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Junction Effects on Work Hardening Rates in Face-Centered Cubic Metals

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Ryan Sills[1,2], Amin Aghaei[2], Nicolas Bertin[2], Wei Cai[2]

[1]Sandia National Laboratories, Livermore, CA

[2]Department of Mechanical Engineering, Stanford University

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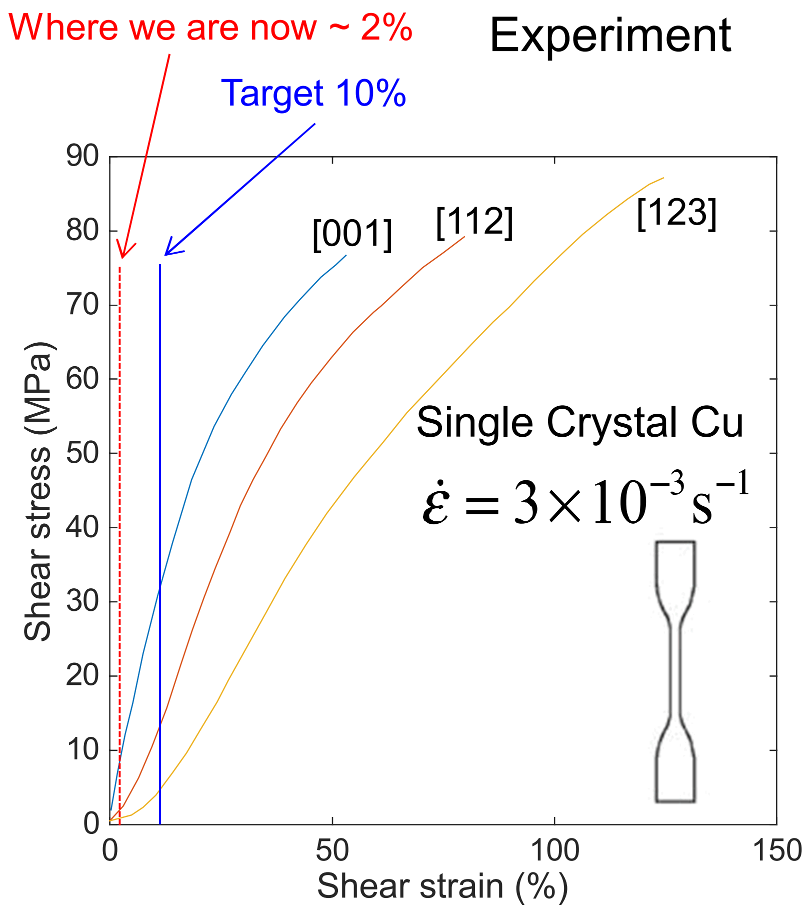
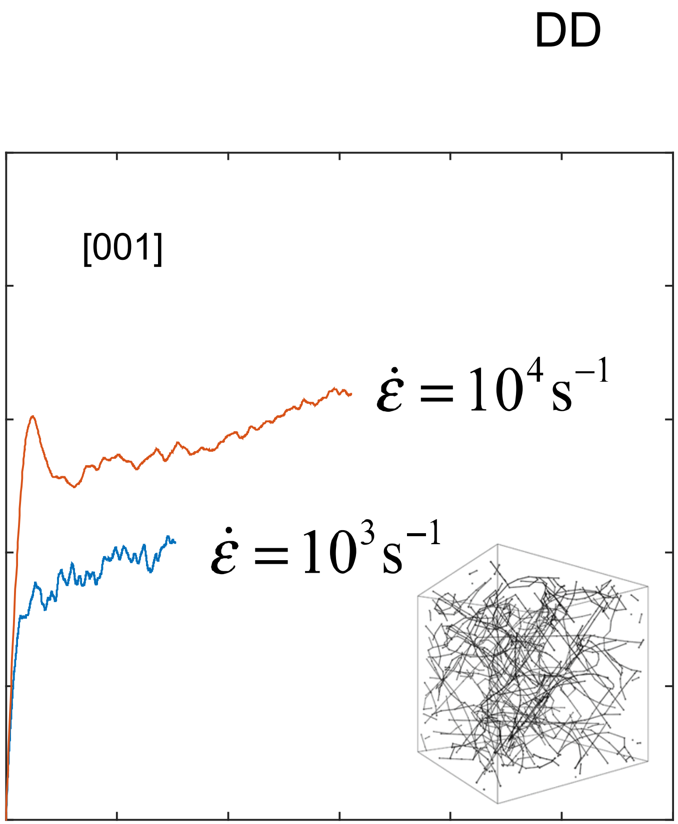
Strain Hardening from Dislocation Dynamics (DD)



T. Takeuchi, Trans. JIM, 16, 629 (1975)



- Strain too low
- Strain rate too high
- Hardening rate looks OK

Outline

1. Efficient Time Integrators for DD

Sub-cycling algorithm

2. Observations from DD Simulations

Strain hardening Rate

Junction effects

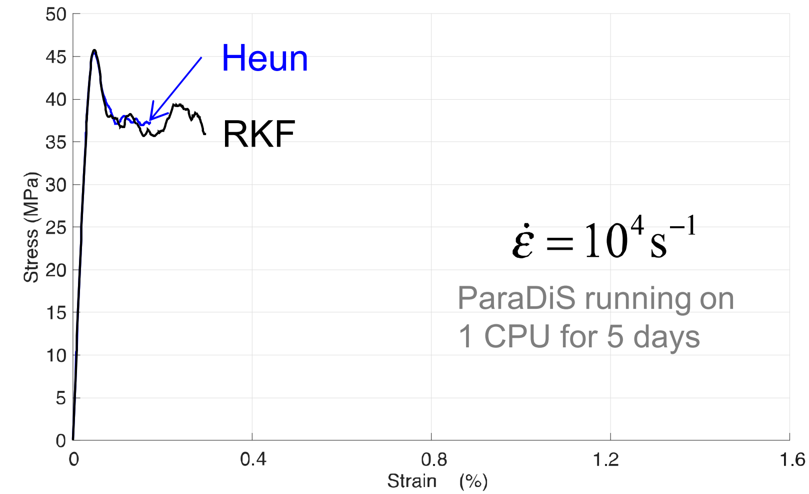
Dislocation length distribution

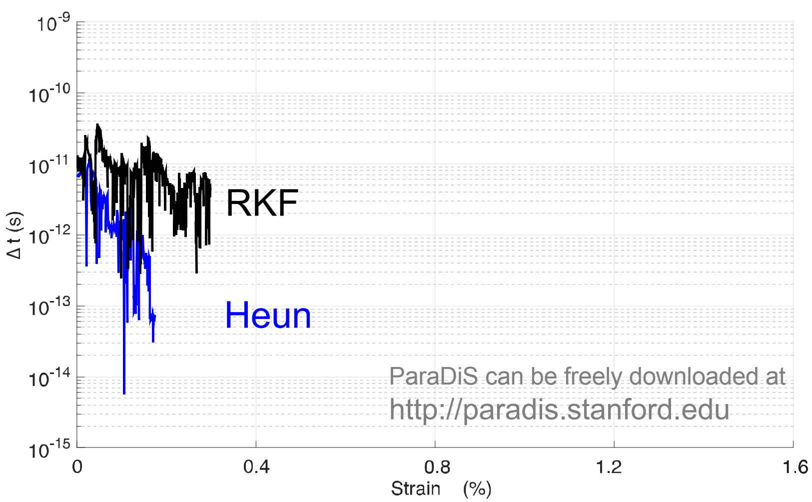
3. Theory / Explanations

“Boltzmann equation” for dislocation segments

Junction effects on strain hardening

Small Time Steps Limit Total Strain





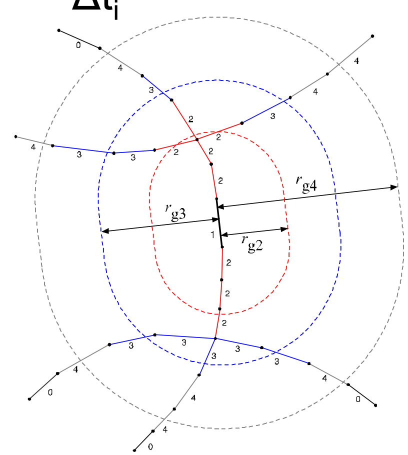
Integrators (Heun or RKF) take very small time steps Δt, because

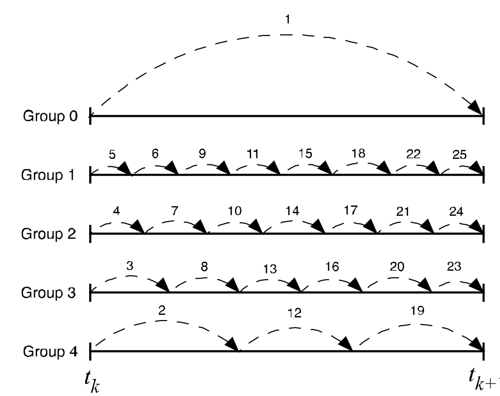
1/r interactions between close-by segments requires small Δt, and

time step Δt is global

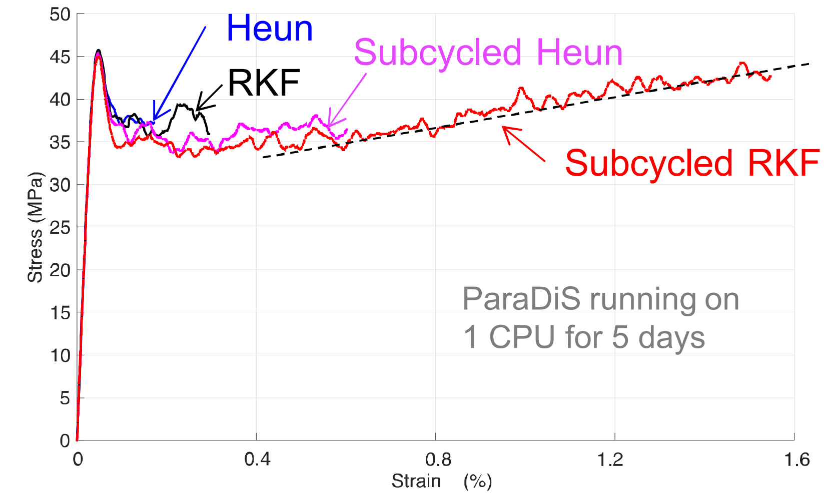
Sub-cycling idea:

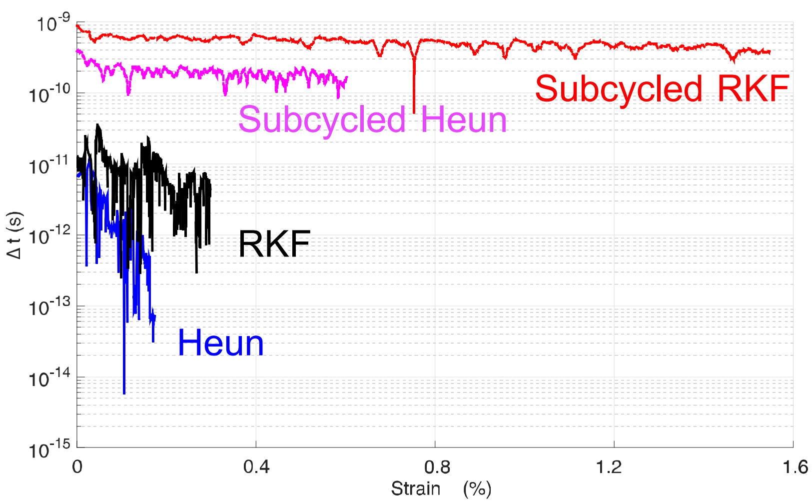
separate pair interactions into groups each with a different time step Δt_i





Efficient Time Integrators for DD



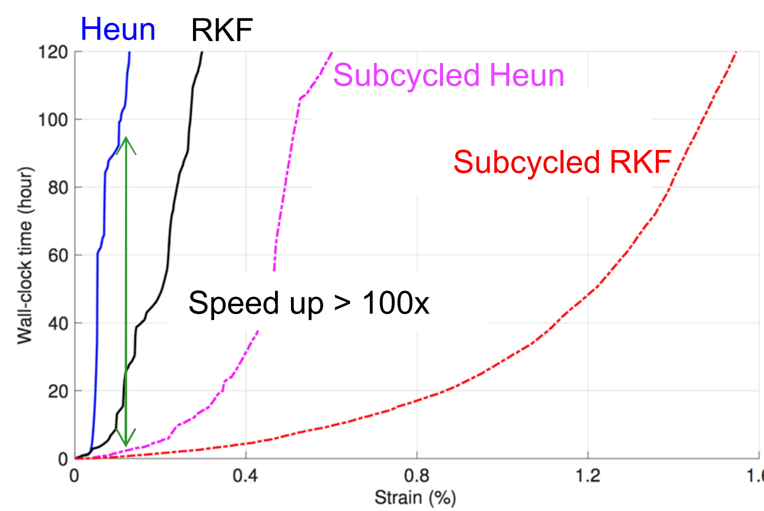


More than 100x increase of global Δt

More than 100x reduction of compute time to the same strain

Less impressive gain in maximum strain

Strain hardening rate can now be extracted



Sills, Cai, MSMSE 24, 025003 (2014).
Sills, Aghaei, Cai, MSMSE 24, 045019 (2016). featured article

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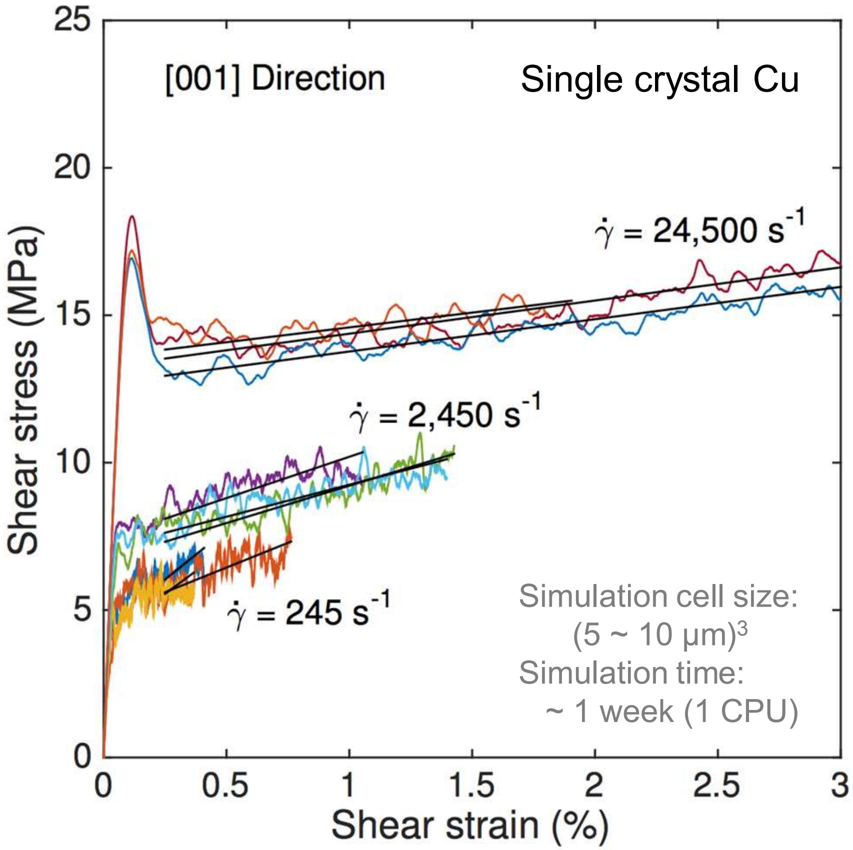
Strain Hardening Rates Predicted by DD

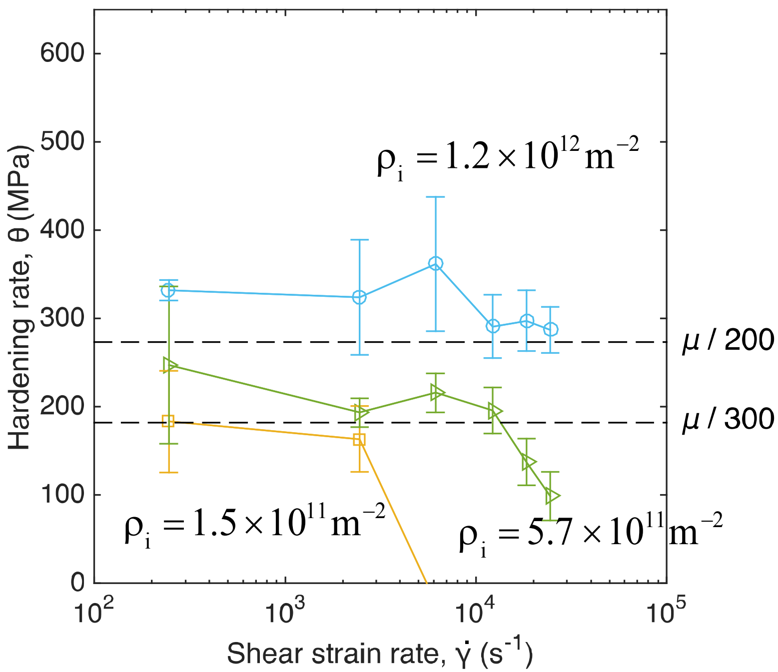


R. B. Sills, PhD Thesis, Stanford University (2016).

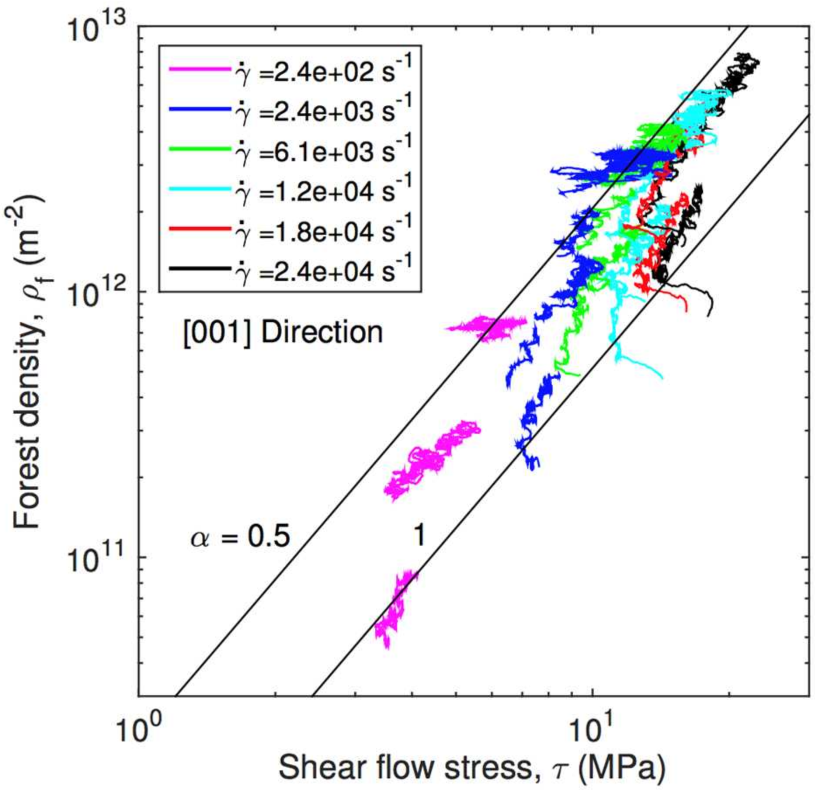
Convergent strain hardening rate Θ below critical strain rate

Critical strain rate decreases with increasing initial dislocation density ρ_i

$\Theta \sim \mu / 200$ consistent with experiment (Stage II)



Hardening Rate vs Dislocation Multiplication Rate



Flow stress vs dislocation density satisfies Taylor relation ($\alpha \approx 0.5$):

$$\tau = \alpha \mu b \sqrt{\rho}$$

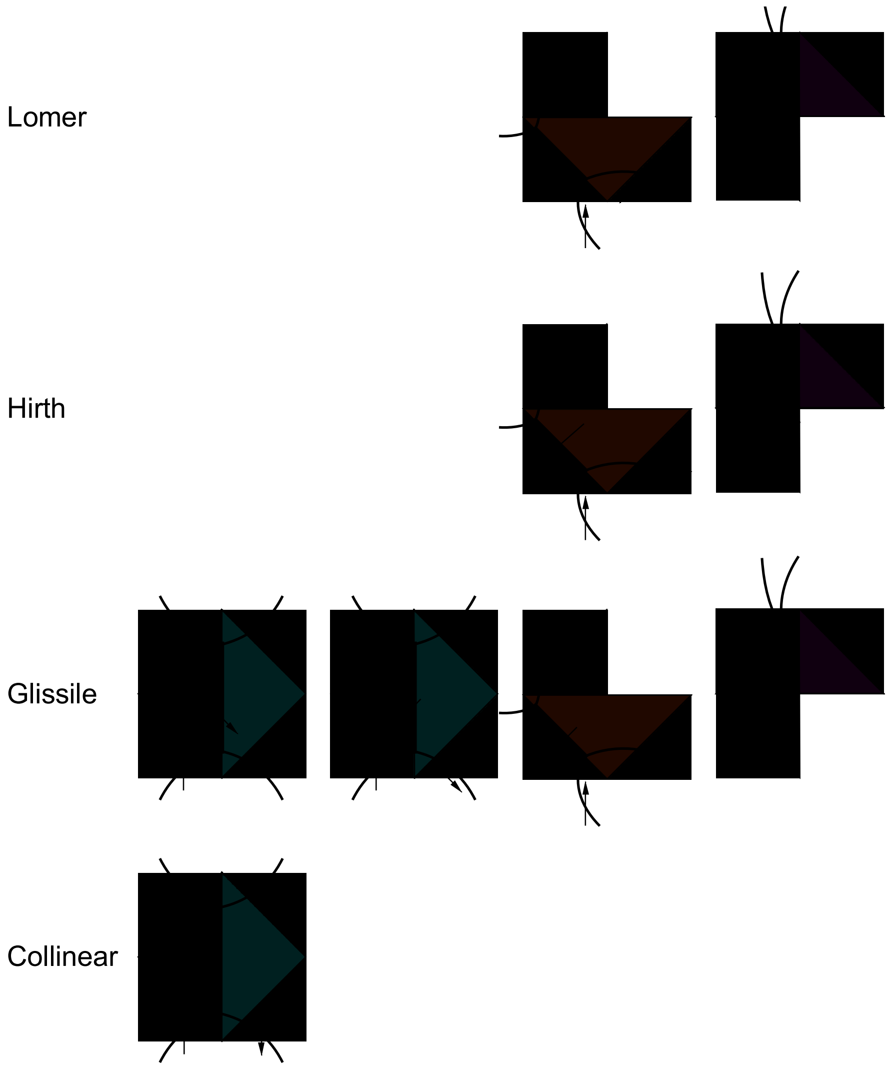
Strain hardening rate is linked to dislocation multiplication rate

$$\Theta = \frac{\dot{\tau}}{\dot{\gamma}} = \frac{1}{2} \alpha \mu b \sqrt{\frac{1}{\rho}} \frac{\dot{\rho}}{\dot{\gamma}}$$

$\dot{\gamma} = \rho b \overline{v}$ is strain rate

$\overline{v}$ is average dislocation velocity

What controls strain hardening rate?



Junctions are believed to be essential for strain hardening?

Four types of junctions in FCC

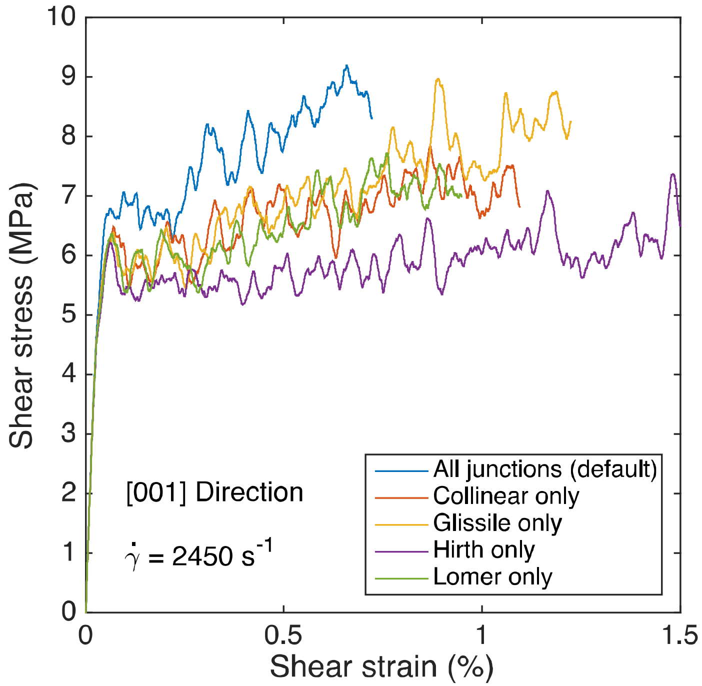
- Lomer
- Collinear
- Glissile
- Hirth

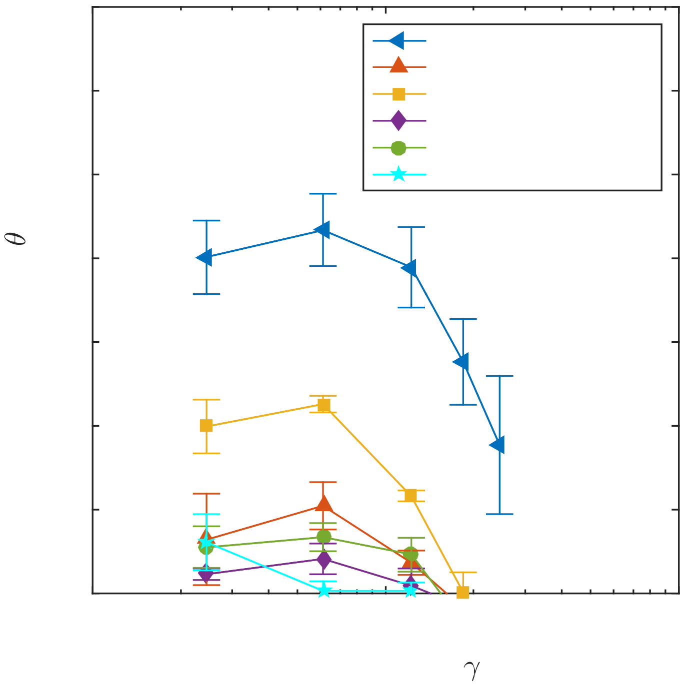
Q: Which junction is most important for strain hardening?

Turn off different junctions in DD (disable node-splitting in ParaDiS)

and see the effect

Hardening Rate with Only One Type of Junction





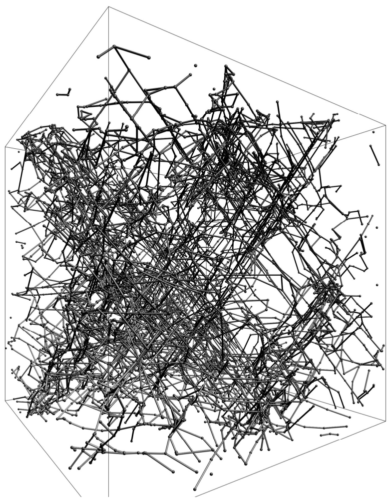
Importance for hardening: Glissile > Collinear ≈ Lomer > Hirth

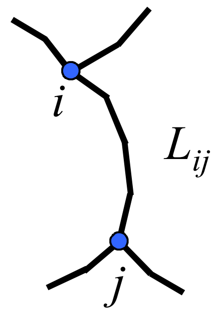
Why?

Collinear junction was ranked highest in strength
(Madec et al. Science 301, 1879, 2003)

Glissile junction makes a dominant contribution to plastic flow
(Stricker & Weygand, Acta Mater 99, 130, 2015)

Dislocation Line Length Distribution





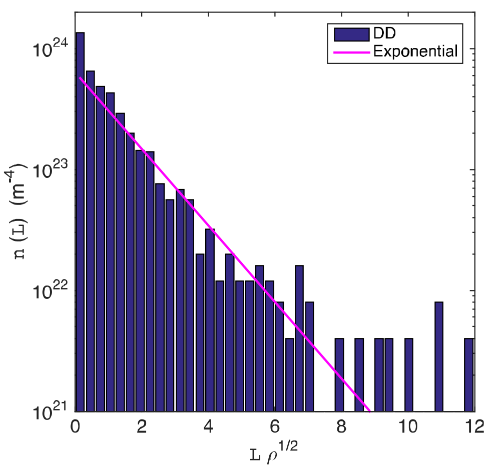
Analyze dislocation microstructure

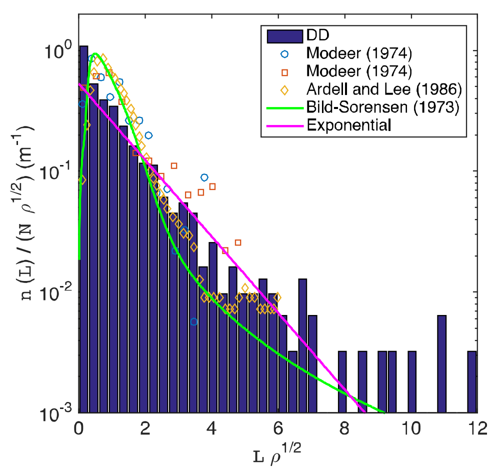
Exponential distribution of segment length

$$n(L) = \varphi\, \rho^2 \exp[-(\varphi\, \rho)^{1/2}\, L]$$

$\rho_f = \varphi\, \rho$ is forest density

ρ is total density, $\varphi \approx 0.53$





all exp't data for unloaded creep microstructures

Total number of segments

$$N = \int_0^\infty n(L)\, dL = \sqrt{\phi}\, \rho^{3/2}$$

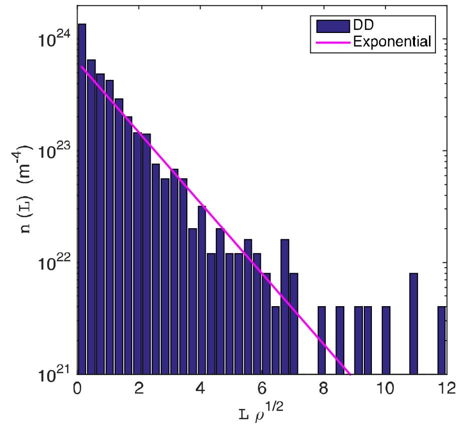
Average segment length

$$\bar{L} = \frac{N}{\rho} = \frac{1}{\sqrt{\phi\, \rho}}$$

Questions:

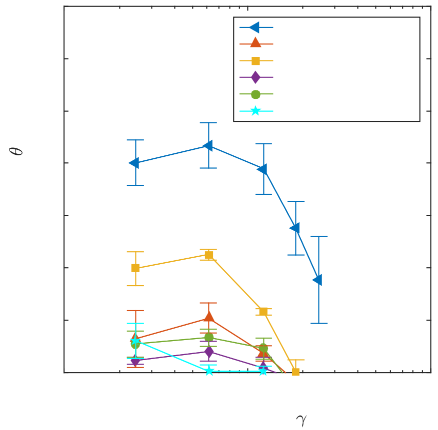
What causes this particular exponential distribution?

$$n(L) = \varphi\, \rho^2 \exp[-(\varphi\, \rho)^{1/2} L]$$



Can this help us explain different junction's contribution in strain hardening?

Glissile > Collinear ≈ Lomer > Hirth



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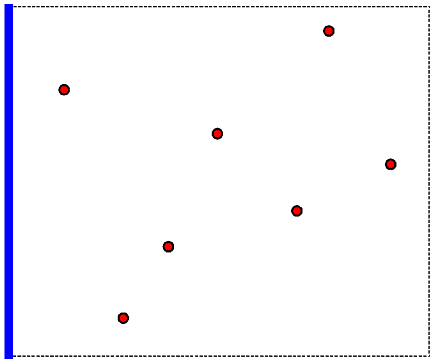
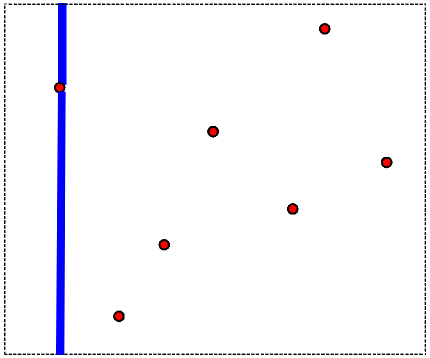
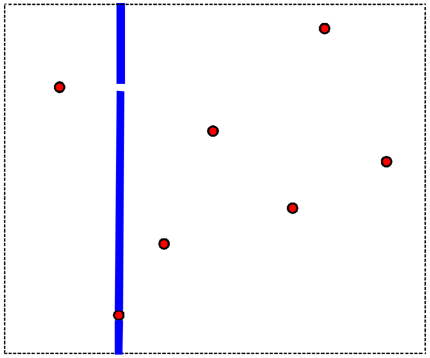
Poisson Process in 1D

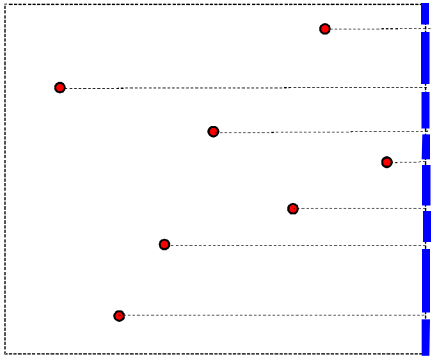


Assume:
1. random (uniformly) distribution of points
2. segment move over some distance
3. segment cut into two when intersecting a point

Result:
Exponential distribution of segment lengths







"Boltzmann-Equation" for Dislocation Line Segments

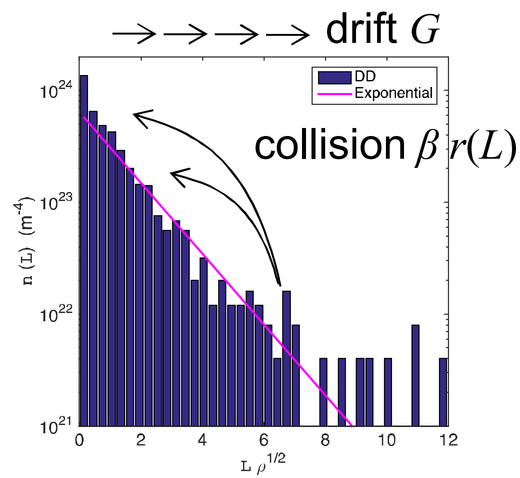
Goal: the simplest model for the evolution of segment length distribution that captures the exponential distribution

$$\frac{\partial}{\partial t} n(L,t) = \dot{n}_{\mathrm{drift}}(L) + \dot{n}_{\mathrm{coll}}(L)$$

$$\dot{n}_{\mathrm{drift}}(L) = -\frac{\partial}{\partial t}\big(n(L)\cdot G\big)$$

$$\dot{n}_{\mathrm{coll}}(L) = -\beta\, r(L)\, n(L) + 2\int_L^{\infty} \frac{1}{l}\,\beta\, r(l)\, n(l)\, dl$$

$$r(L) = \phi\, \rho\, \bar{v}\, L$$ intersection rate of segment L



Input parameters: G segment length growth rate

β probability of collision → stable junction

Link length evolution equation proposed in:
Lagneborg and Forsen, Acta Met. 21 (1973). Ardell and Przystupa, Mech. Mater. 3 (1984).

Requirement for the Exponential Distribution

Reproduces the exponential distribution $n(L) = \varphi\,\rho^2 \exp[-(\varphi\,\rho)^{1/2} L]$ if

$$G = 2\beta\,\bar{v}$$

segment length growth rate

junction formation probability

$\bar{v}$: average dislocation velocity

physical interpretation:

a dislocation of length L forms a stable junction →
length of the dislocation network is allowed to increase by L.
similar idea was proposed in Devincre et al. Science 320, 1745 (2008)

Strain hardening rate:

$$\Theta = \frac{\dot{\tau}}{\dot{\gamma}} = \frac{1}{2}\alpha\,\mu\,b\sqrt{\frac{1}{\rho}}\,\frac{\dot{\rho}}{\dot{\gamma}} = \frac{1}{2}\alpha\,\mu\,b\sqrt{\frac{1}{\rho}}\,\frac{G\,N}{\rho\,b\,\bar{v}} = \boxed{\alpha\,\mu\sqrt{\phi}\,\beta}$$

$$\Theta \approx \frac{\mu}{200}\,,\ \alpha \approx 0.5,\ \varphi \approx 0.53$$

$\beta \approx 0.014$ i.e. only 1.4% of collisions leads to stable junctions → dislocation storage

Junction Contribution to Strain Hardening Rate

Junction Type	Intersection Fraction (I) from DD	Formation Fraction (F) from DD	(I x F)	
Collinear	0.07 ± 0.005	0.52 ± 0.02	0.036	
Glissile	0.37 ± 0.015	0.30 ± 0.01	0.11	# of slip systems
Hirth	0.35 ± 0.03	0.02 ± 0.01	0.007	very unstable
Lomer	0.21 ± 0.01	0.31 ± 0.01	0.065	

Junction contributes to strain hardening through

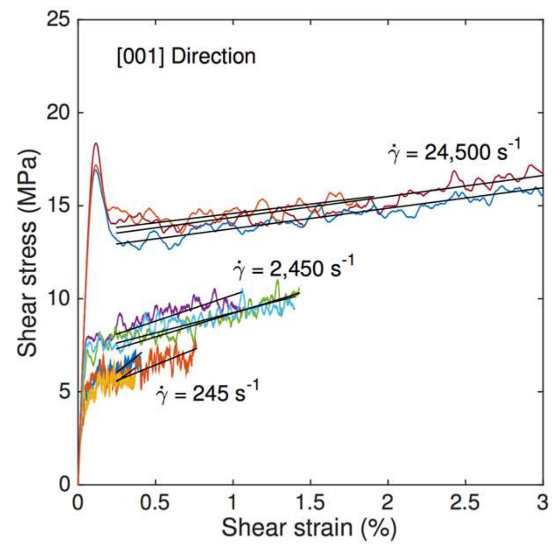
stable junction formation probability: $\beta = S \sum_{i=\mathrm{C,G,H,L}} I_i F_i$

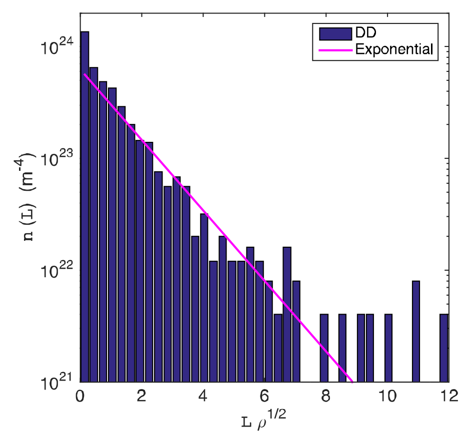
storage fraction: $S = 0.066$,

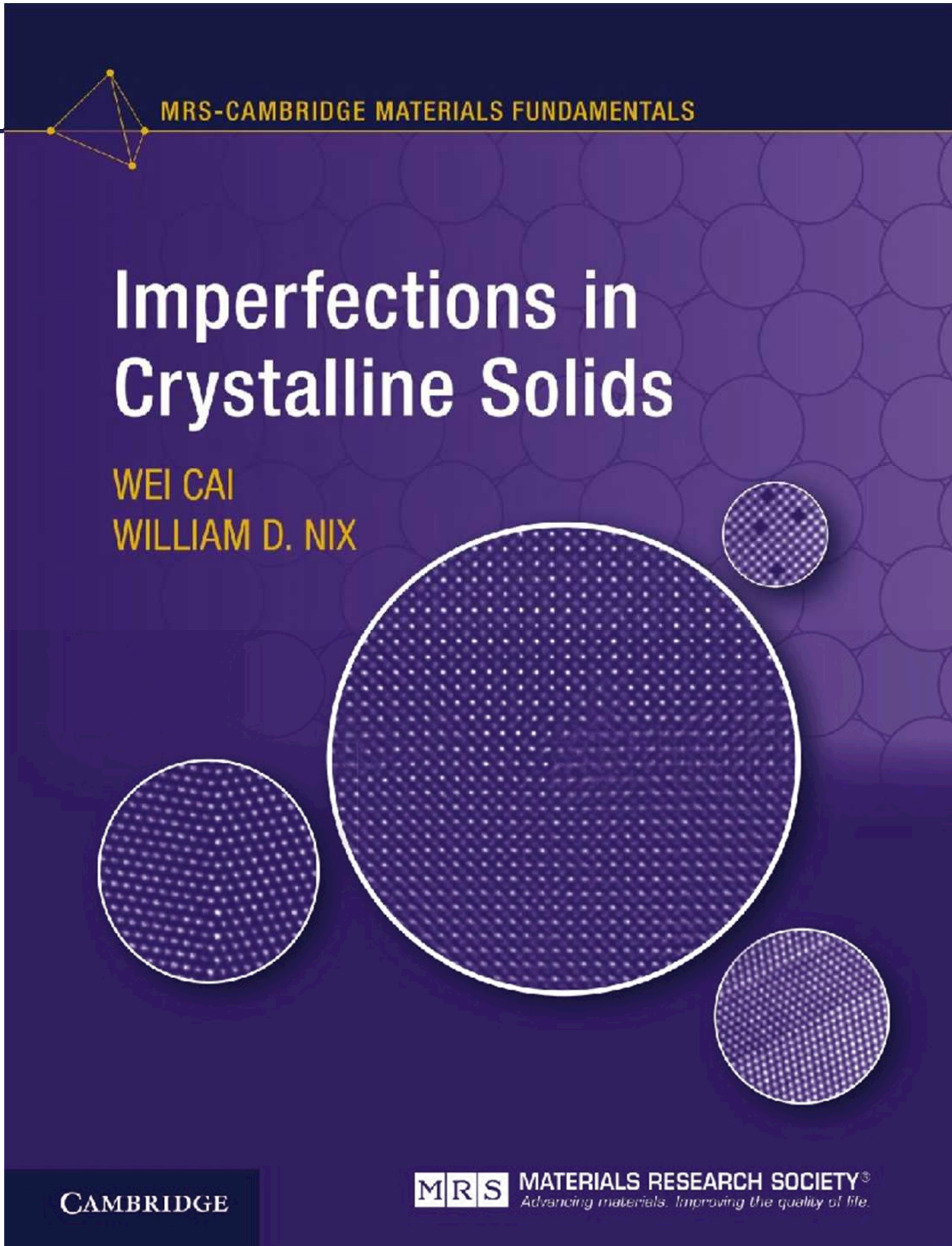
so that $\beta \approx 0.014$, strain hardening rate $\Theta = \alpha\, \mu \sqrt{\phi}\, \beta \approx \mu / 200$

Summary

- Hardening rate can now be predicted (rapidly and repeatedly) by DD
- Importance for junctions in hardening: Glissile > Collinear ≈ Lomer > Hirth
- Dislocation segment length is exponentially distributed ([001] loading)
- Exponential distribution can be explained by a drift-collision equation if dislocation storage rate is proportional to junction formation rate
- Glissile junction formation rate is highest because of high collision rate and “good enough” stability.







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Point defects

Dislocations

Grain boundaries

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if you teach a crystal defects course

Backup Slides

Subcycling Performance in Parallel

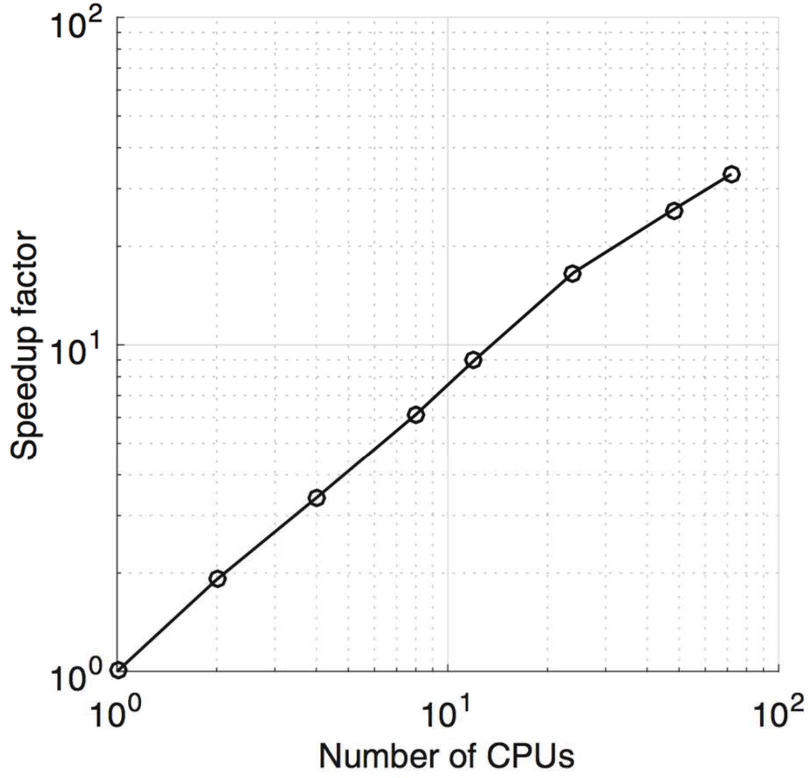
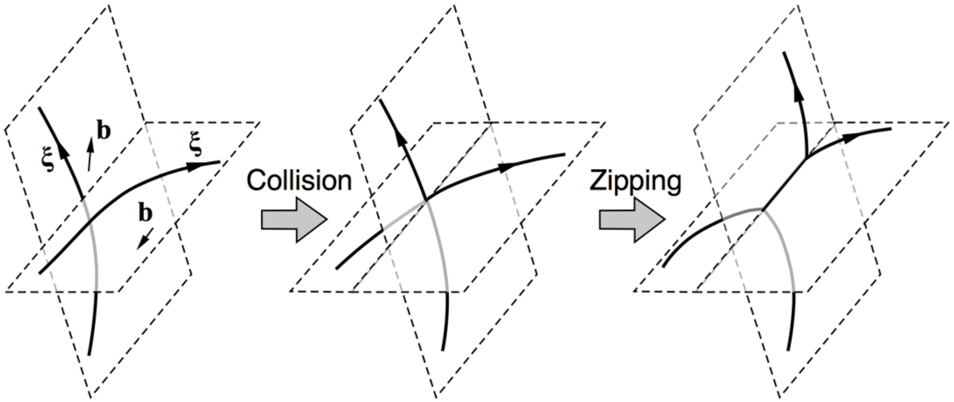


Figure 8. Parallel scalability of the RKF subcycling integrator, showing the speedup factor relative to serial for a configuration at 1.5% strain containing about 27 500 nodes.

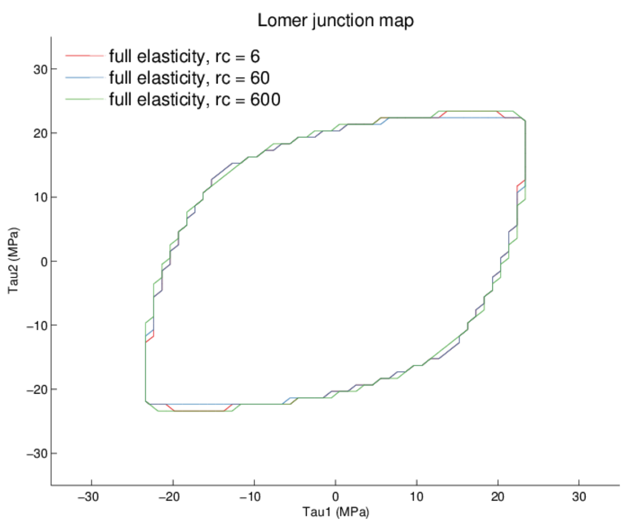
Turn off specific types of junctions in DD

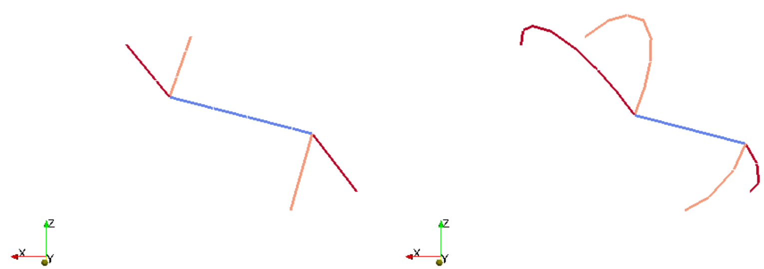


Disable Node-splitting that leads to (specific type of) junction formation

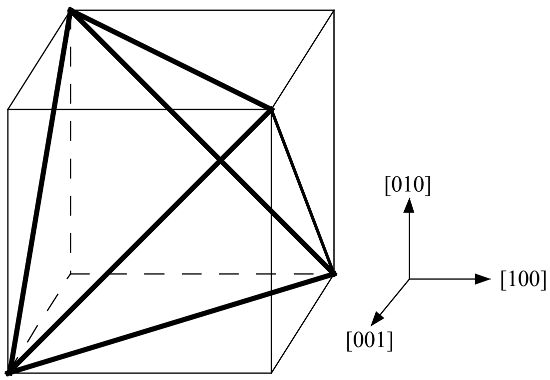
Increase core radius r_c to prevent junction formation by segment reaction

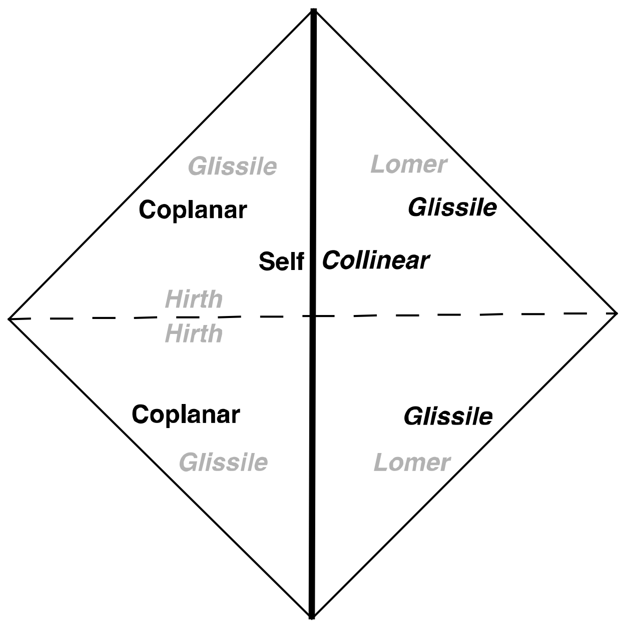
Junction strength (stress map) unchanged by increasing r_c





What controls strain hardening rate?





Which junction?

Harding is different from strength

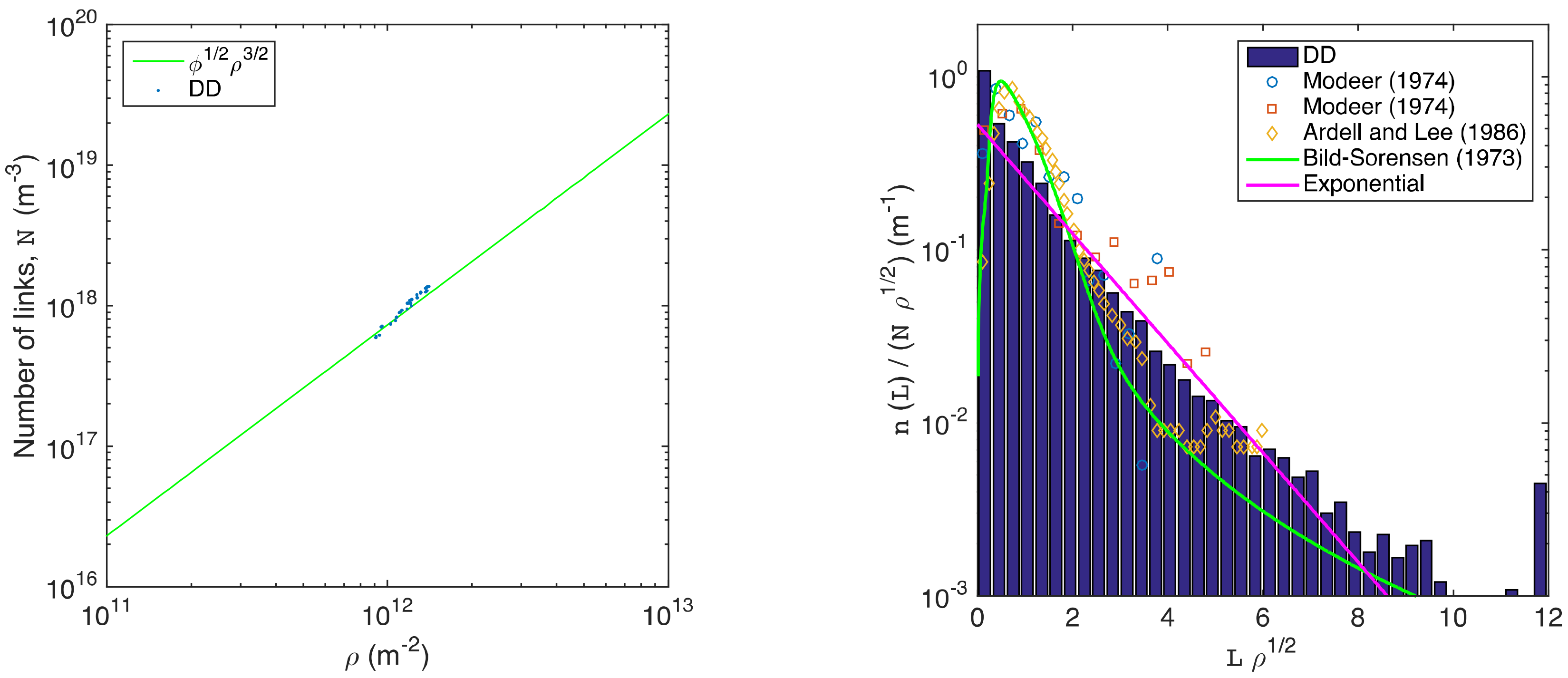
Four types of junctions

- Lomer
- Collinear
- Glissile
- Hirth

DD Evidence

Evidence for

$$N = \varphi^{1/2} \rho^{3/2}$$



"Boltzmann-Equation" for Dislocation Line Segments

Goal: the simplest model for the evolution of segment length distribution that captures the exponential distribution

$$\frac{\partial}{\partial t} n(L,t) = \dot{n}_{\text{drift}}(L) + \dot{n}_{\text{coll}}(L)$$

similar to Boltzmann's equation for position-momentum distribution of molecules in gas

drift term: $$\dot{n}_{\text{drift}}(L) = -\frac{\partial}{\partial t}\left(n(L) \cdot G\right)$$

$G = \dot{\rho} / N$ — rate of segment lengthening independent of L (for simplicity)

collision term: $$\dot{n}_{\text{coll}}(L) = -\beta\, r(L)\, n(L) + 2\int_L^\infty \frac{1}{l} \beta\, r(l)\, n(l)\, dl$$

$r(L) = \phi\, \rho\, \bar{v}\, L$ — rate of a segment in collision proportional to L (intuitive)

β — probability of collision → stable junction independent of L (for simplicity)

Requirement for the Exponential Distribution

PDE

$$\frac{\partial}{\partial t} n(L,t) = \dot{n}_{\text{drift}}(L) + \dot{n}_{\text{coll}}(L)$$

$$\dot{n}_{\text{drift}}(L) = -\frac{\partial}{\partial t}\left(n(L)\cdot G\right)$$

$$\dot{n}_{\text{coll}}(L) = -\beta\, r(L)\, n(L) + 2\int_L^\infty \frac{1}{l}\beta\, r(l)\, n(l)\, dl$$

$$r(L) = \phi\, \rho\, \bar{v}\, L$$

reproduces the exponential distribution $n(L) = \varphi\, \rho^2 \exp[-(\varphi\, \rho)^{1/2} L]$ **if**

$$G = 2\beta\, \bar{v}$$

segment length growth rate

junction formation probability

analogous to Einstein relation $D = \mu\, k_B T$

Strain hardening rate:

$$\Theta = \frac{\dot{\tau}}{\dot{\gamma}} = \frac{1}{2}\alpha\, \mu\, b\sqrt{\frac{1}{\rho}}\,\frac{\dot{\rho}}{\dot{\gamma}} = \frac{1}{2}\alpha\, \mu\, b\sqrt{\frac{1}{\rho}}\,\frac{G\, N}{\rho\, b\, \bar{v}} = \boxed{\alpha\, \mu\sqrt{\phi}\, \beta}$$

Junction Formation and Strain Hardening Rate

What is the meaning of $G = 2\beta\,\overline{v}$?

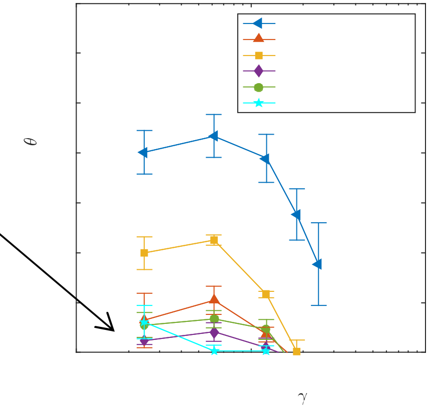
segment length growth rate → $\overline{v}$

junction formation probability → β

a physical interpretation:

a dislocation of length L forms a stable junction → length of the dislocation network is allowed to increase by L.

strong DD evidence that: no junction formation → no multiplication → no strain hardening



so it seems reasonable that junction formation event → dislocation storage of length L

$$\Theta = \alpha\,\mu\sqrt{\phi}\,\beta \qquad \Theta \approx \frac{\mu}{200}, \ \alpha \approx 0.5, \ \varphi \approx 0.53$$

$\beta \approx 0.014$ i.e. only 1.4% of collisions leads to stable junctions → dislocation storage

Junction Contribution to Strain Hardening Rate

Junction Type	Intersection Fraction (I)	Formation Fraction (F)	Estimated Storage Fraction (S)	Contribution to β (I x F x S)
Collinear	0.07 ± 0.005	0.52 ± 0.02	*0.066*	0.0024
Glissile	0.37 ± 0.015	0.30 ± 0.01	*0.066*	0.0073
Hirth	0.35 ± 0.03	0.02 ± 0.01	0	0
Lomer	0.21 ± 0.01	0.31 ± 0.01	*0.066*	0.0043
(Total)	1.0			0.014

Due to the number of slip systems

From DD, we observe:

1. intersection fraction (I) for each junction type
2. fraction (F) of each intersection leading to a junction
3. all Hirth junctions destroyed soon after they are formed ($S = 0$)

Assumption:

storage fractions (S) for Collinear / Glissile / Lomer are the same

So that $\beta \approx 0.014$, and strain hardening rate $\Theta = \alpha\, \mu \sqrt{\phi}\, \beta \approx \mu / 200$

No Junction, No Multiplication

Similar to Devincre et al. Science 320, 1745 (2008)

Intersection rate x a fraction forms junction x adds some length to total density

β ←→p0\sqrt{a_bar} = 0.117*0.35 = 0.04

Junction form leads to length increase
??L ←→ l_i_bar