

Exceptional service in the national interest



Dislocation junctions and work hardening in FCC metals

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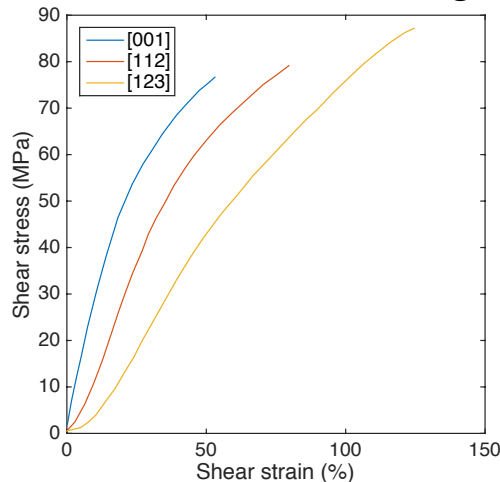
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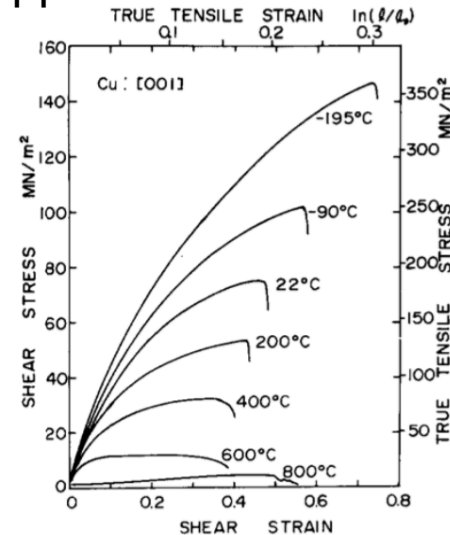
DDD—a tool for studying hardening?

- Grand vision circa 1990s: Compute stress-strain curves with discrete dislocation dynamics (DDD)
 - Understand fundamental mechanisms governing hardening, recovery,...

Single crystalline copper



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

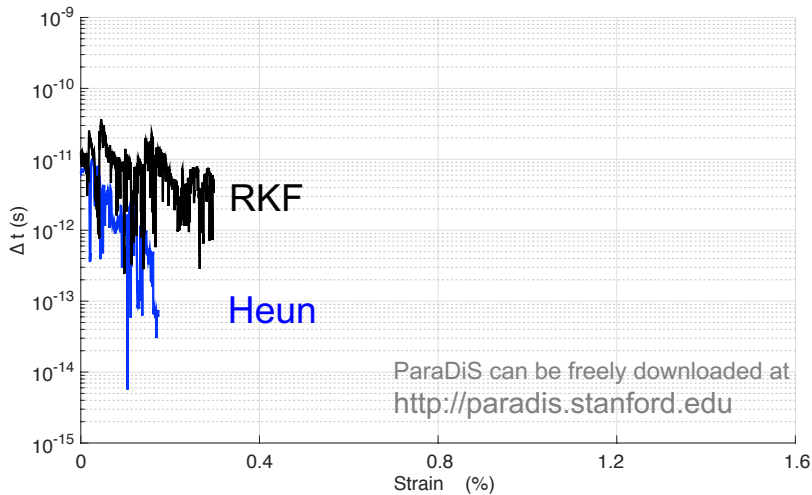
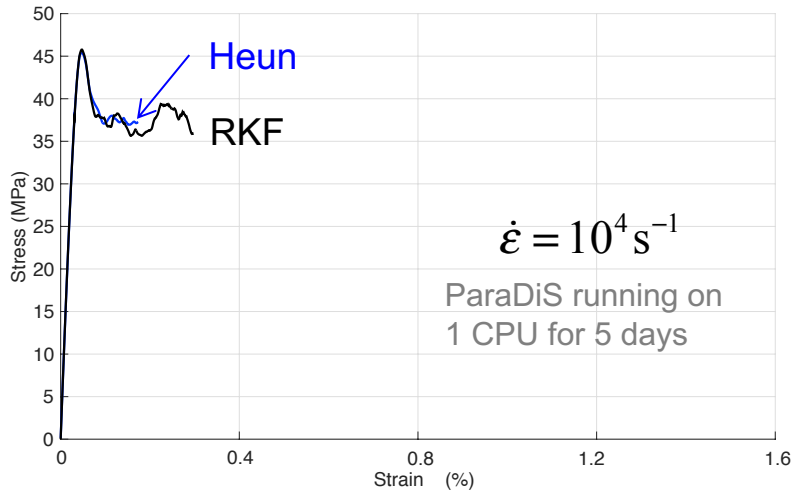


Kawasaki and Takeuchi, Scripta Metall., 14 (1980)

- But... progress has been slow
 - Computationally difficult to simulate a stress-strain curves
 - ~1% strain usually requires many months of computation time

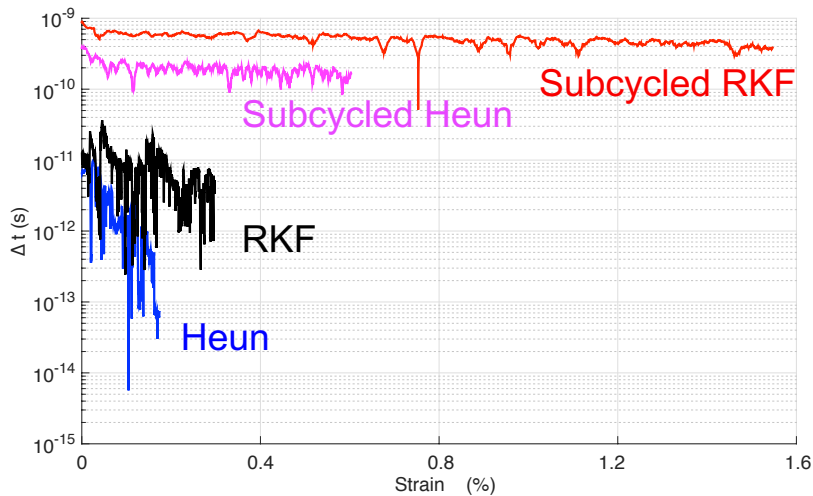
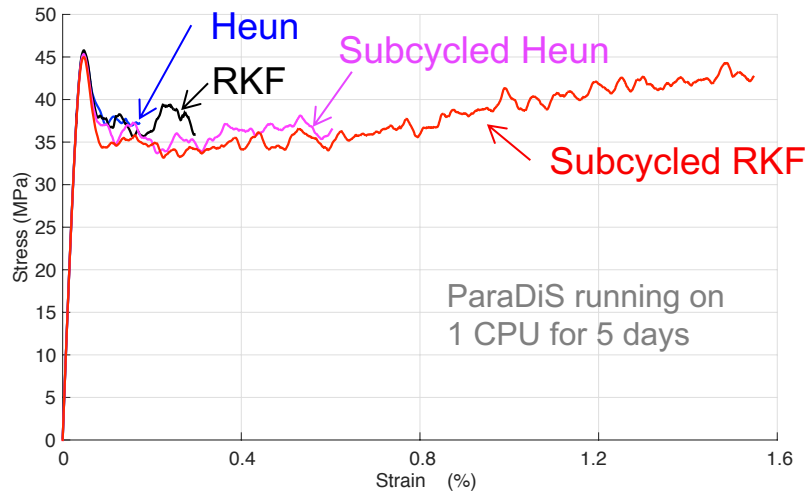
More efficient time integration

- Ordinary explicit & implicit integrators are slow
- Developed “sub-cycling” scheme to increase efficiency



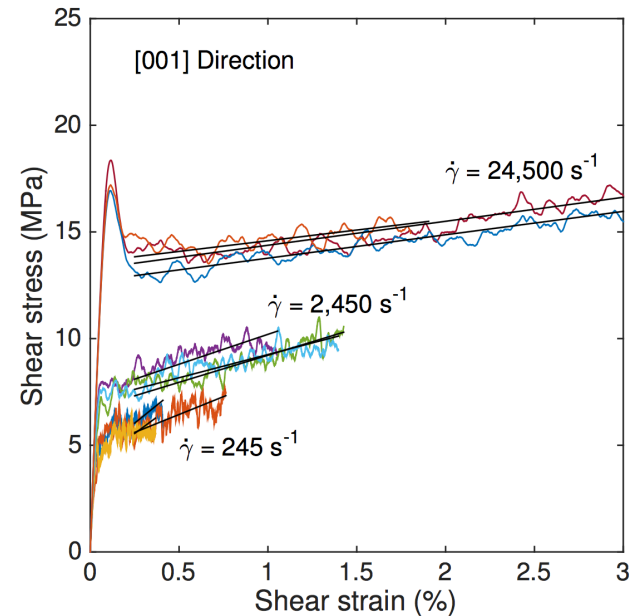
Better time integration

Sills et al. Modell. Simul. Mater. Sci. Eng. 24 (2016)



- Ordinary explicit & implicit integrators are slow
- Developed “sub-cycling” scheme to increase efficiency
 - Achieve 100X speedup

Sills, PhD Thesis, Stanford University, (2016)



Hardening and multiplication

Convergent strain hardening rate Θ
below critical strain rate

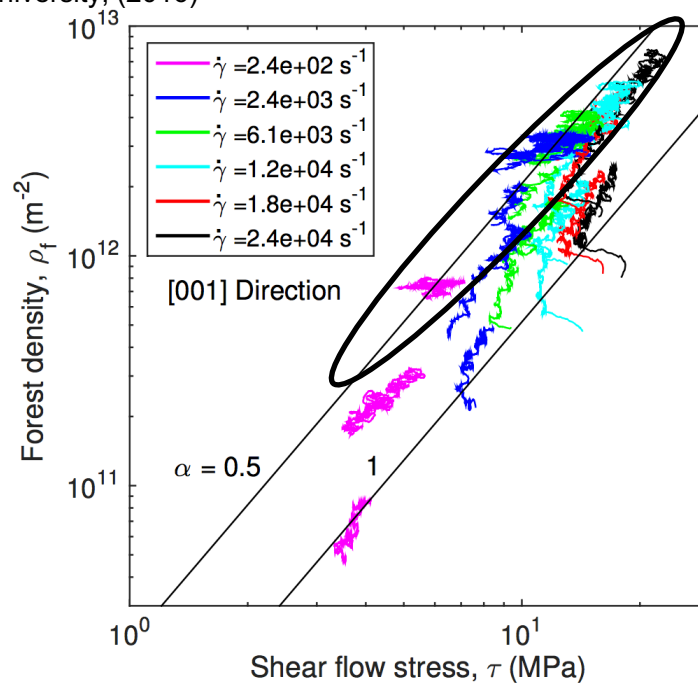
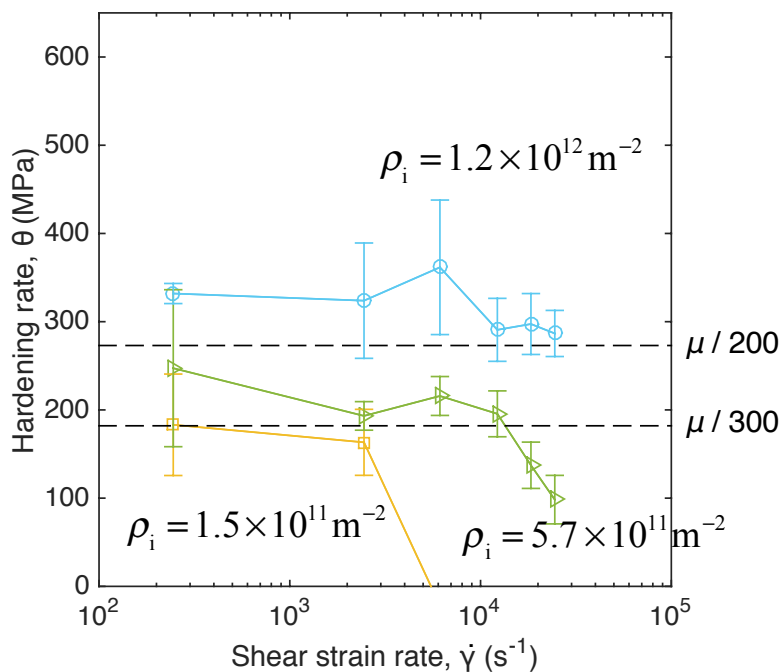
$\Theta \sim \mu / 200$ consistent with experiment
(Stage II, expected for [001])

Hardening is due to multiplication:

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

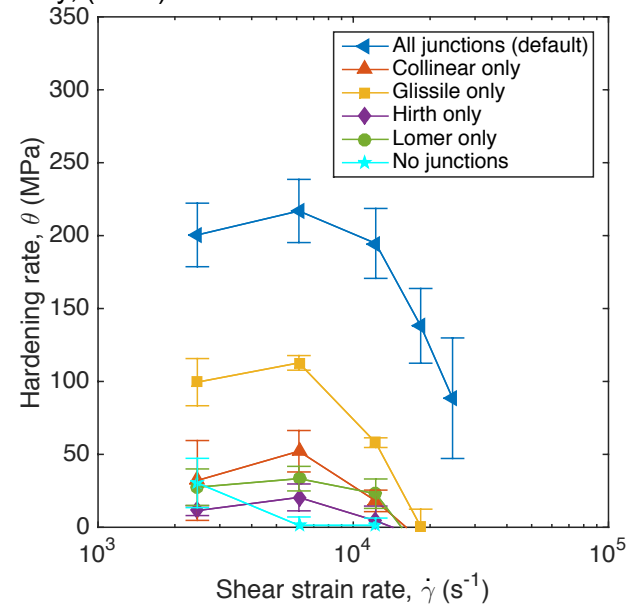
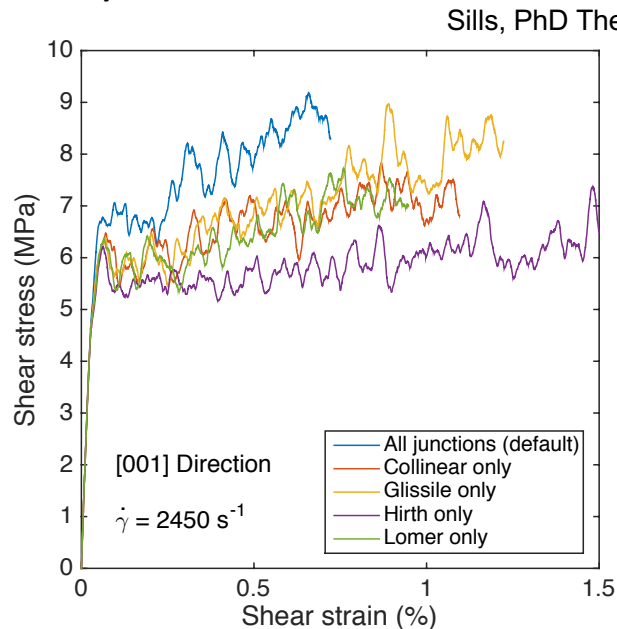
Low strain rate/larger initial density
gives $\alpha \approx 0.5$ (Mecking & Kocks, 1981)

Sills, PhD Thesis, Stanford University, (2016)



Mechanism for hardening?

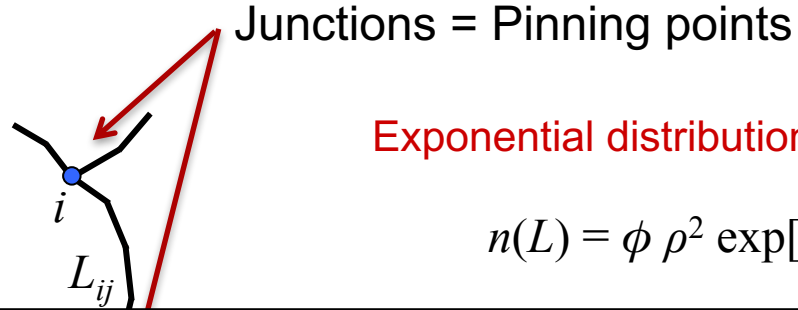
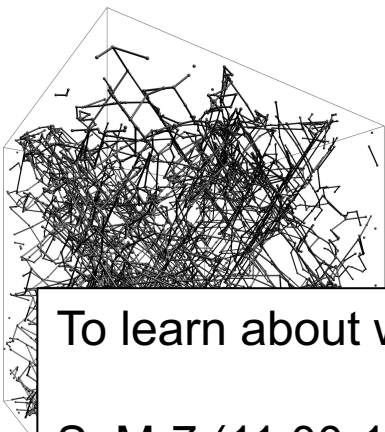
- Junction formation? Which junction types?
- Our approach: Suppress junction formation (node splitting)
 - Key benefit of DDD!



Importance for hardening: Glissile > Collinear \approx Lomer > Hirth

Why? Related to stable junction formation rate

Junctions and microstructure

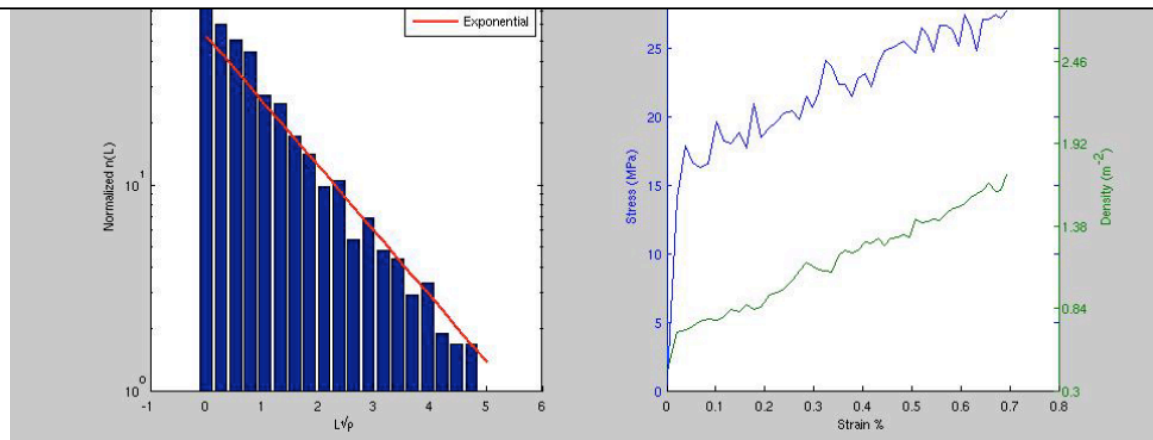


Exponential distribution of segment length

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

To learn about work we are doing to develop governing equations for $n(L)$:

SaM-7 (11:00-12:30) *Constitutive Modeling of Plasticity*
**Coarse-graining dislocation dynamics with length distributions:
a new paradigm for crystal plasticity**



Conclusions

- New sub-cycling-based time integration scheme enables 100X speedup with ParaDiS
- DDD reproduces Stage II hardening in [001] loading and obeys Taylor relation
- Hardening is due to junction formation
 - glissile > collinear > Lomer > Hirth for [001]
- Junction formation leads to exponential link length distribution