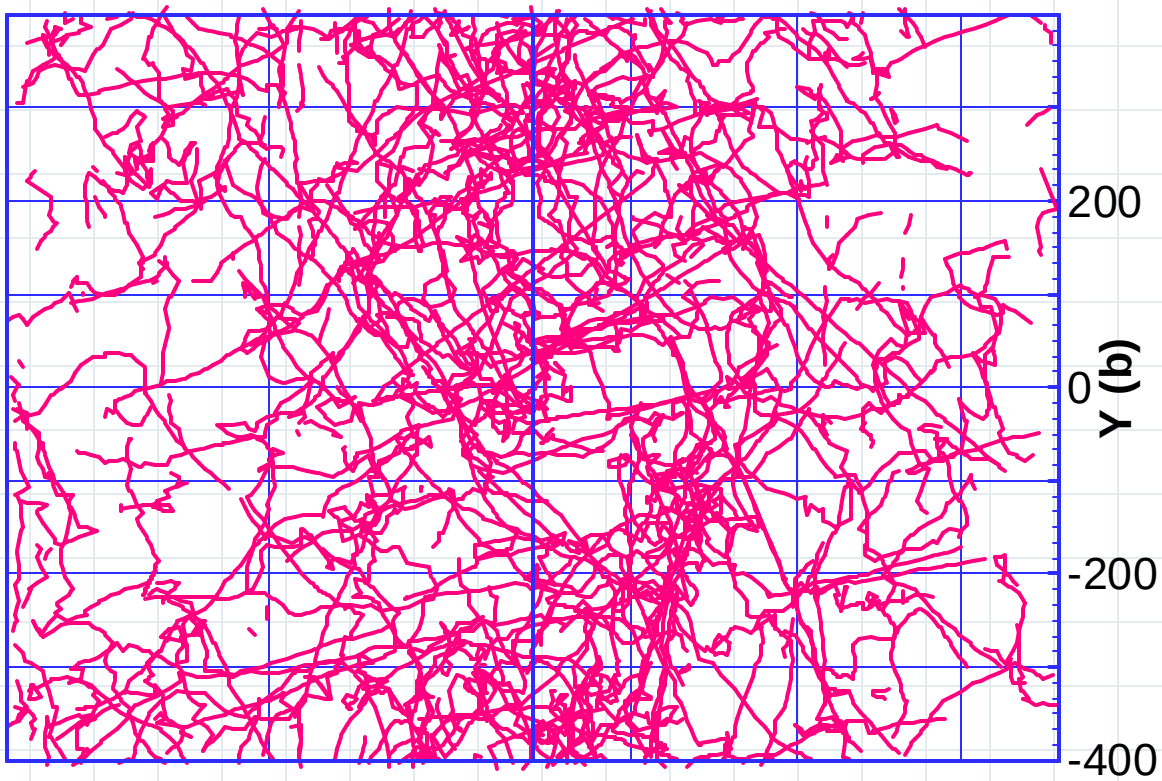
(exy = 3.2%, r =3.69 x 10^{16}/m^2)

After Unloading

(exy = 2.7%, r =2.71 x 10^{16}/m^2)

SDD: Relaxation

(210) plane



- At 0.5 ns after unloading
- εyz = 3.1%, ρ=3.05 x $10^{15}/m^2$

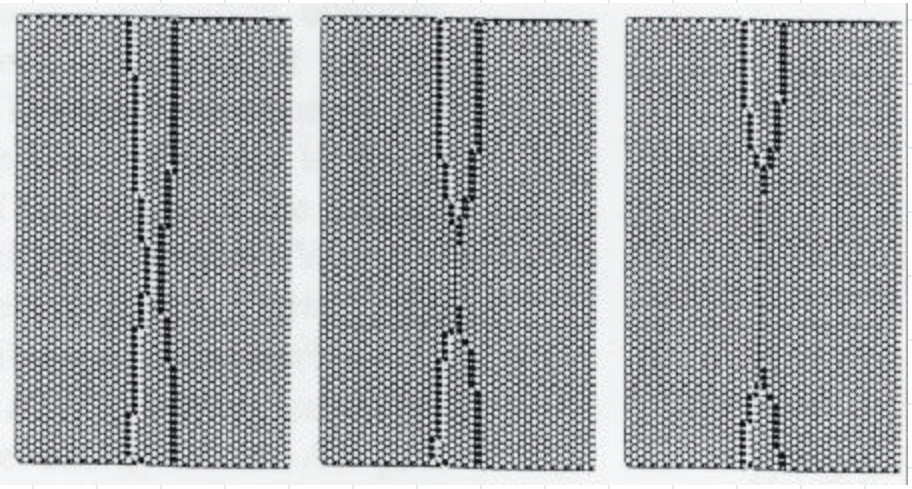
Cross-Slip

Cross-slip in DD

1. Cross-slip by bowing out onto the secondary plane to form a super-double kink configuration (Shoeck-Seeger mechanism).
2. Isotropic for loading direction
3. No consideration of time duration

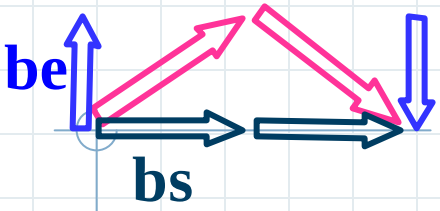
Cross-slip in SDD

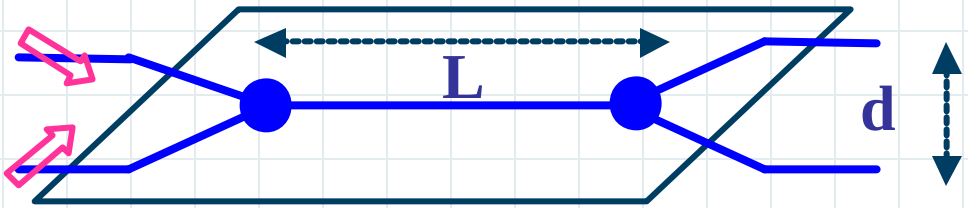
1. Cross-slip by immediate dissociation and expansion of Shockley partials (Escaig-Friedel mechanism)
2. Anisotropic for loading direction
3. Time duration is naturally included in the stochastic process.



(MD by Rasmussen et al 1997)

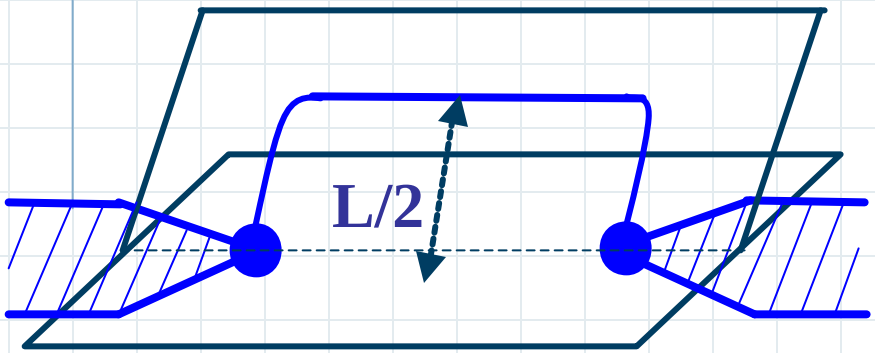
Implementation of Cross Slip Mechanism

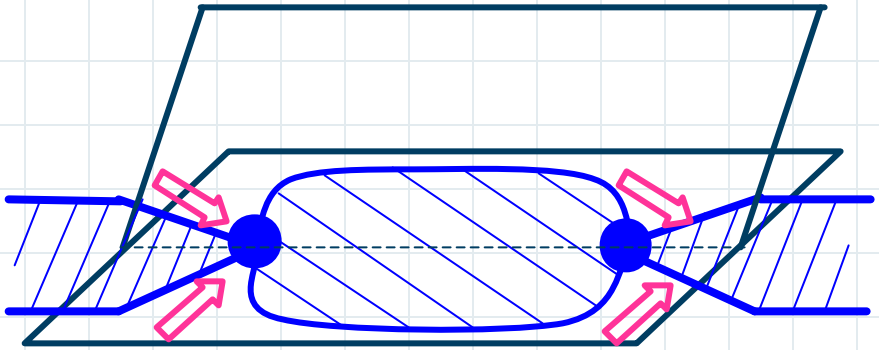




DD: Schoeck-Seeger mechanism

SDD: Escaig-Friedel mechanism





Screw Type **Edge Type**

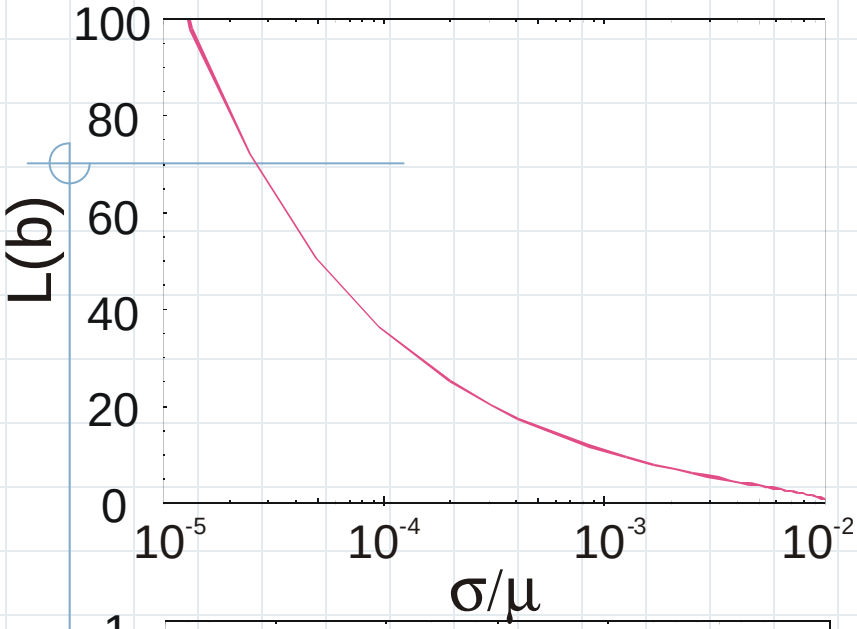
ΔG (Schoeck-Seeger mechanism) > ΔG (Escaig-Friedel mechanism)

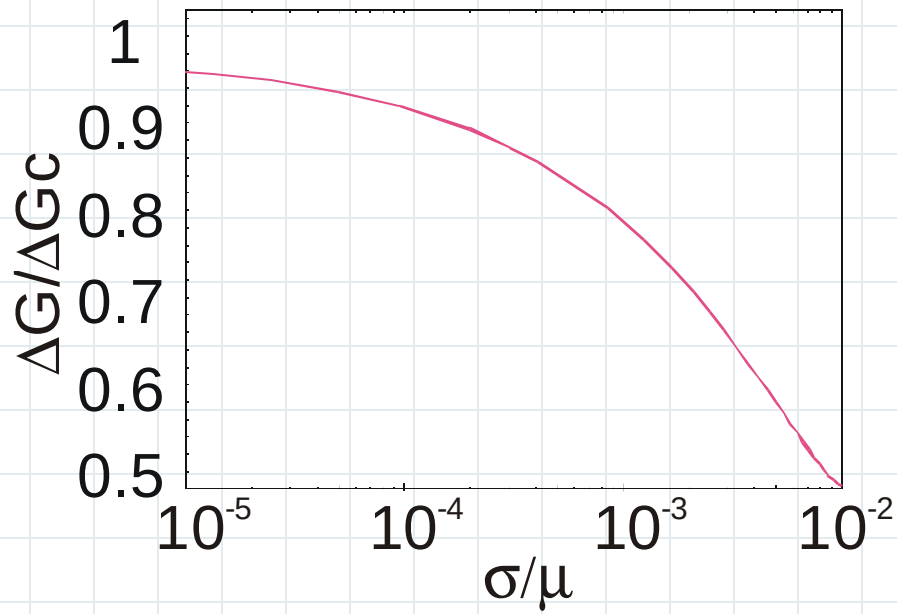
Escaig-Friedel mechanism is much more likely.

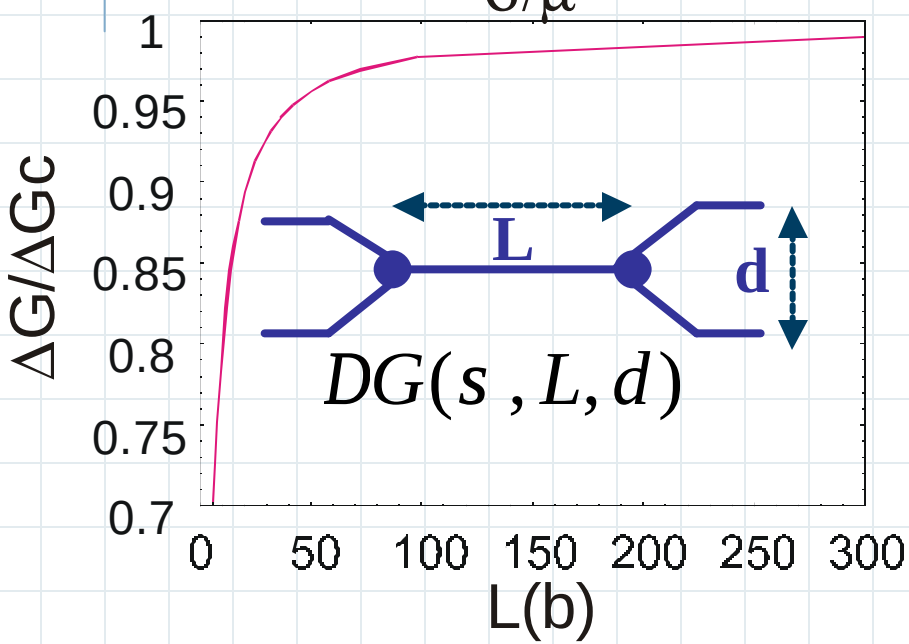
Edge type constriction
→Positive elastic energy

Screw type constriction
→Negative elastic energy

Cross Slip Energetics







MD data for Cu:

Activation free energy DGc

= 1.2 eV (Rao et al 1999)

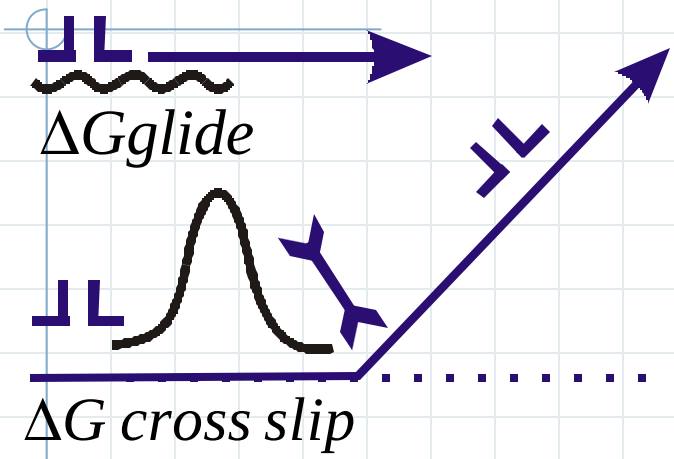
= 2.7 eV (Rasmussen et al 1997)

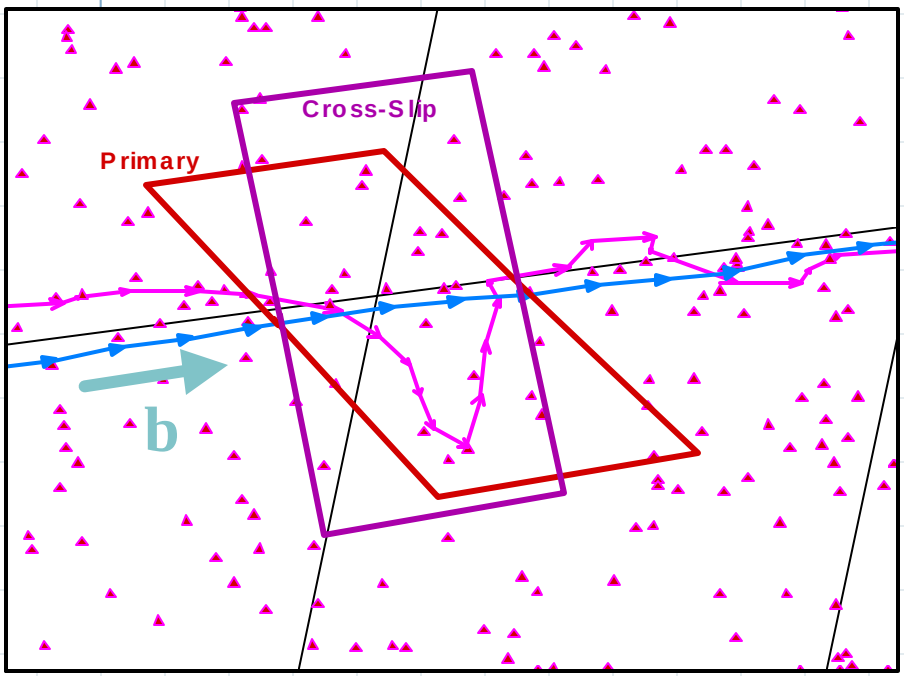
Typically, L = 20 ~ 80 b, d = 6.7 b for

Stacking fault energy γ = 0.045J/m^2

Implementation of Cross Slip Mechanism

Mode of motion of screw:

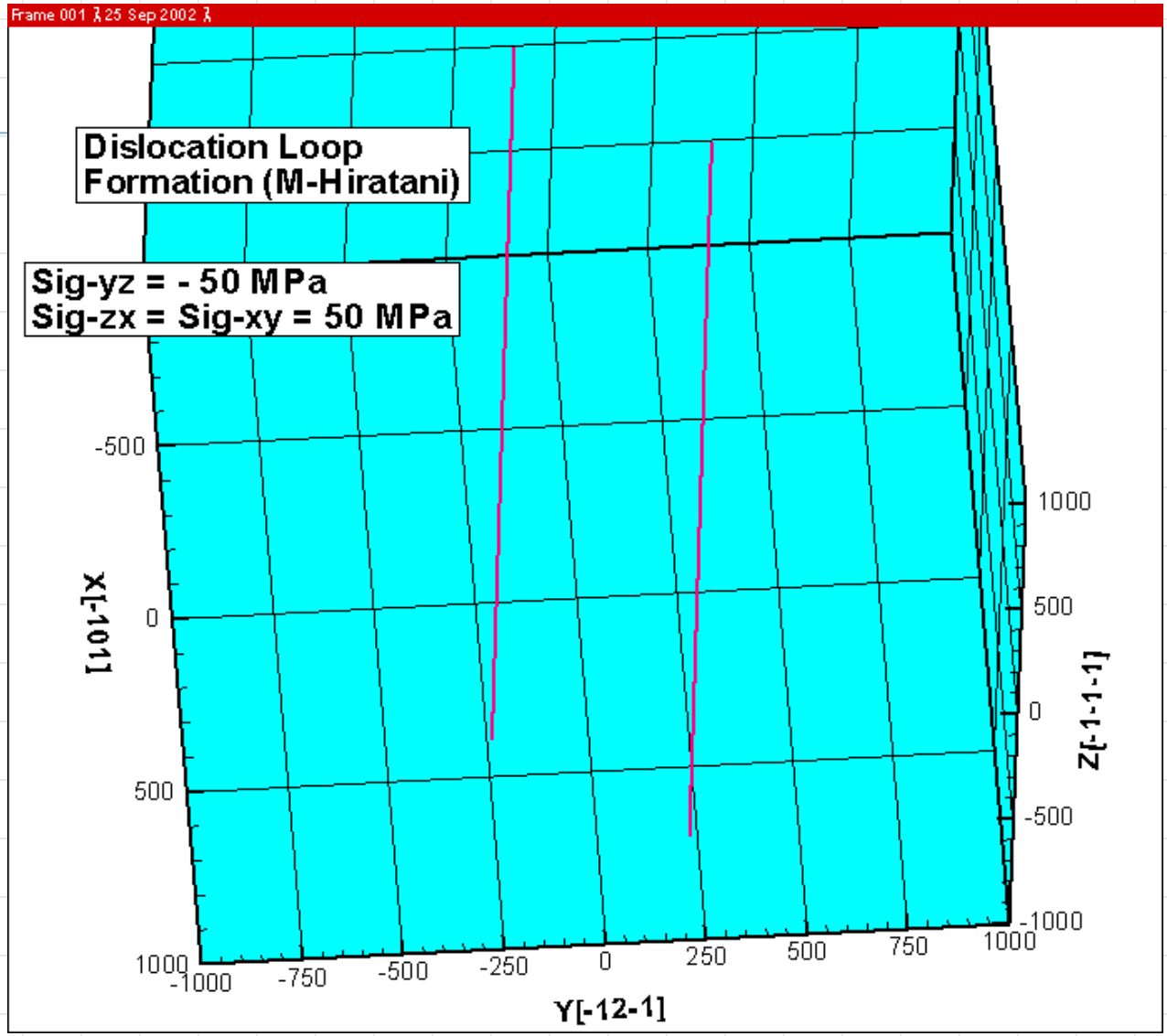


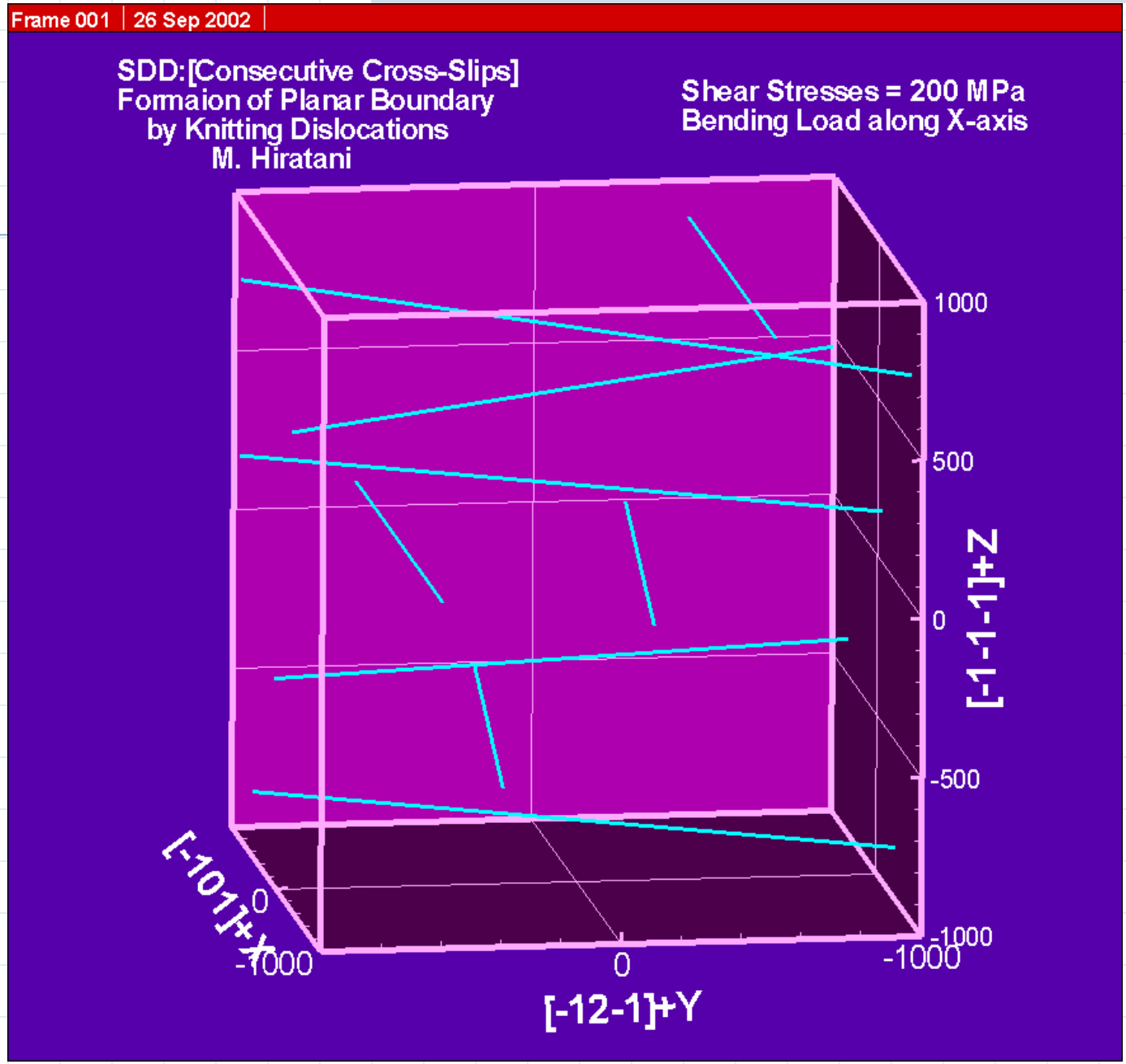


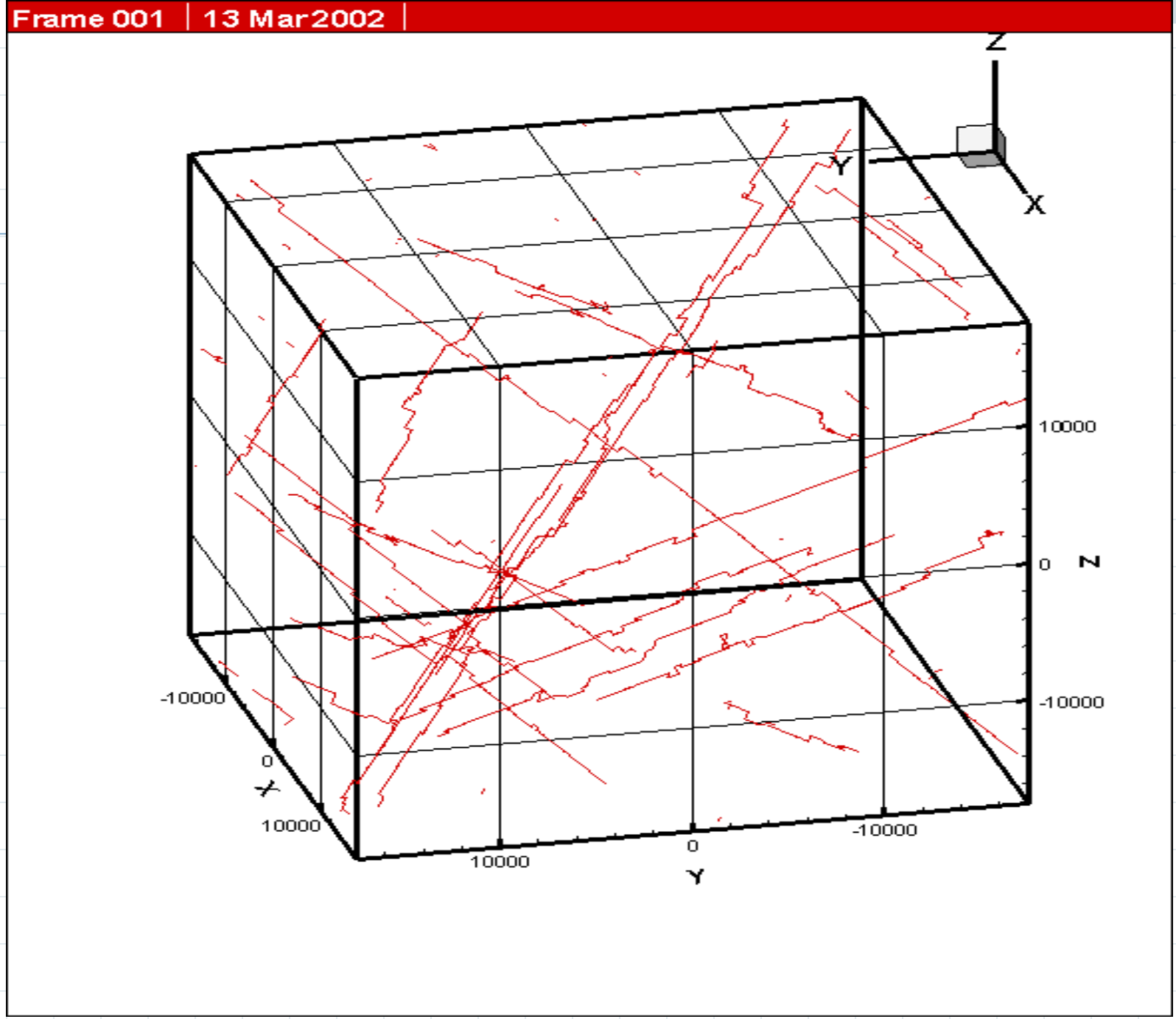
Algorithm

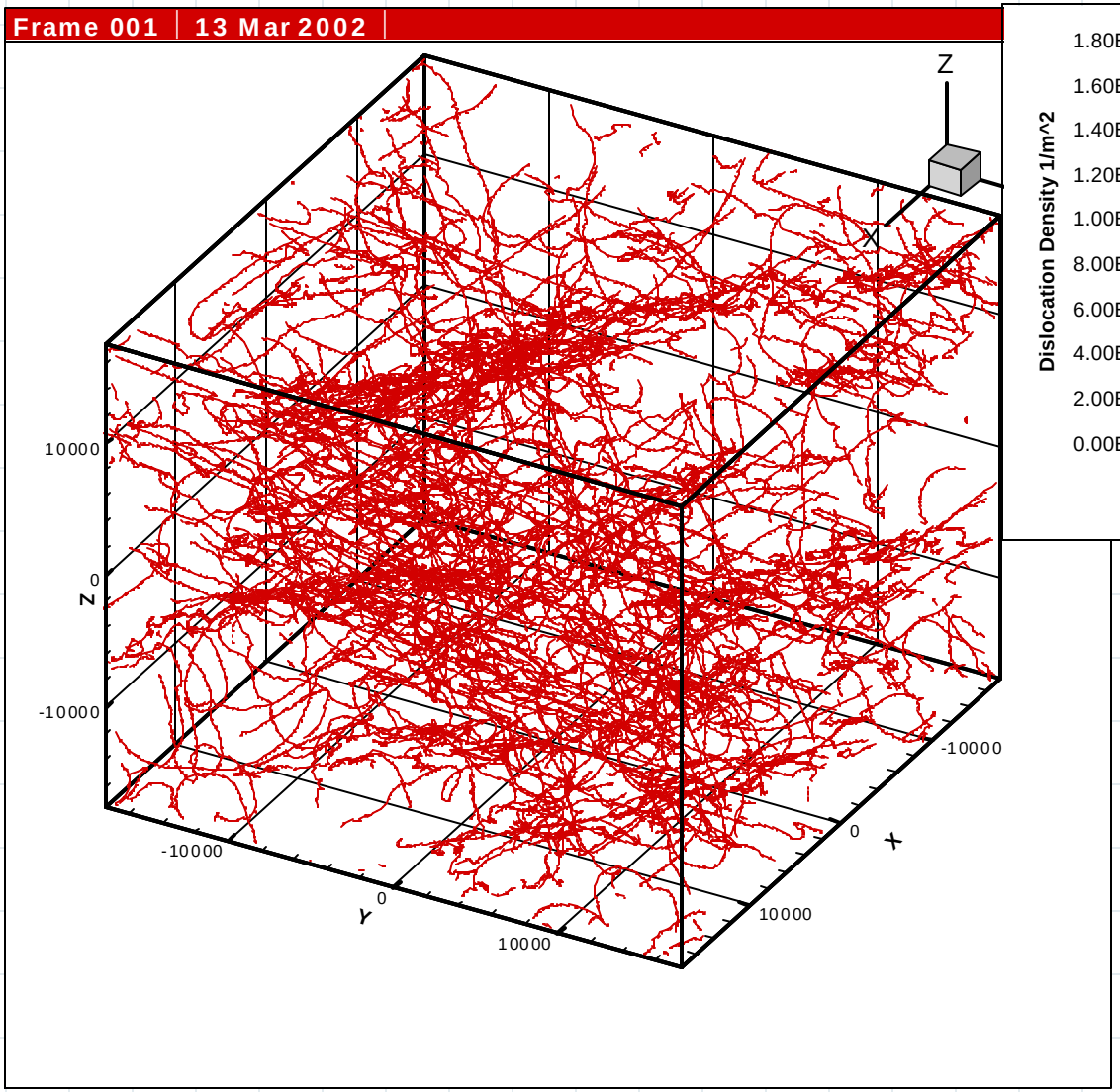
1. Generate a random number and choose a plane according to the activation enthalpy
2. Introduce parallel Shockley partials using coordinates of perfect screw.
3. Place a corresponding effective force barrier around the partials
4. Move dislocations according to the Langevin forces + systematic forces.

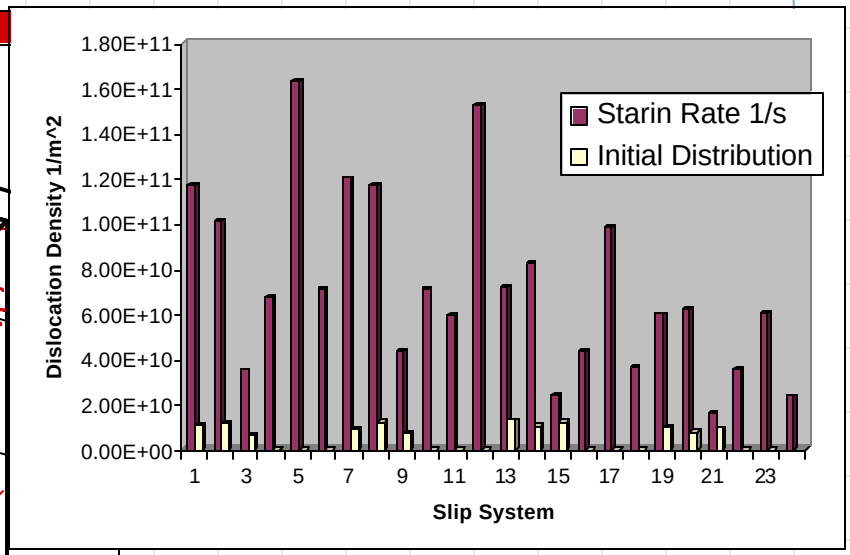
- **Random Distribution of SFTs with average interval of 40b**
- **Snap shot after 50 ps**
- **PBC, T=300K**

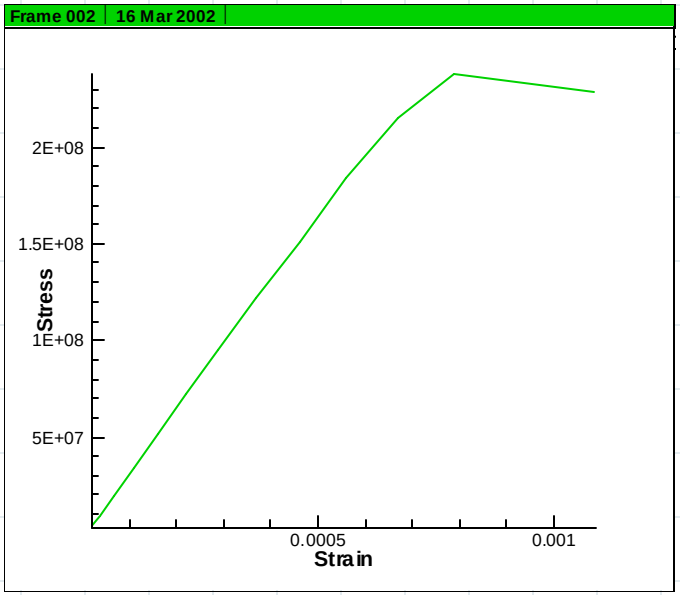

Frame 001 25 Sep 2002
Dislocation Loop
Formation (M-Hiratani)
Sig-yz = - 50 MPa
Sig-zx = Sig-xy = 50 MPa
X[-101]
-500
0
500
1000
Y[-12-1]
-1000
-750
-500
-250
0
250
500
750
1000
Z[-1-1-1]
1000
500
0
-500
-1000


Frame 001 | 26 Sep 2002
SDD:[Consecutive Cross-Slips]
Formaion of Planar Boundary
by Knitting Dislocations
M. Hiratani
Shear Stresses = 200 MPa
Bending Load along X-axis
1000
500
0
-500
-1000
[-1-1-1]+Z
[-101]+X
0
-1000
0
-1000
[-12-1]+Y

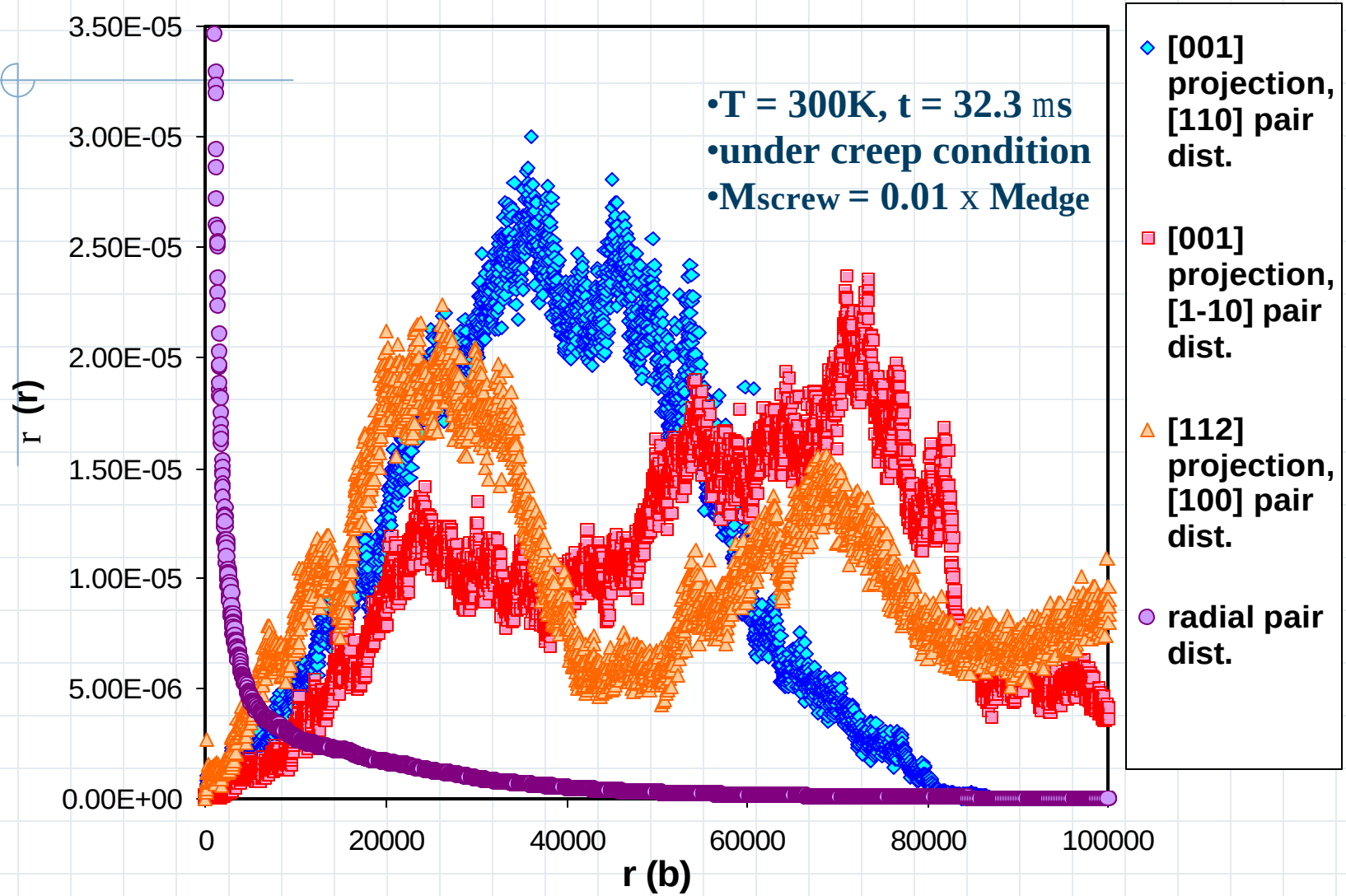

Frame 001 | 13 Mar 2002 |
Z
Y
X
10000
0
Z
-10000
-10000
0
X
10000
10000
0
-10000
Y


Frame 001
13 Mar 2002
Z
X
10000
0
Z
-10000
-10000
0
Y
10000
-10000
0
X
10000


1.80E+11
1.60E+11
1.40E+11
1.20E+11
1.00E+11
8.00E+10
6.00E+10
4.00E+10
2.00E+10
0.00E+00
Dislocation Density 1/m^2
Starin Rate 1/s
Initial Distribution
1
3
5
7
9
11
13
15
17
19
21
23
Slip System

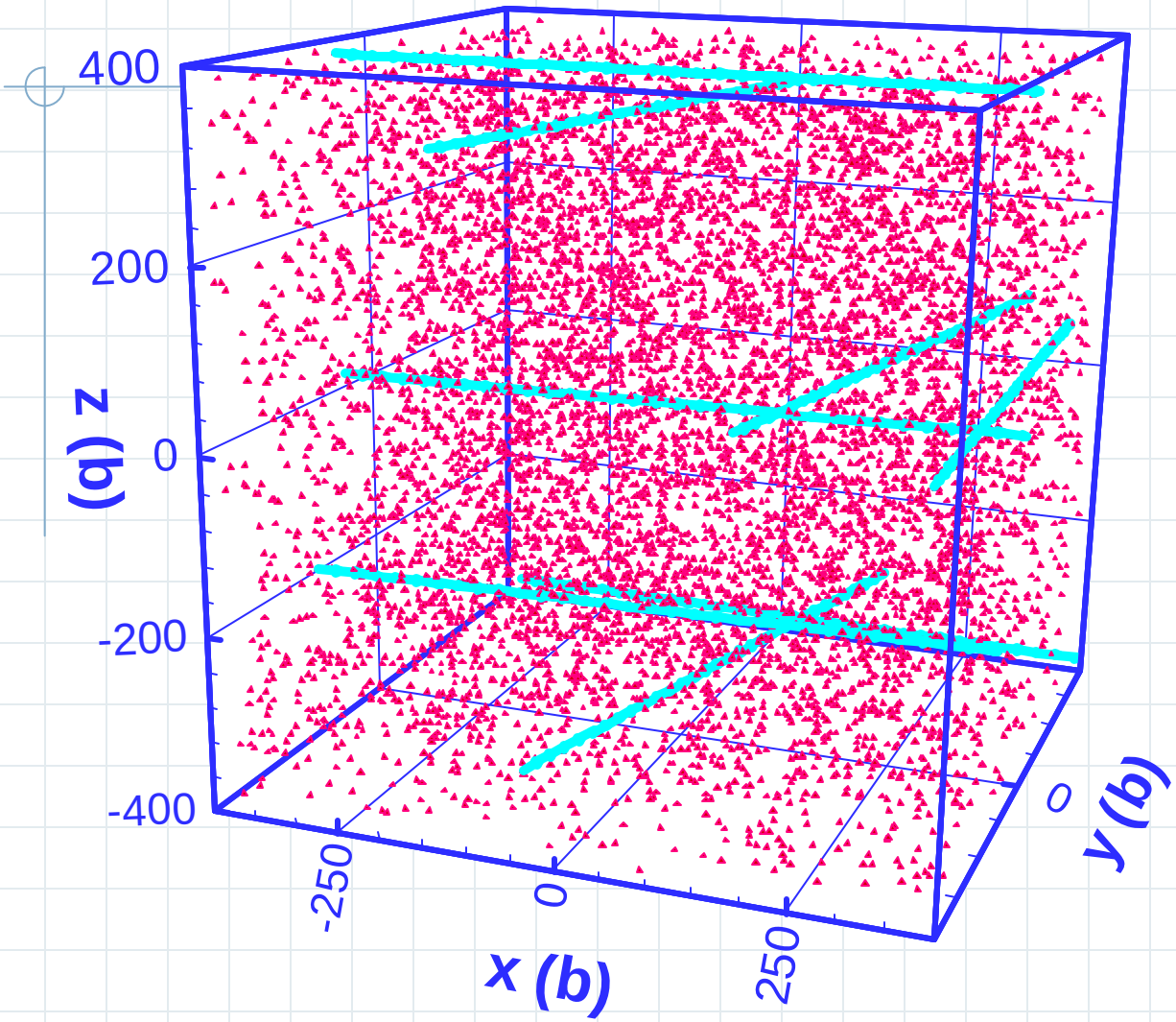

Frame 002
16 Mar 2002
2E+08
1.5E+08
1E+08
5E+07
Stress
0.0005
0.001
Strain

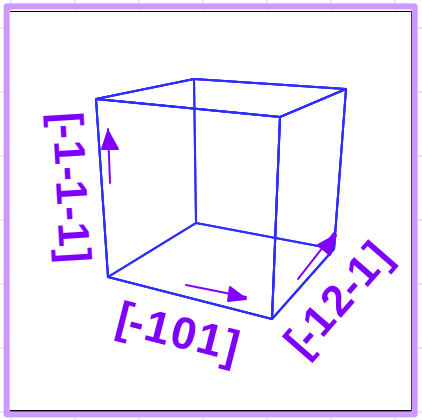
Dislocation Structure in Molybdenum



Pair Distribution Functions

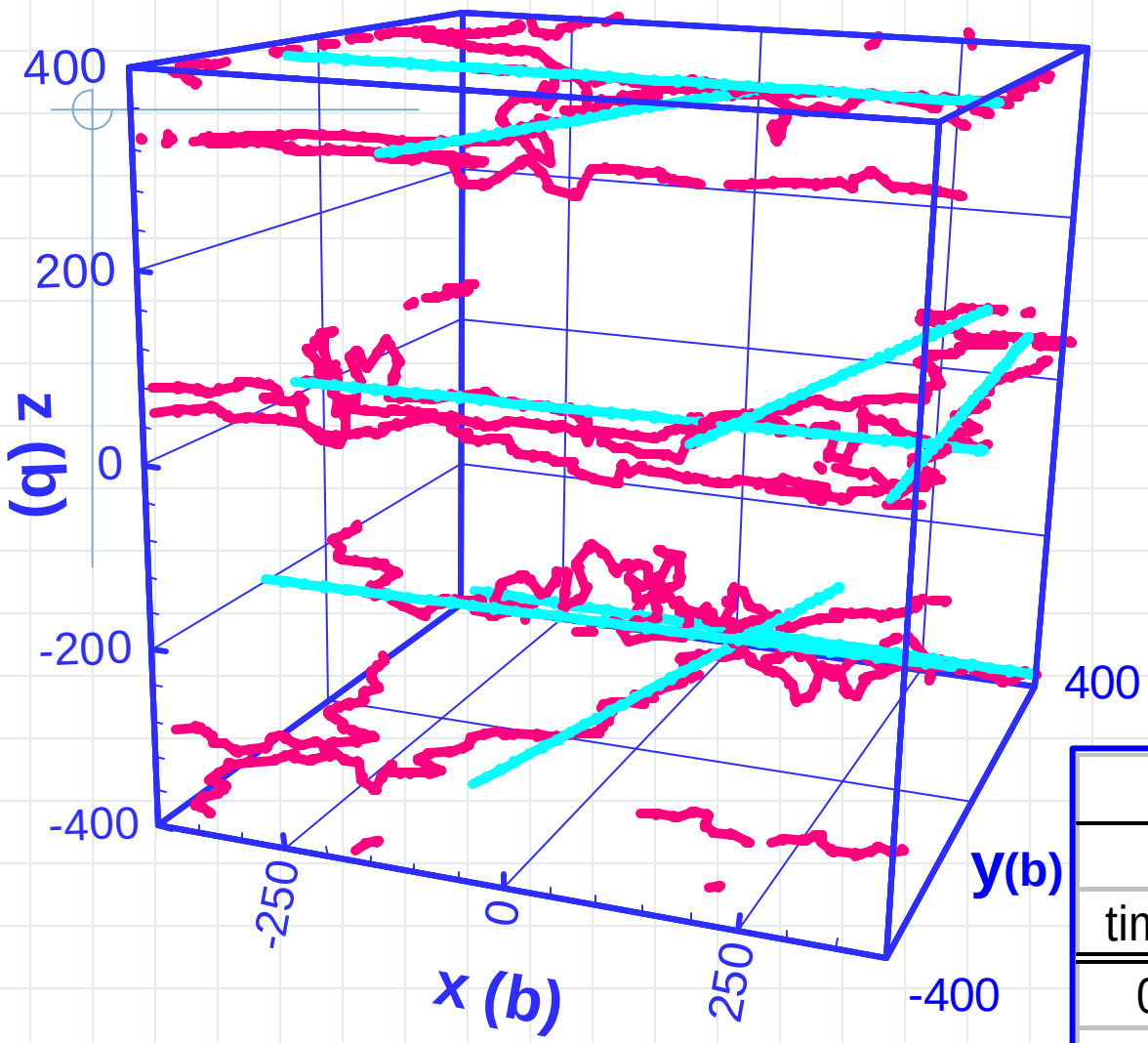
SDD: Cross Slip in Irradiated Copper (before deformation)





- Random distribution of dislocations on (111) planes with b = a/2[-101]
- Average SFT size = 10b & spacing = 50b

SDD: Cross Slip in Irradiated Copper (after 1ns)



- Dislocation shapes before and after loading
- s_{31}=20 MPa for 1ns
- SFTs are removed for clear view

Density in the unit of 10^{14} /m^2			
	primary	x-slip	
time	(111)	(-1-11)	total
0	1.93	0	1.93
1 ns	3.49	1.88	5.37

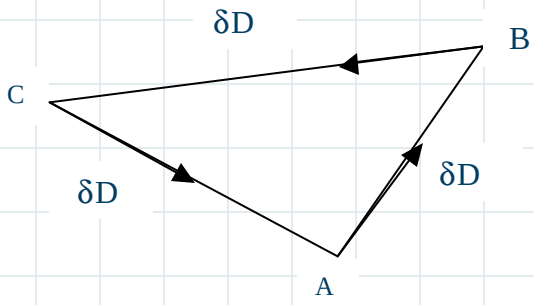
Statistical study of dispersion hardening by point-like obstacles II

M. Hiratani and H.M. Zbib

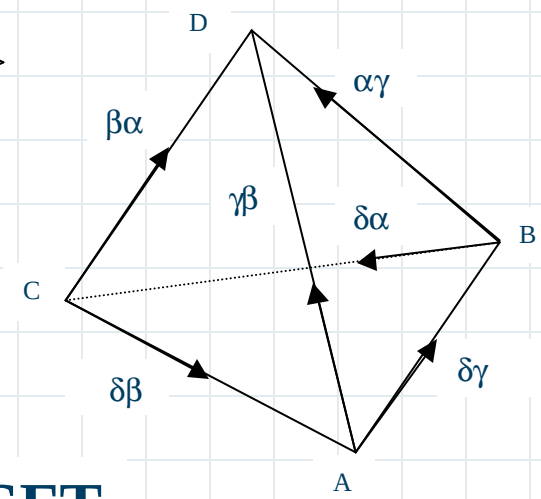
The critical resolved shear stress for a dislocation percolating through unlike penetrable obstacles is derived using Kocks-Friedel type dislocation model. The partition function and density function are determined under the extreme condition of the partition function and geometrical condition. The analytical result implies a superposition law for the concentration of pinning obstacles on a dislocation, and the Pythagorean type-hardening rule for the critical resolved shear stress in the limit of weak obstacle strength. Additionally, the analytical results are compared with computational data for a modeled irradiated bcc metal by the discrete dislocation dynamics.

SFT versus FS loop!

Interaction between a defect (Frank sessile loop or SFT) and a glide edge dislocation



Frank-sessile loop



SFT

In the DD code the SFT is constructed from six dislocations segments with **Stair Rods Dislocations: e.g.**

$$\boldsymbol{b}_{db} = \boldsymbol{b}_{dA} + \boldsymbol{b}_{Ab} = \frac{\boldsymbol{a}}{6}[1\bar{2}1] + \frac{\boldsymbol{a}}{6}[\bar{1}1\bar{2}] = \frac{\boldsymbol{a}}{6}[0\bar{1}\bar{1}]$$

Etc..

Criterion for FS Loop Unfaulting and Loop Absorption Scheme

unfaulting from a sessile Frank partial loop (with a Burgers vector of a<111>/3 type) to a perfect generally prismatic loop (with a Burgers vector of a<110>/2 type)

$$\Delta E = \textit{faulted state} - \textit{unfaulted state}$$

$$\Delta E(\textit{stressed}) = A^{(2)}g + \underbrace{A^{(2)} n_i^{(2)} s_{ij}^{(1)} b_j^s}_{E^{int}} - \frac{RGa^2}{24}\left(\frac{2-n}{1-n}\right) \ln\left(\frac{2R}{e_o}\right)$$

$A = \textit{loop area} = pR^2$

$g = \textit{surface tension} = \textit{stacking efault energy}$

$e_o = \textit{characteristic core dimension} = \frac{b}{2} - 4b$

$b_j^s = b_j^f - b_j^p = \textit{Shockley partial}$

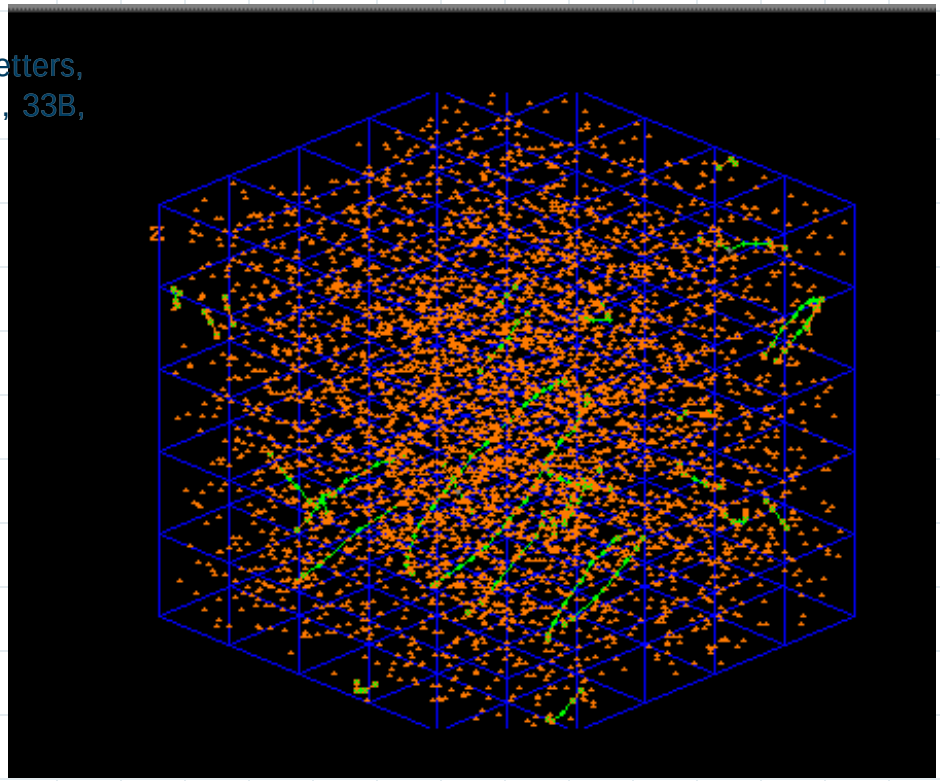
For any given Frank partial, there are three different Shockley partials (of type a<112>/6) that would transform it to a perfect dislocation of type a<110>/2.
All conjugate Shockley partials for a given Frank partial have been tabulated.

Kharishi, T, Zbib, H.M., T. Diaz de la Rubia and M. Victoria,

Nature, 406, 871-874, 2000. Philosophical Magazine Letters, 81, 583-593, 2001. Metallurgical and Materials Transactions B, 33B, 285-296, 2002.

Kharishi, T, Zbib, H.M., T. Diaz de la Rubia and M. Victoria

Nature, 406, 871-874, 2000. Philosophical Magazine Letters, 81, 583-593, 2001. Metallurgical and Materials Transactions B, 33B, 285-296, 2002.



What is the relationship between increase in flow stress and defect density?

Possible mechanisms being investigated:

1. **Defects decorating the dislocations (hard obstacles)**
2. **Dispersed defects (soft obstacles)**
3. **Combination of 1 and 2.**

How do channels form?

•Defects are absorbed by the dislocation core.

Absorption criterion? Dislocation core-defect interaction (input from MD simulation)

What controls the size of the channel?

Cross-slip

Super-jogs (due to loop absorption?)

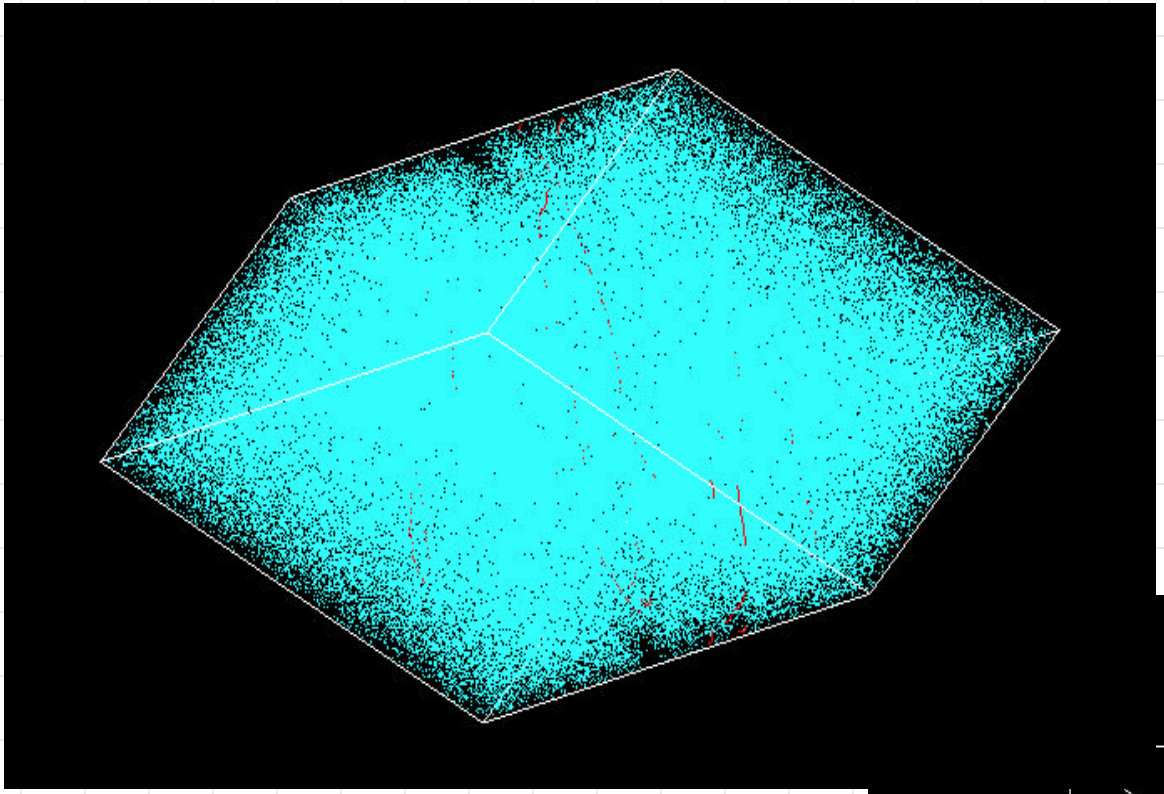
Material: Pd single crystal / and Cu

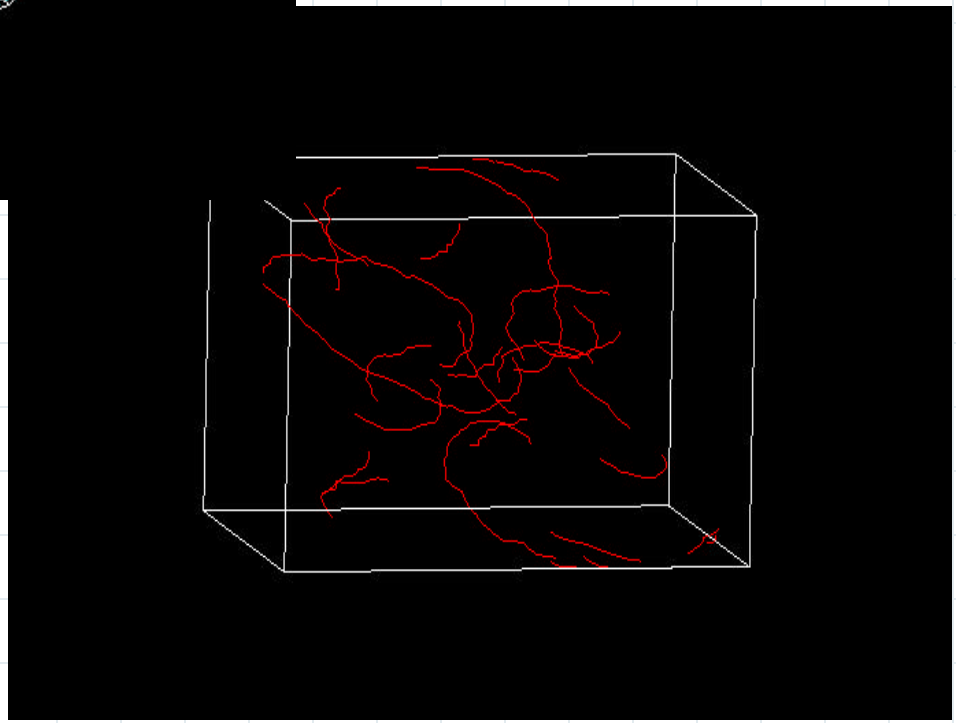
Defect density = 10^{20} - 10^{22} /m^3

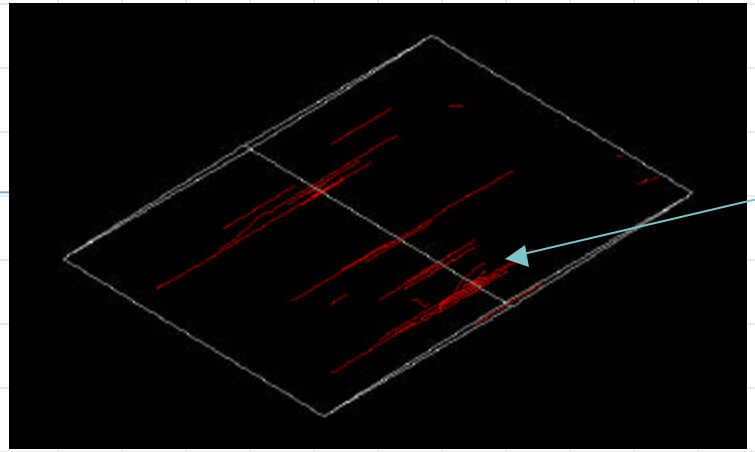
Initial dislocation density 10^{11} - 10^{12} /m^3

Loop size 1.28 nm to 3.48 nm

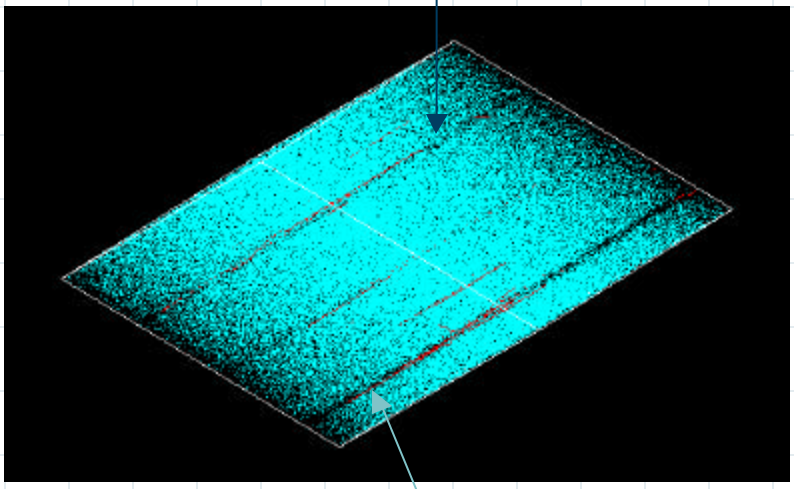
Random distribution of 10^5 - 4×10^6 point defects (prismatic loops/SFT's). Loops are on {111} planes with <111> Burgers vectors.

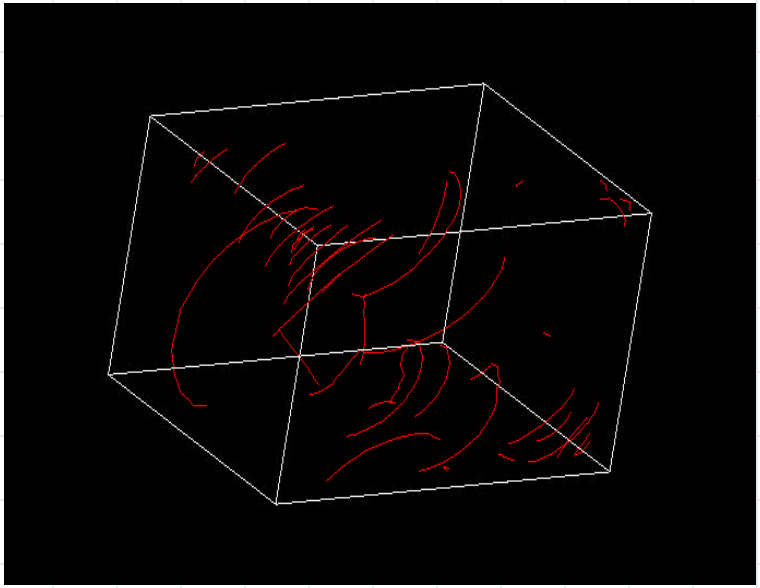




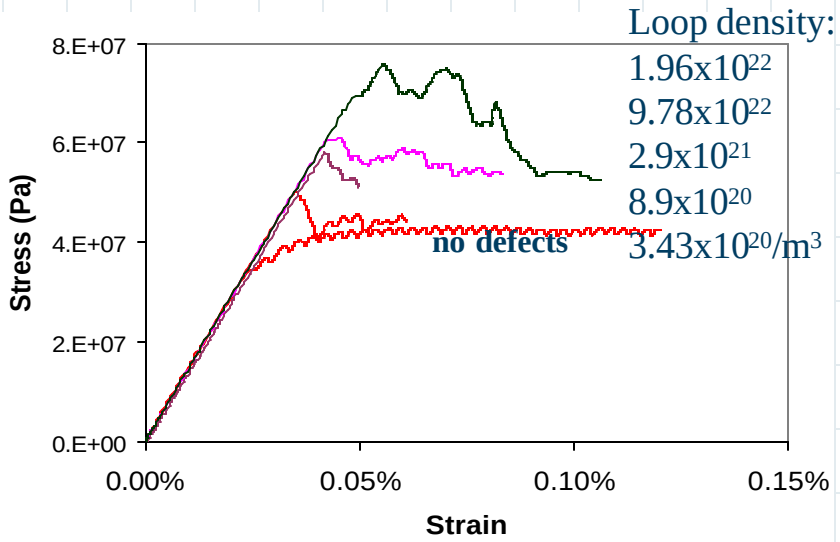


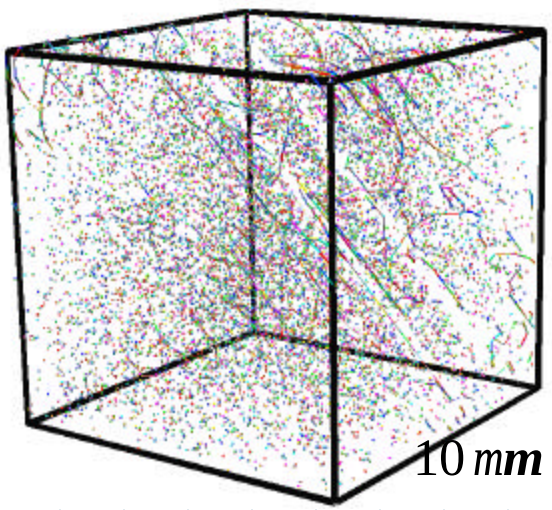
Starting from a single FK source, dislocations cross-slip and double cross-slip spreading normal to the original slip plane. Spreading is restrained by mutual trapping of dislocations segments on parallel planes (e.g. dipoles)



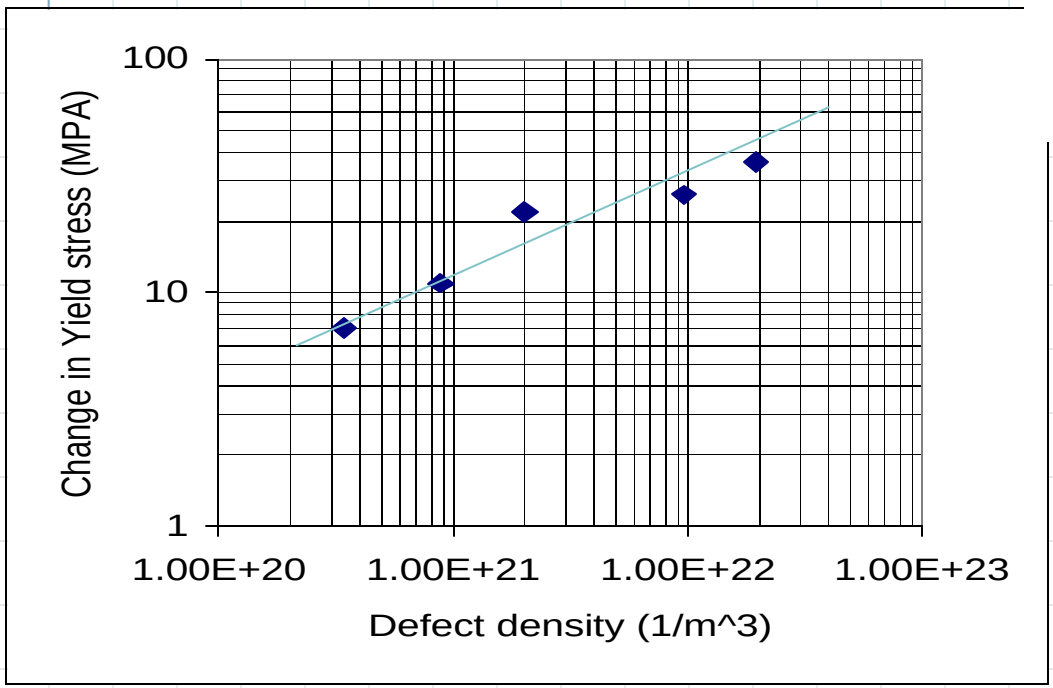


Bands cleared from defects (width: 200-300 nm)


Loop density:
1.96x10^22
9.78x10^22
2.9x10^21
8.9x10^20
3.43x10^20/m^3
no defects
Stress (Pa)
8.E+07
6.E+07
4.E+07
2.E+07
0.E+00
0.00%
0.05%
0.10%
0.15%
Strain


10 mm

B

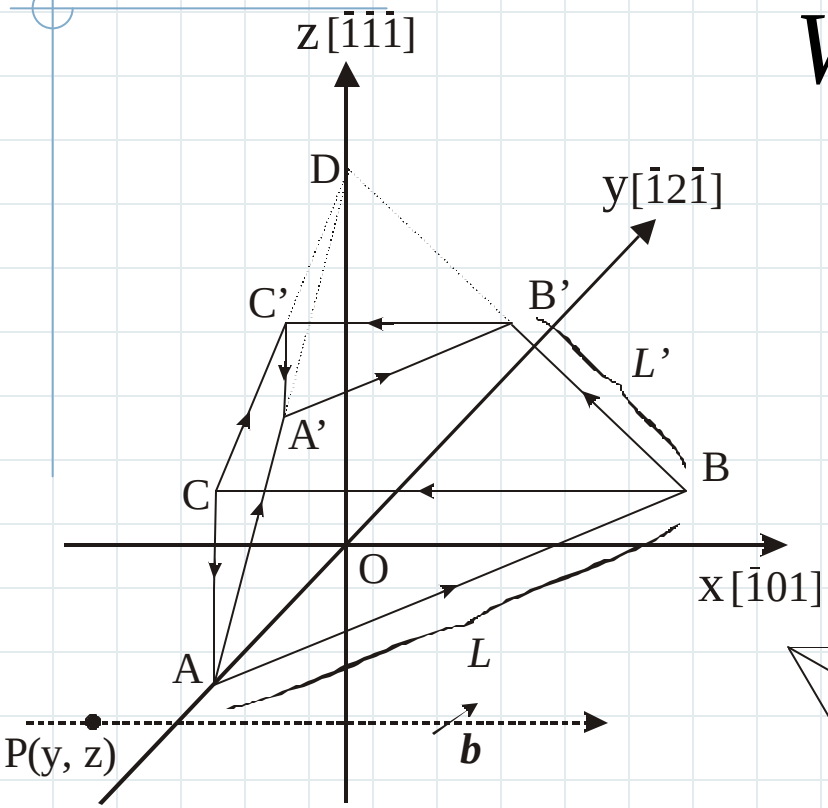

Change in Yield stress (MPA)
100
10
1
1.00E+20
1.00E+21
1.00E+22
1.00E+23
Defect density (1/m^3)

Interaction of Complete and Truncated Stacking Fault Tetrahedra with Glissile Dislocations in Irradiated Metals

Hiratani, H. M. Zbib, and B.D. Wirth Phil Mag. 2002

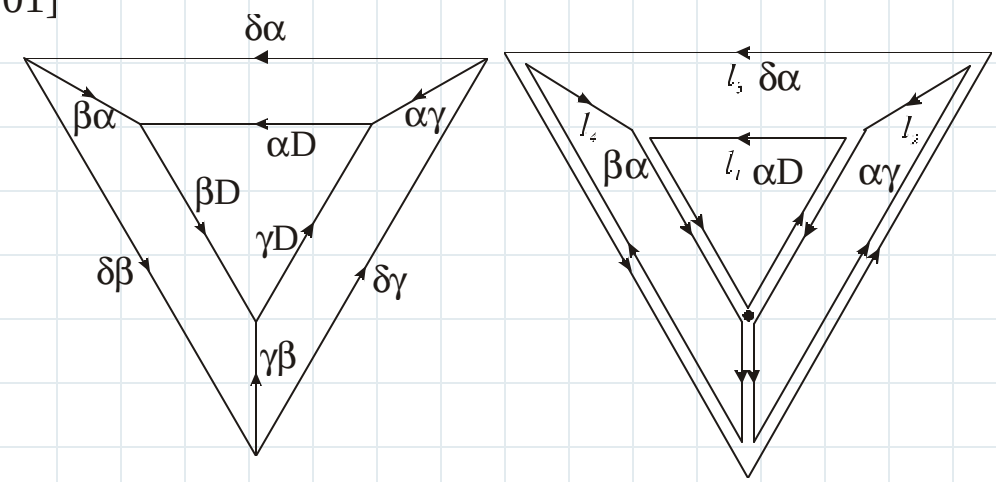
Collapse and absorption mechanism of truncated stacking fault tetrahedra (SFTs) by approaching dislocations are proposed. Both self-energy and elastic interaction energy in a straight dislocation-SFT system are calculated analytically. Although an isolated SFT is in many cases more stable than a complete dislocation loop or Frank sessile loop, it can become metastable under the influence of strain fields of surrounding dislocations. Interaction between incident dislocations and SFTs can cause instability of the complete SFT relative to truncated SFT, Frank sessile loop, and complete dislocation loop. In general, interaction energy due to a single dislocation is found to be not large enough to overcome elastic barriers between a metastable truncated SFT and stable unfaulted loop by thermal activations. Pinning through core reactions and dislocation piled-ups in certain glide systems approaching the SFT are shown to lower the barriers considerably. These collapse and absorption mechanisms can explain flow localization and defect free channels in irradiated materials.

Evaluation of Elastic Interaction Energy

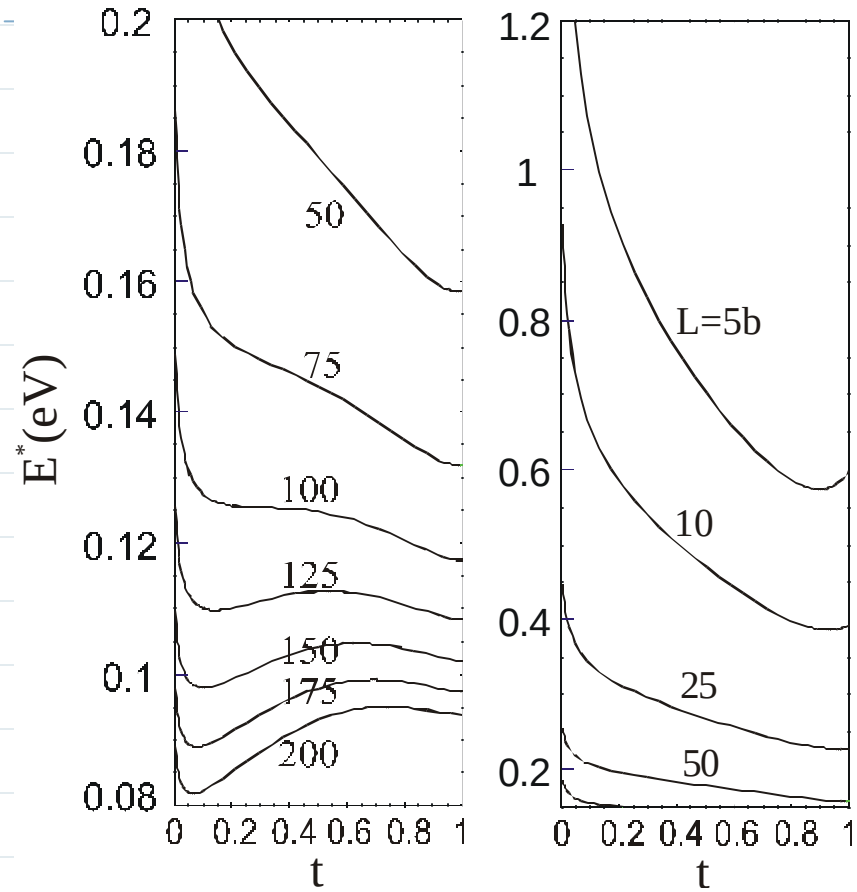


$$W_{12} = \int_{A_1} \boldsymbol{b}_1 . s_2 . dA_1$$

1. Blins Formula for 2 closed loops
2. Decomposition of SFT into Volterra loops



Stability of truncated SFT w/o Dislocation



t = 1: complete SFT

t = 0: Frank Sessile loop

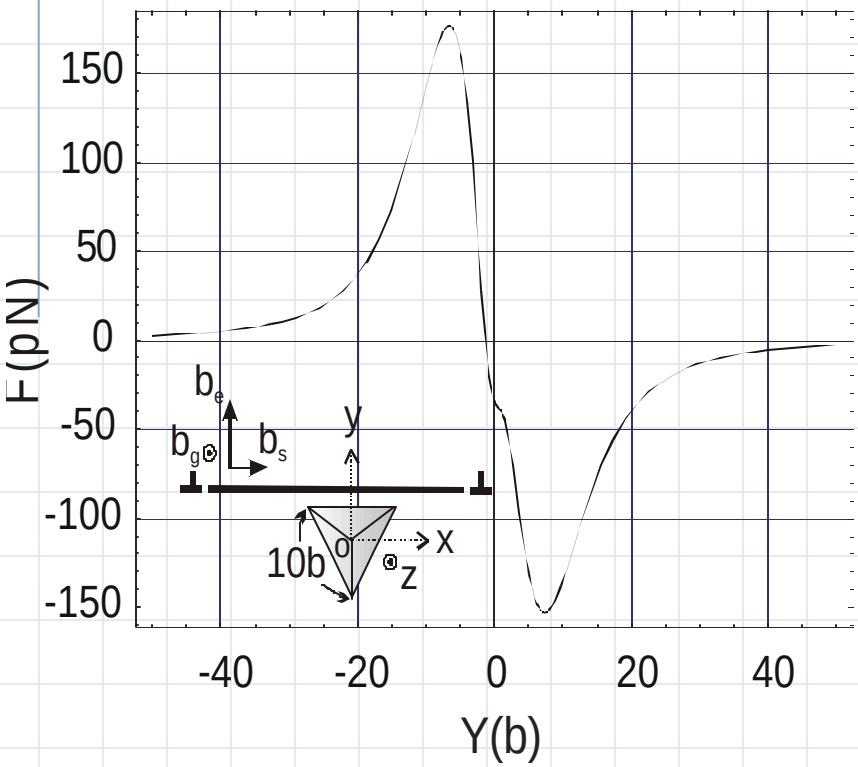
- Self-energy as a function of degree of truncation *t*
- Complete SFT is more stable than truncated SFT at small size
- Truncated SFT becomes metastable at L~100b
- Truncated SFT becomes more stable than complete SFT at L~125b

t= L'/L

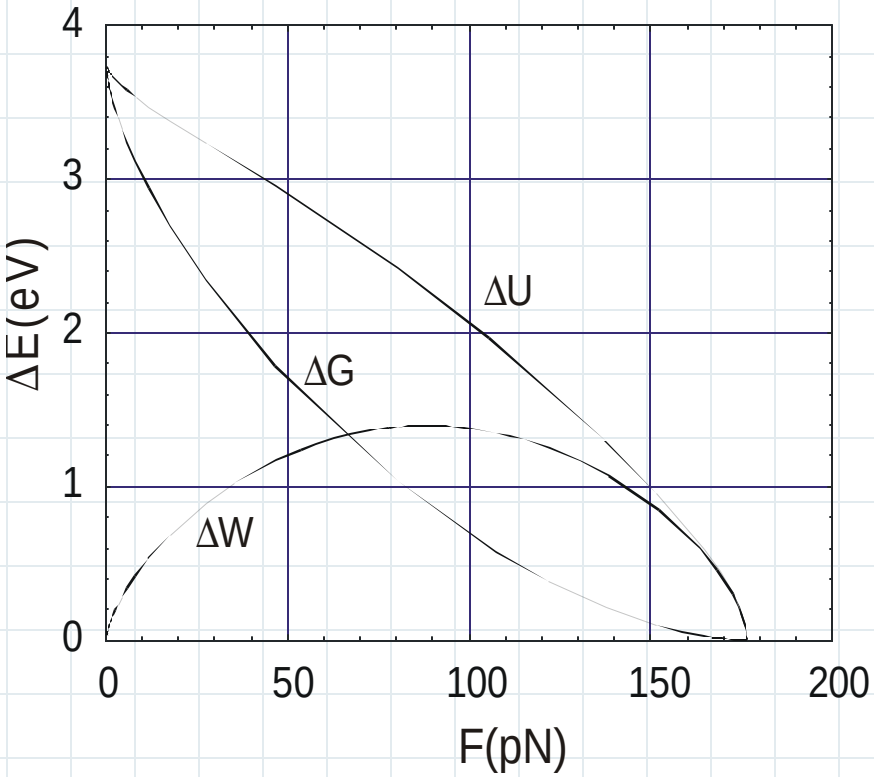
Stability of Complete SFT with Dislocation

Defect-Glissile Dislocation Interactive Force

Force profile

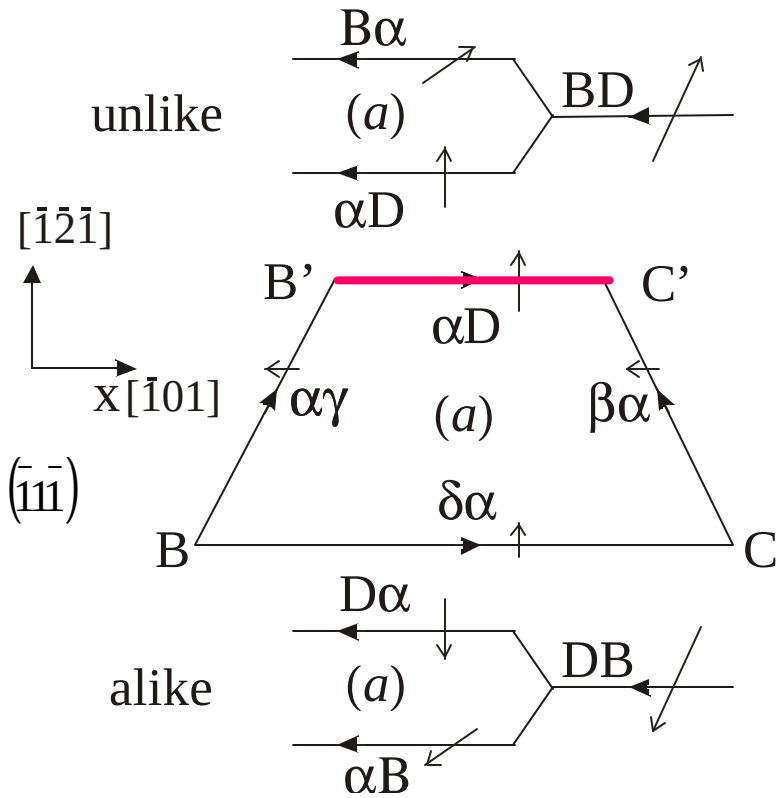


Activation Energy profile



Case for a perfect dislocation gliding on a base plane of SFT (d-plane)

Stability of truncated SFT with Dislocation (I)



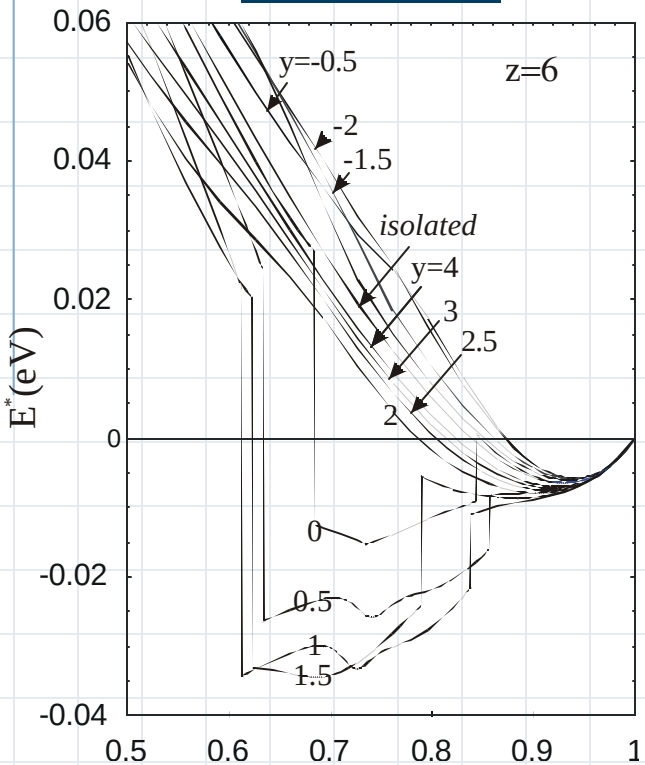
- Schematics for incident dislocation (Shockley Partial dislocations) on Truncated SFT with Burgers vectors.
- Segment B'C' is glissile on a side-plane of SFT .
- Alike case and Unlike cases are possible.
- Stability of truncated SFT is checked by system energy defined as

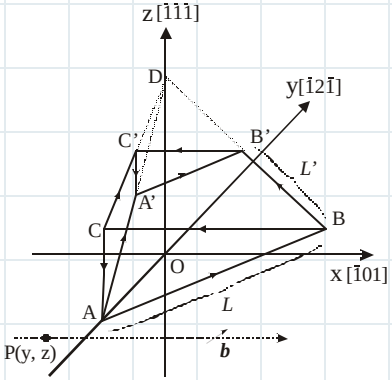
$$\Delta E = E_{\text{int}}(tSFT) + E_{self}(tSFT) - E_{\text{int}}(pSFT) - E_{self}(pSFT)$$

Case for a perfect dislocation gliding on a side plane of SFT (a-plane)

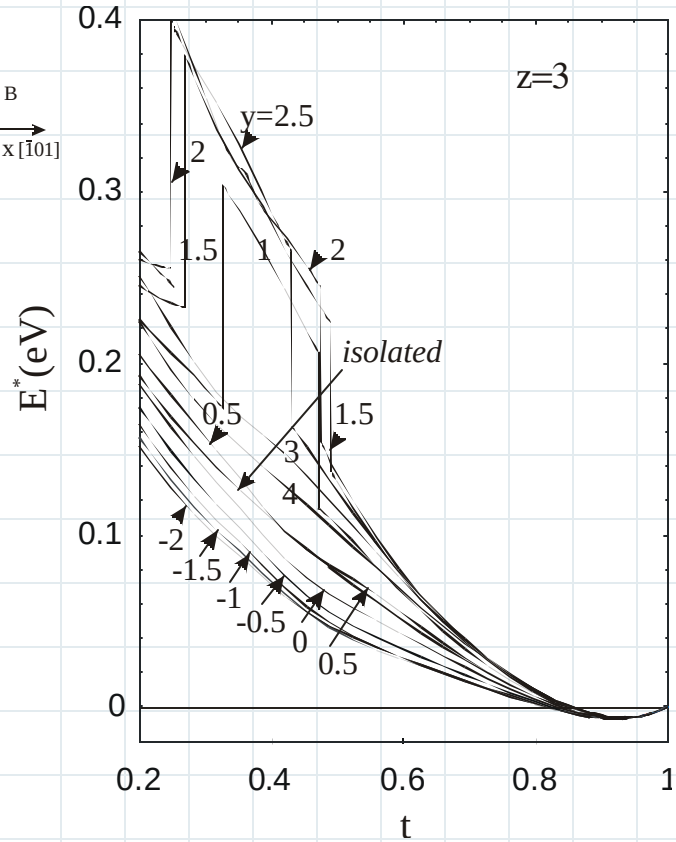
Stability of truncated SFT with Dislocation (II)

Unlike case





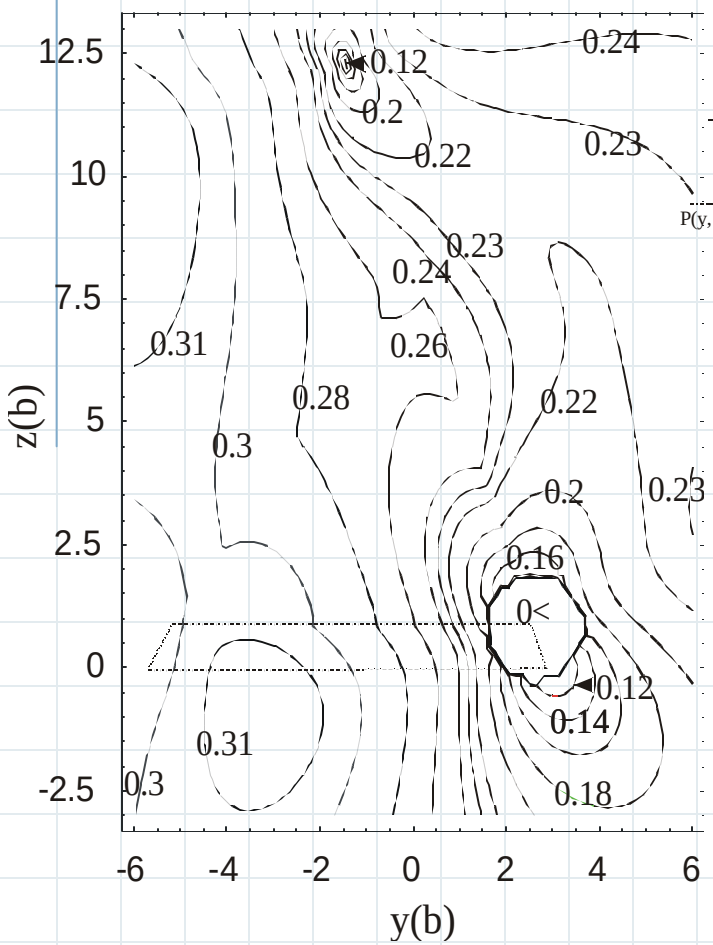
Alike case

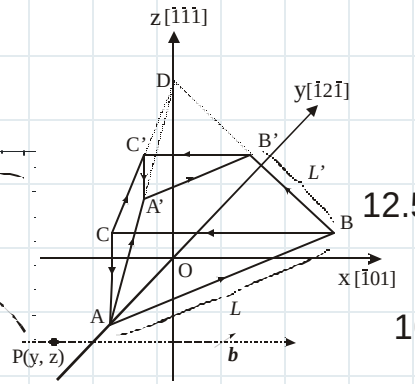


system energy at various positions of incident Shockley partials.

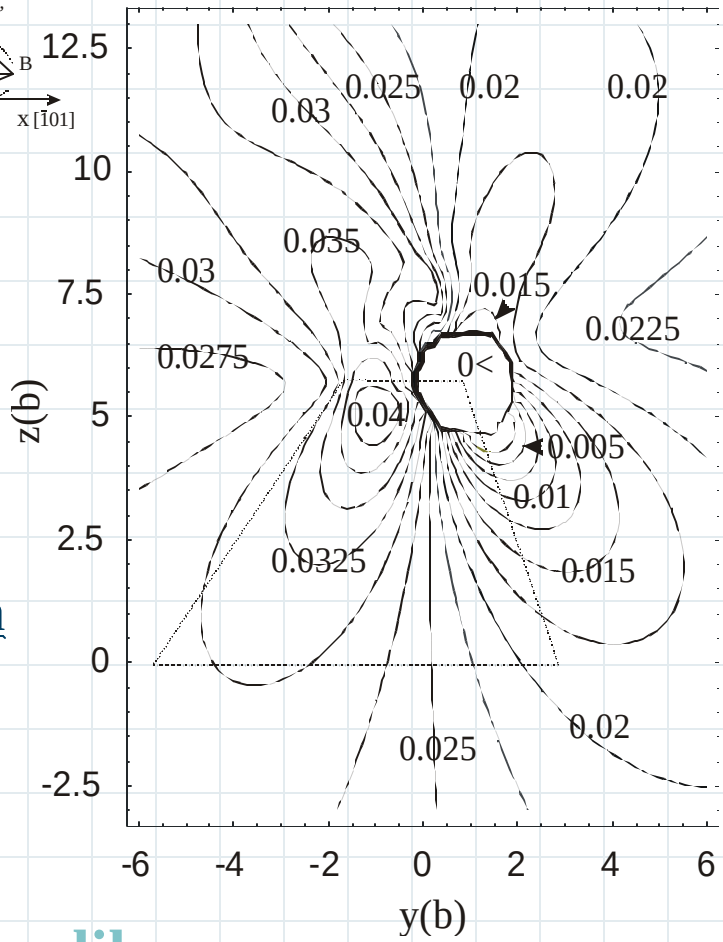
Stability of truncated SFT with Dislocation (III)

Unlike case at t = 0.1





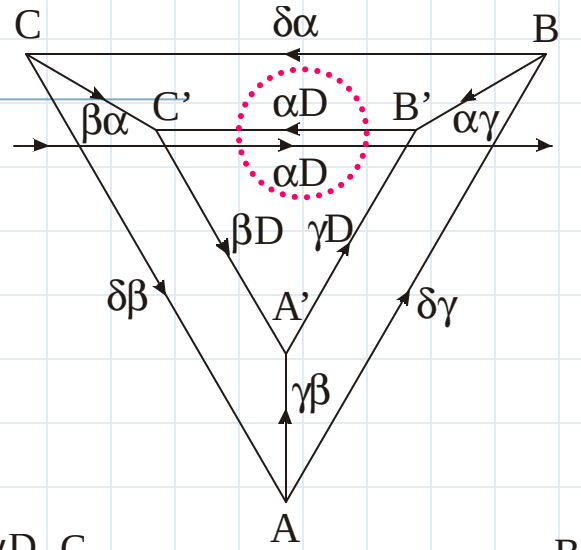
Unlike case at t = 0.7



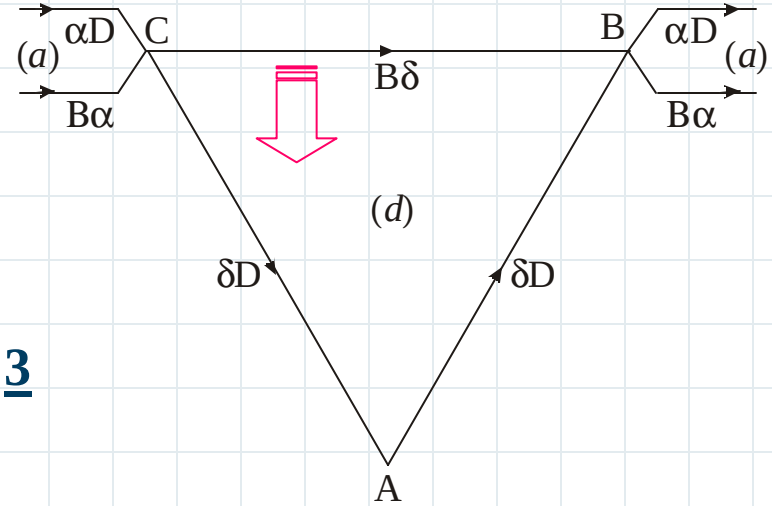
Energy / vacancy in eV

Contour Maps for unlike cases

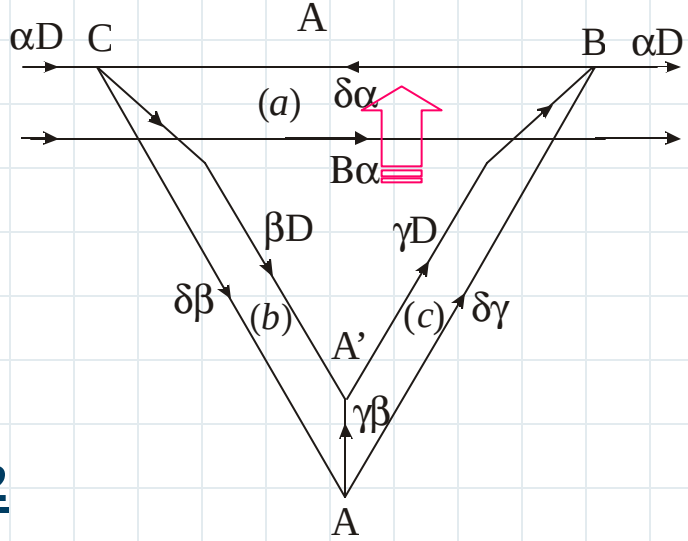
Destruction of SFT by Annihilation



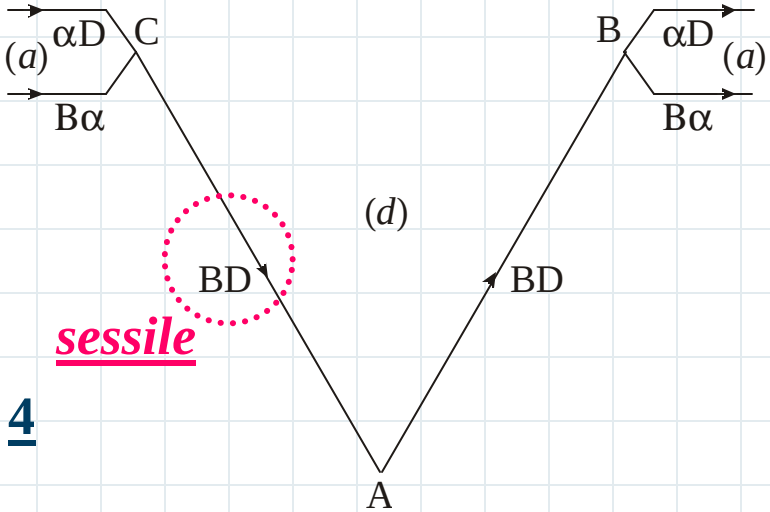
1



3



2

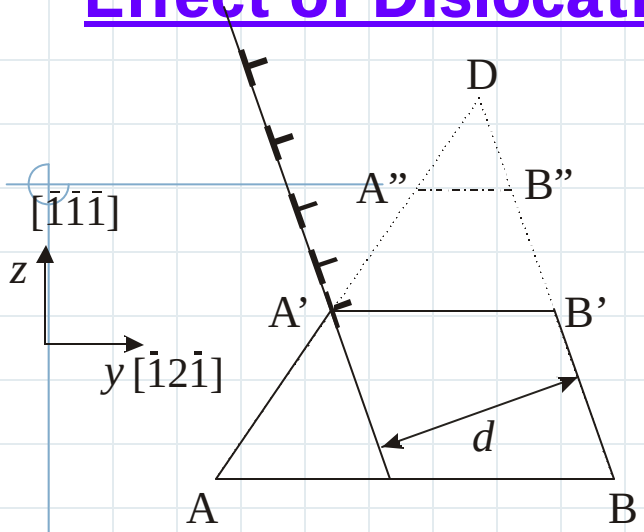


sessile

4

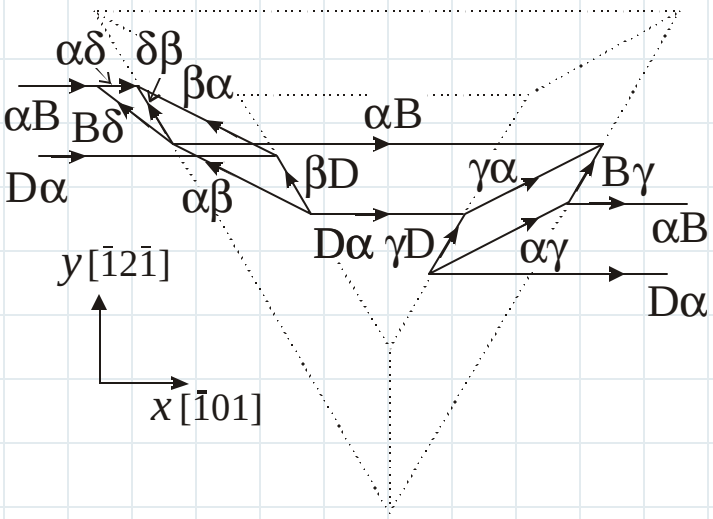
Vacancy Absorption → Superjogs are introduced

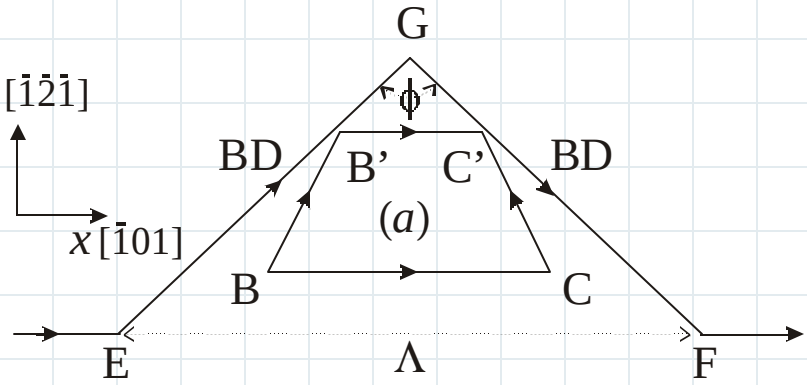
Effect of Dislocation Pile-ups & Core-Reactions (I)



Pile-ups anchored with glissile Shockley partials

Potential jog formation by core-reaction





Bowed dislocation pressing SFT down

- ***Once incident dislocation cut Shockley partials of SFT in truncated part, SFT will collapse by either mechanical work or core-reactions.***

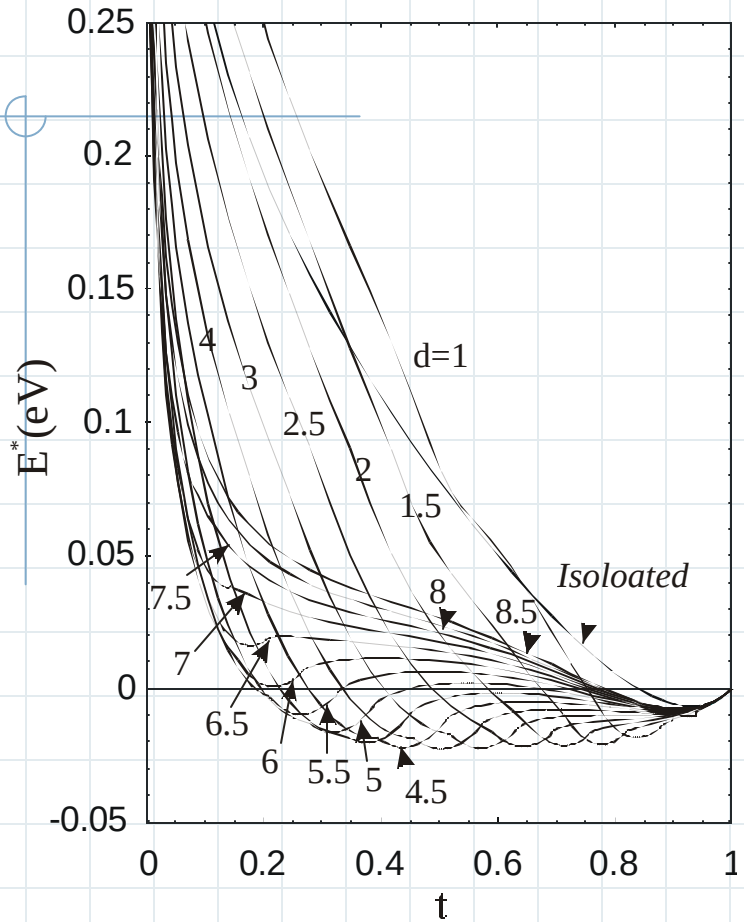
$$\Gamma = -\frac{2\sin^2(f/2)}{\Lambda\cos(f/2)}\frac{\partial E}{\partial f}\bigg|_{f\to f_p}$$

$$E_f = \frac{mb^2\Lambda}{16p(1-n)}\left\{\frac{4-2n+n\cos(2f)}{\cos f}\log\left[\frac{\Lambda}{2(1+\cos f)er}\right]-(4-n)\log\left[\frac{(1+\sec f)^2\Lambda}{16er}\right]\right\}$$

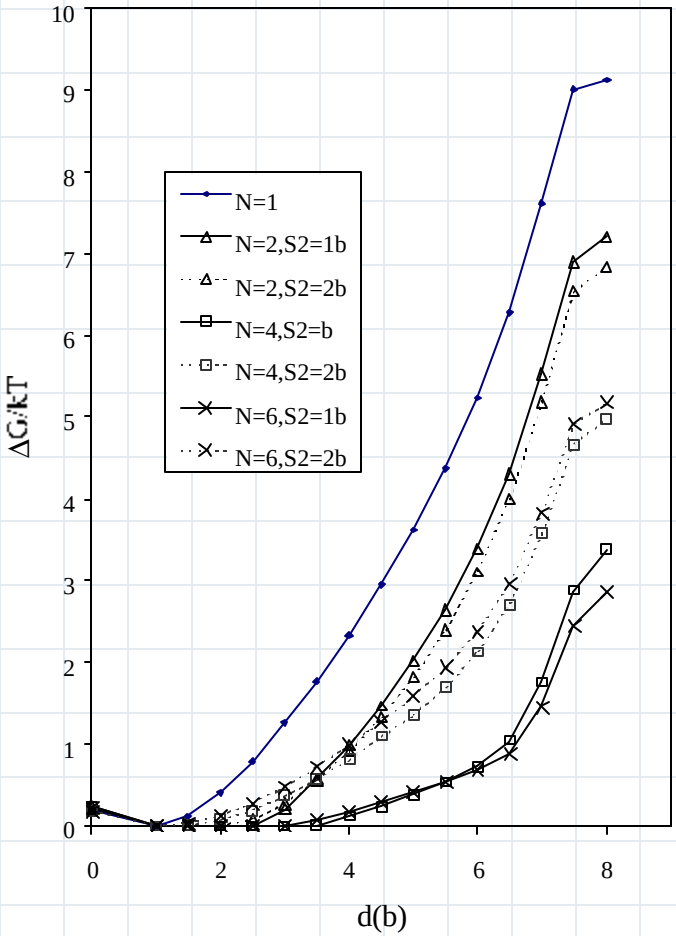
For $f_p = 60°$,
$\Gamma = 610.4$ pN and $F_p = 1.057$ nN,
For $f_p = 80°$,
$\Gamma = 535.0$ pN and $F_p = 819.7$ pN
for $f_p = 100°$,
$\Gamma = 473.2$ pN and $F_p = 608.4$ pN
If the leading dislocation is incident on the two SFT segments, the SFT can hold the dislocation until the exerted force reaches $2F_p = 1.2 \sim 2.1$ nN.

However, the force required to truncate the SFT reaches its maximum at $t = t_0$ just before transformation into FSL, and it is usually comparable to the pinning force of SFT segments except regimes where annihilation or combination between two parallel segments takes place. For instance, $F_c = 3.47$ nN for the isolated case, and in unlike cases, $F_c = 1.99$ nN at $N = 4$, $s_{12} = 1b$ and $P = (0, 4b)$, and $F_c = 1.75$ nN at $N = 4$, $s_{12} = 1b$ and $P = (-b, 6.5b)$.

Effect of Dislocation Pile-ups & Core-Reactions (II)



System energy vs t for 4 alike dislocation pile-ups



Activation energy at various glide plane distance in pile-ups (alike cases)

CRSS for Cases of Weak Obstacles of 2 Different Kinds

Results in the limit of large obstacle dislocation arrays, and in the limit of weak obstacle strengths F1 (F2):

- Obstacle concentration on *pinned dislocation* x1 (x2)

$$x_i = \frac{y_i F_i^3}{y_1 F_1^3 + y_2 F_2^3} \qquad (x_1 + x_2 = 1, \quad y_1 + y_2 = 1)$$

- CRSS (Pythagorean type)

$$t_{tot}^2 = t_1^2 + t_2^2 + O\left[\left(\frac{F_1 - F_2}{F_1 + F_2}\right)^2\right]$$

ref: Koch et al (1986)

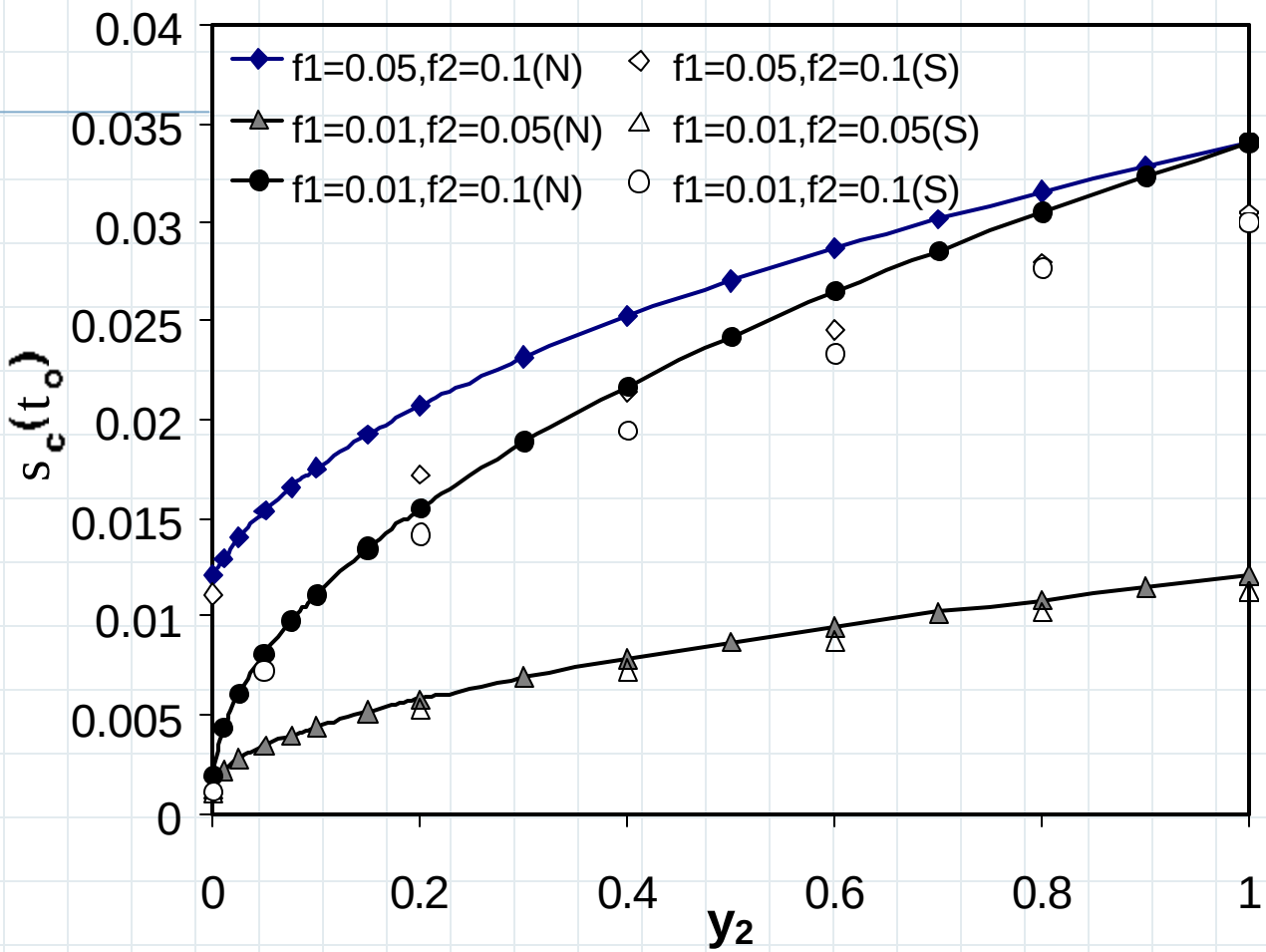
ad hoc superposition

$$t_{tot}^a = t_1^a + t_2^a$$

empirical rule of mixture

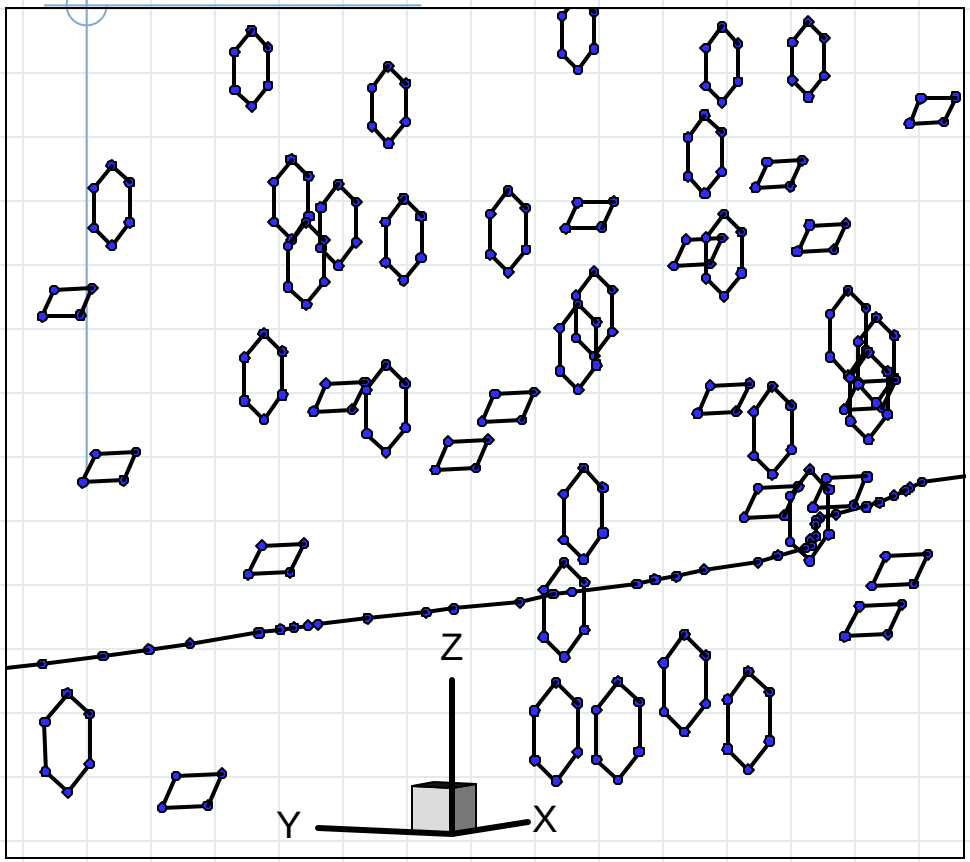
$$t_{tot}^p = y_1^q t_1^p + y_2^q t_2^p$$

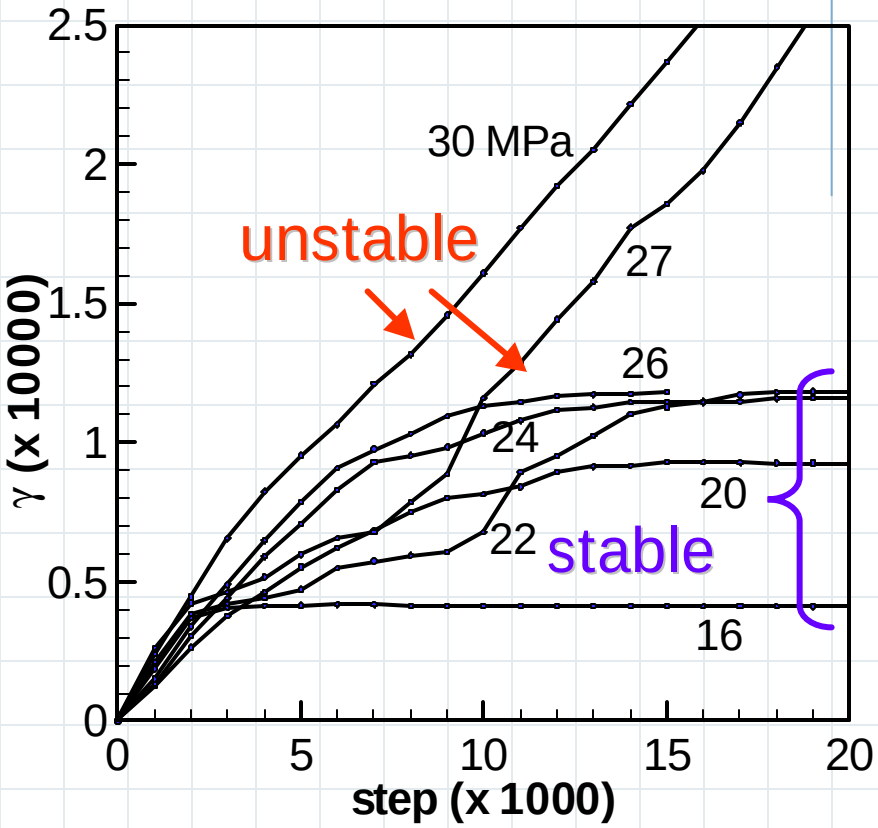
Effect of Concentration on CRSS



- The CRSS is normalized by the Orowan stress. (N) and (S) denote data obtained by numerical calculations in this work and simulation by Altintas (1978), respectively.

DD simulations

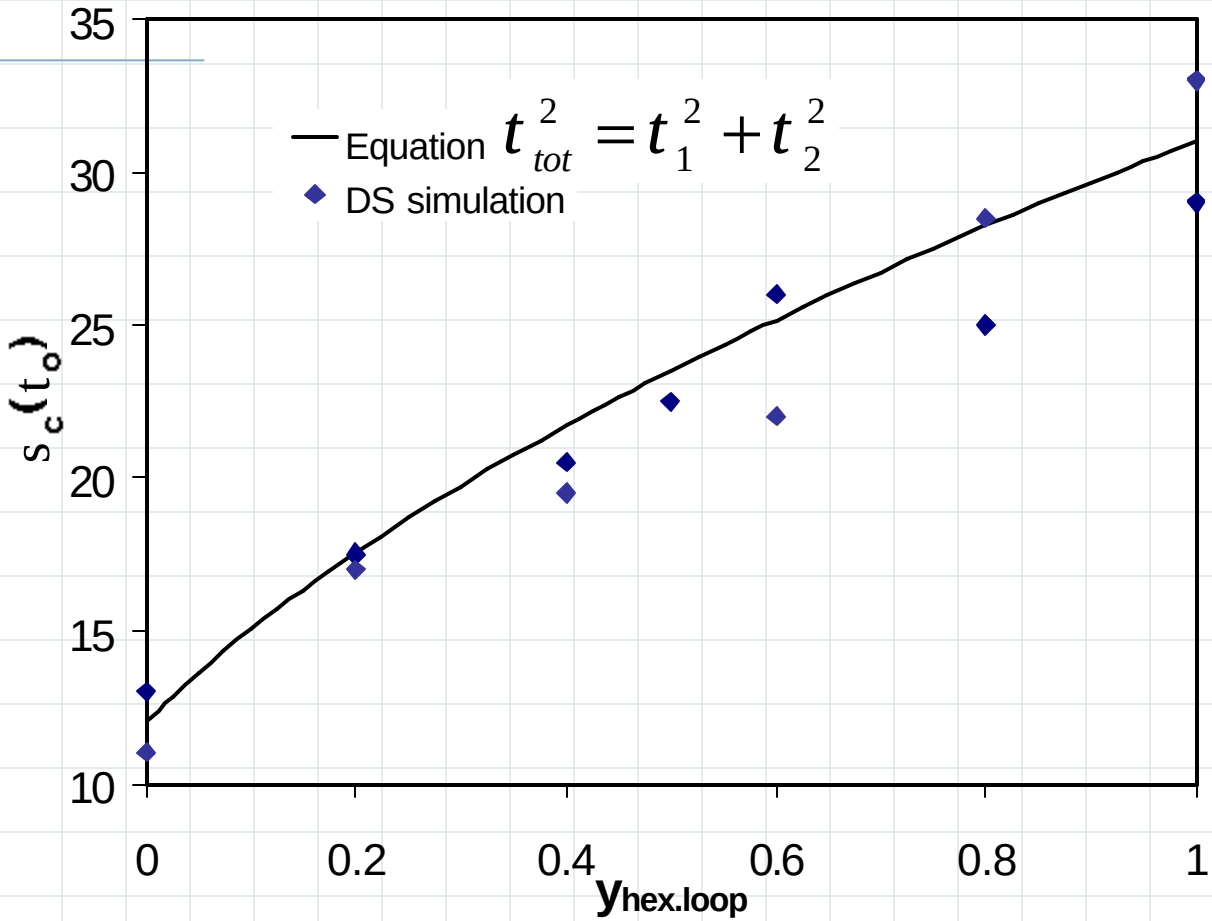




- Snap shot of DD simulation

- DD simulation data for plastic strain vs comp. time step.

CRSS obtained by DD



- CRSS as function of the relative concentration of the hexagonal loops ($y_{hex.loop}$).

Conclusion

• Without incident dislocations, complete and truncated SFTs are more stable than Frank sessile loops or perfect loops, and possess a high activation energy that prevents them from collapsing.

• The energy difference between a slightly truncated SFT and a complete SFT at typically observed sizes is small, a fraction of thermal energy of RT.

•Interaction between a SFT and single dislocation is not strong enough to cause collapse of the SFT at RT except annihilation cases.

•Annihilation by core-reactions and formation of bow-out configuration with super-jogs are proposed.

•The activation energy can be significantly increased by pile-ups and the to transform truncated SFT to Frank sessile loops may be comparable to the thermal energy at room temperature.

•Mechanical work and core-reactions are regarded as main collapse mechanisms after Shockley partials in SFT are intersected by incident dislocations.