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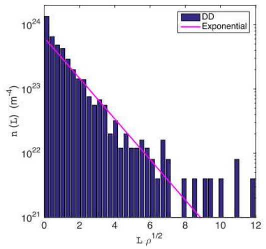
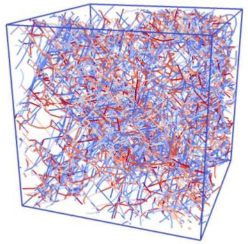
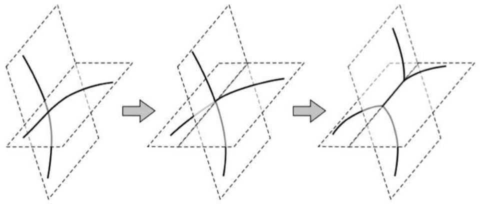
Dislocation Network Evolution and Strain Hardening







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Relating microstructure to mechanical properties

A key goal of mesoscale modeling is to relate microstructure to mechanical properties

The prime example is the Taylor relation

Microstructural variable

Mechanical property → $$\tau = \alpha \mu b \sqrt{\rho}$$

But how does dislocation density ρ evolve with strain γ ? This controls the hardening rate via:

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

Discrete dislocation dynamics (DDD) is a tool that can link microstructure with properties

Dislocation Properties
- Junctions
- Cross-slip
- Climb rate
- …

→

Microstructure
- Dislocation networks
- Patterning
- …

→

Mechanical Properties
- Yield strength
- Hardening rate
- Creep rate
- …

Discrete dislocation dynamics simulations

Single crystalline Cu

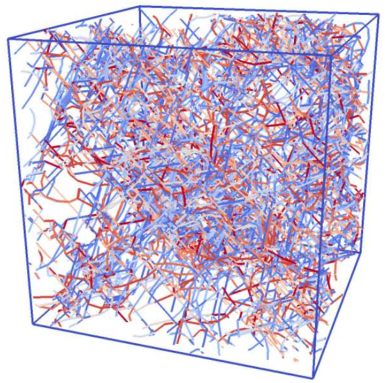
15 μm box with periodic boundary conditions

Initial dislocation densities ~ 10^{12} m^{-2}
- Relaxed straight lines, no pinned sources

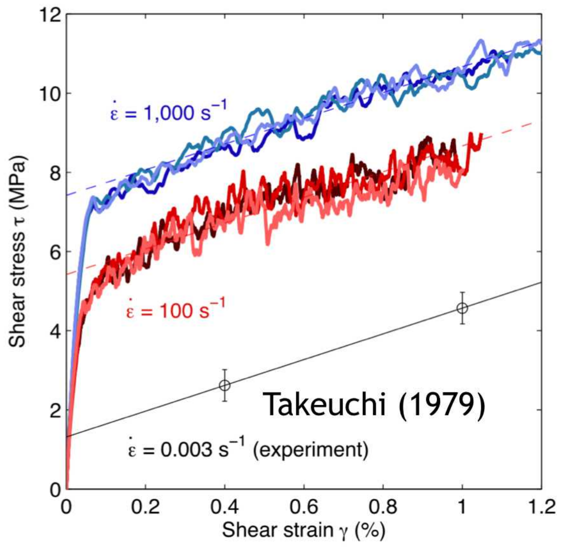
Strictly enforced glide planes
- No cross-slip

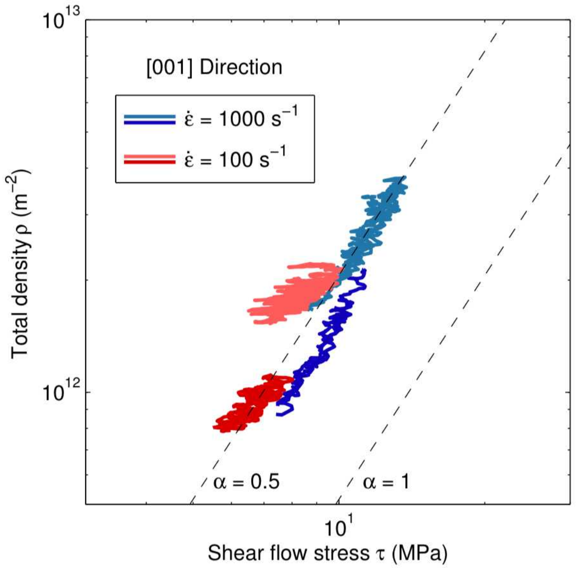
New subcycling-based time integrator with GPU implementation
- Achieve 1% shear strain in ~1 day on 1 GPU, compared with >30 days on >500 CPUs

DDD simulations of [001] loading reproduce quasi-static hardening rate and obey Taylor relation



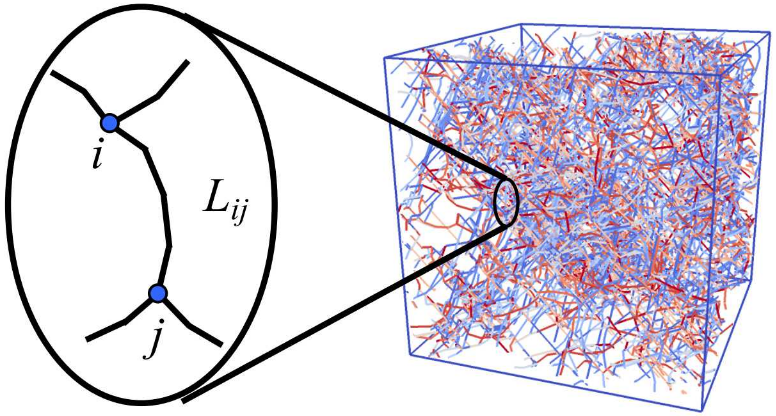
Dislocation configuration at 0.87% shear strain





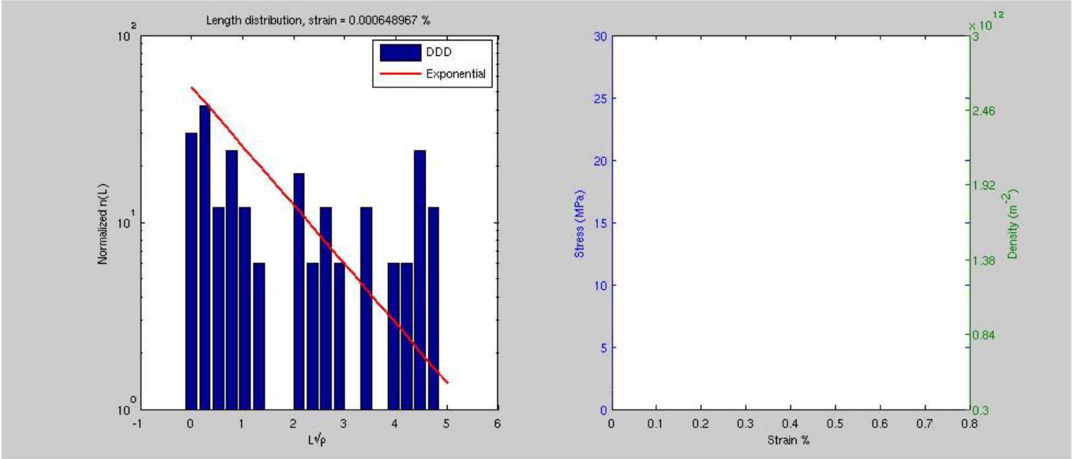
*Collaboration underway with K. T. Ramesh at JHU to perform high strain rate experiments on Cu single crystals

Link length distribution



A number of theorist have proposed that the *link length distribution* is an important feature of the dislocation network

- Lagneborg and Forsen, Acta Met., 1973; Gasca-Neri and Nix, Acta Met., 1974; Ardell and Przystuda, Mech. Mater., 1984



Define distribution function $n(L)$ such that

$$N = \int_0^\infty n(L)dL$$ Number density of links

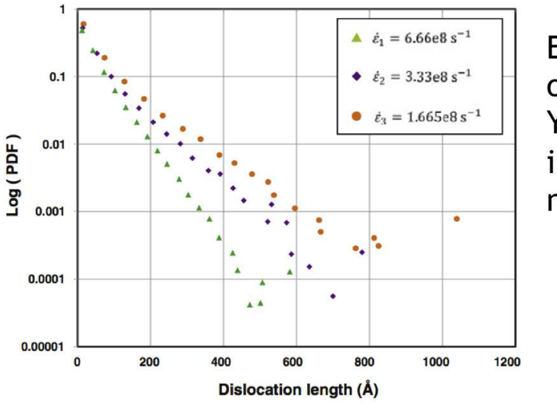
$$\rho = \int_0^\infty Ln(L)dL$$ Dislocation density

Our simulations show that to a good approximation:

$$n(L) = \phi\rho^2 \exp\left(-\sqrt{\phi\rho}L\right)$$

where

$$\bar{L} \equiv \frac{\rho}{N} = \frac{1}{\sqrt{\phi\rho}}$$ Average link length



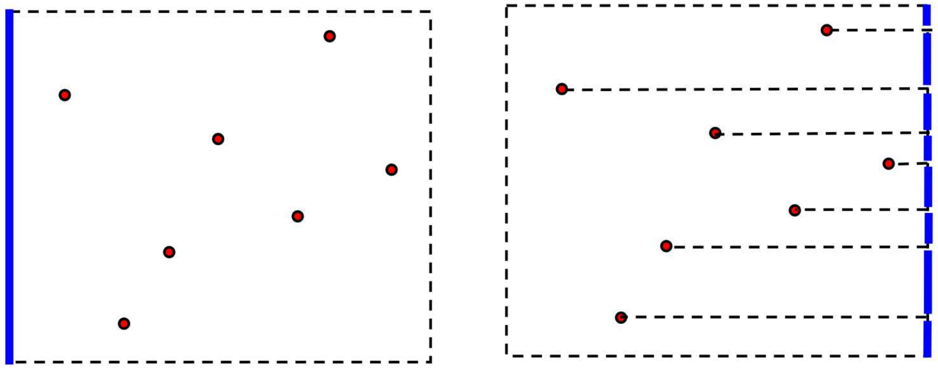
(b) $D = 150$ nm

Exponential length dependence observed by Voyiadjis and Yaghoobi (Scripta Mater., 2017) in MD simulation of Ni nanopillar compression

Origin and consequence of the exponential distribution

Exponential distributions are hallmarks of 1D Poisson point processes

- This means junction formation is spatially random



So what… let's assume that:

$$\dot{N} = 2\beta\rho_f\rho\bar{v} = \frac{2\beta\rho_f}{b}\dot{\gamma}$$

Stable junction formation probability

Forest density $\rho_f = f\rho$

The exponential distribution says that:

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

Combining these together reveals that:

$$\dot{\rho} = \frac{4\beta f\dot{\gamma}}{3b\sqrt{\phi}}\sqrt{\rho} - \frac{\dot{\phi}}{3\phi}\rho$$

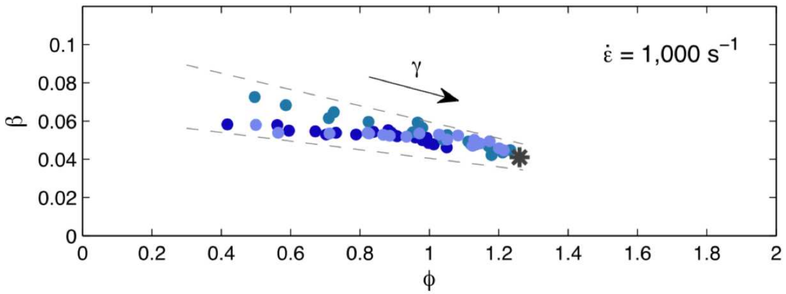
$$\dot{\rho} = K_1\sqrt{\rho} - K_2\rho$$

*Interesting aside: looks like Kocks-Mecking!

Junction formation controls multiplication and strain hardening

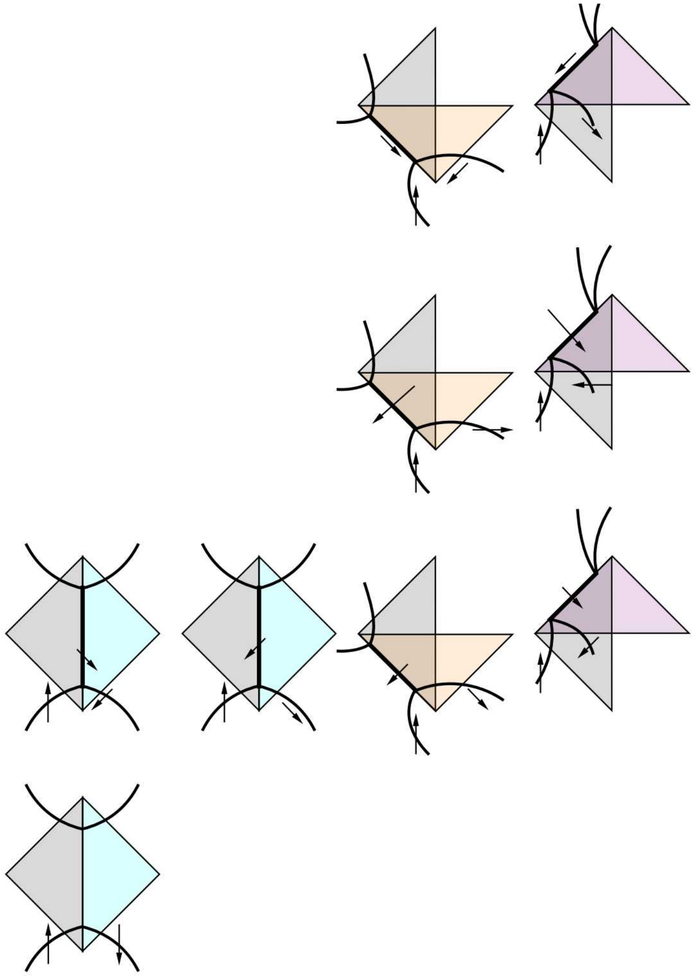
$$\frac{d\tau}{d\gamma} \approx \frac{2\alpha\beta f}{3\sqrt{\phi}}\mu \approx \frac{\mu}{200}$$

$\alpha \approx 0.5, f \approx 0.45, \beta \approx 0.042$



$\beta \approx 0.042$ i.e. only 4.2% of collisions leads to stable junctions → dislocation storage

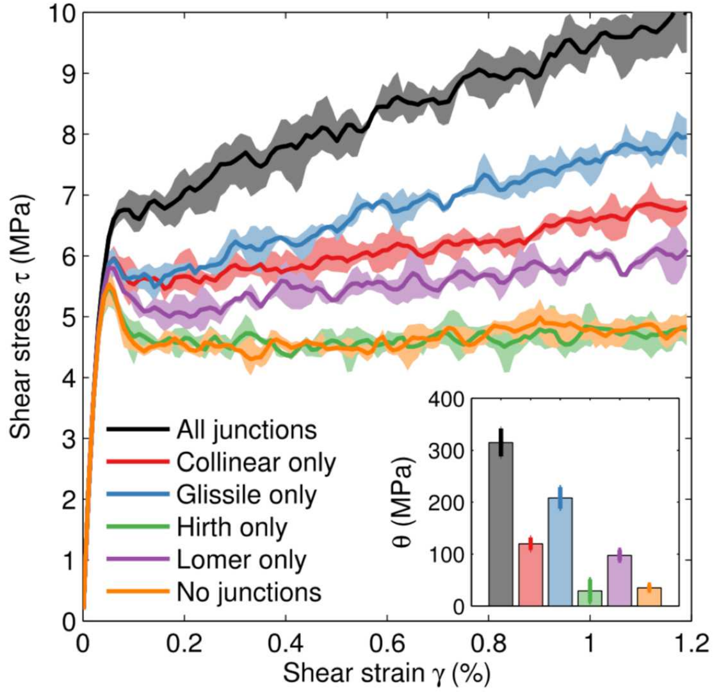
Which junction contributes most to strain hardening?



	$I_{Junction}$
Lomer	2
Hirth	2
Glissile	4
Collinear	1

Number of possible junctions per slip system

Turn off different junctions in DDD and see the effect



Glissile > Collinear > Lomer > Hirth

$I_G\beta_G > I_C\beta_C > I_L\beta_L > I_H\beta_H$

Collinear junction is strongest (largest β)
Glissile junction has more ways to form (largest I)

Summary

DD simulations can now predict (Stage II) strain hardening rate in [001] loading consistently

Dislocation segment length is exponentially distributed in [001] loading

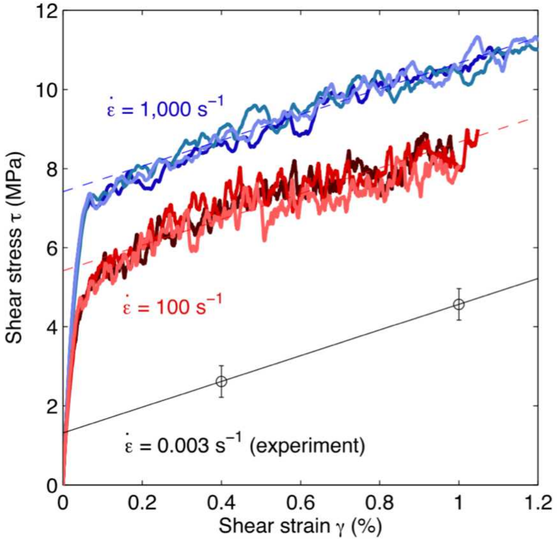
Exponential distribution can be explained if junction formation is a spatially random (Poisson) process

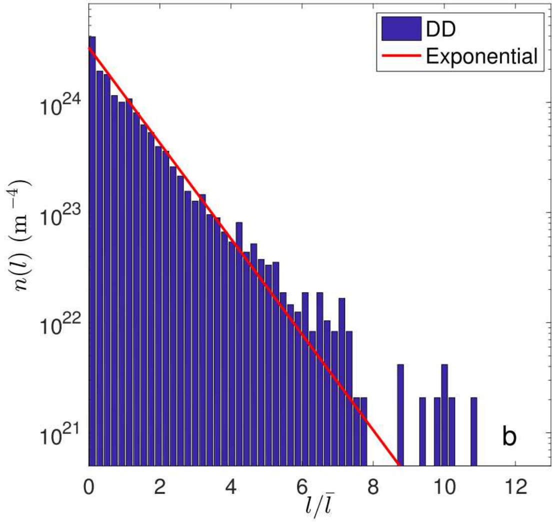
Exponential distribution predicts that junction storage rate β is proportional to strain hardening rate

Dislocation → *Microstructure* → *Property*

$$\beta \rightarrow n(L) = \phi\rho^2 \exp\left(-\sqrt{\phi\rho}L\right) \rightarrow \frac{d\tau}{d\gamma}$$

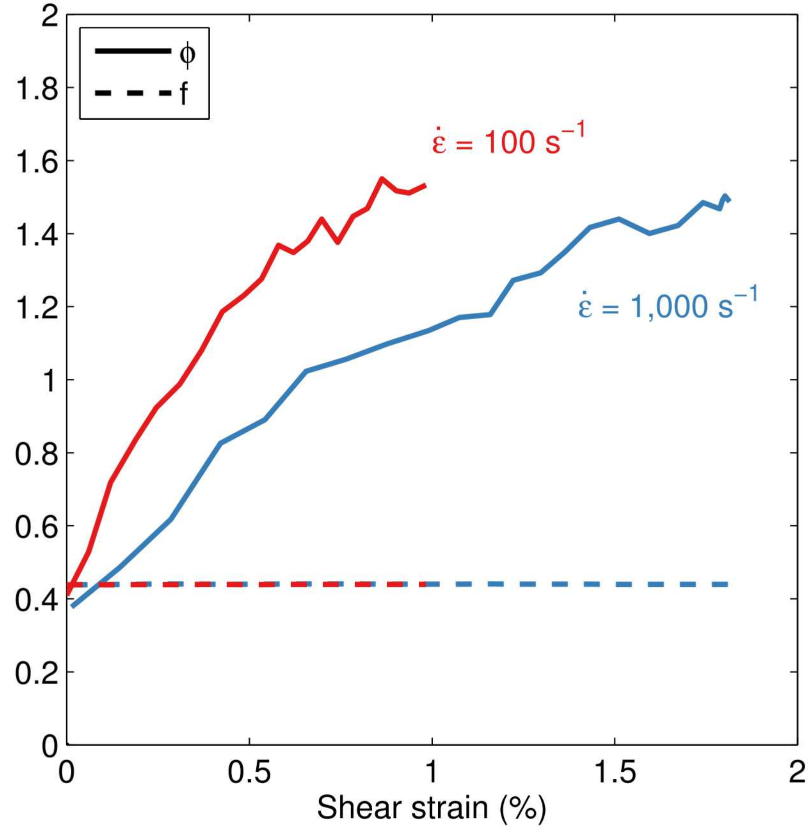
R. B. Sills, N. Bertin, A. Aghaei, and W. Cai, Phys. Rev. Lett. **121**, 085501 (2018)





Backup slides

Extra figures



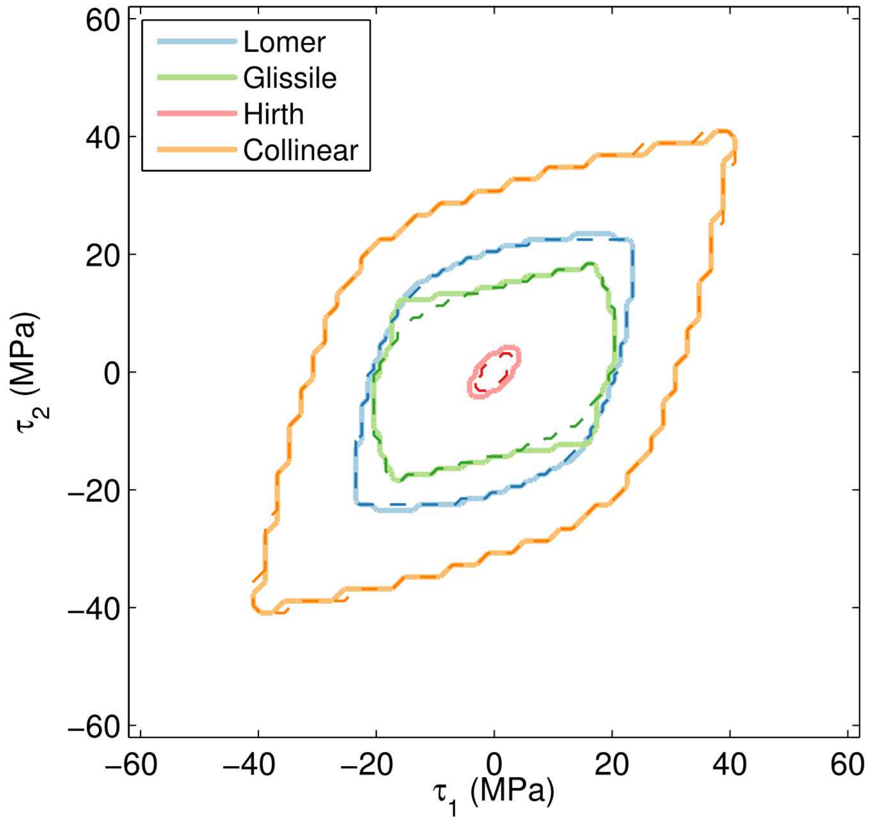


FIG. 5. Example of junction strength maps computed for the four types of FCC junctions resulting from the intersection of two dislocations with initial orientations $\varphi_1 = \varphi_2 = 30°$ with respect to the junction direction. Results are reported for core radii r_c = 6b (solid lines) and r_c = 200b (dashed lines).

Evidence for exponential distribution