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Link Statistics of Dislocation Network during Strain Hardening

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Summary

- Statistical analysis of 118 large-scale Discrete Dislocation Dynamics (DDD) simulations in face-centered cubic (f.c.c.) Cu.
- Link length distributions on active slip systems follow a **double exponential**; inactive systems follow a **single exponential**.
- The long-tail component originates from stress-induced bowing of long links in the dislocation network.
- A generalized Poisson process with link *splitting and growth* reproduces both distributions.
- Provides a quantitative microstructural basis (i.e., network geometry) for constitutive modeling of strain hardening.

Dislocation dynamics simulations

We performed 3D DDD simulations using the ParaDiS code for Cu single crystals under uniaxial loading across the stereographic triangle (as performed in Ref. [1]).

Each configuration contains $\sim 2\times 10^4$ dislocation links, averaged over strain windows ($\gamma_d \in [0.9, 1.05]\%$) for statistical robustness.

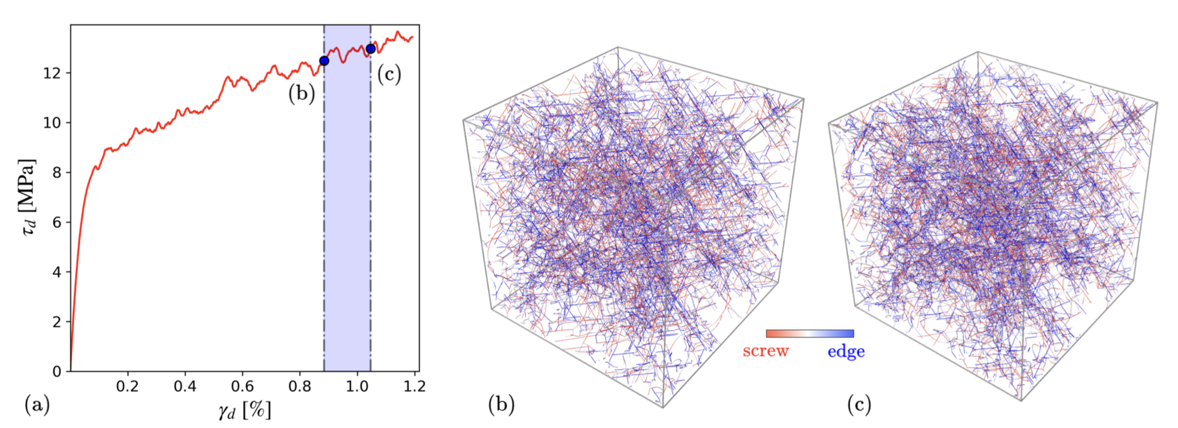

Figure 1: Loading and DDD setup for link statistics extraction.

The schematic illustrates the uniaxial loading geometry applied to the Cu single crystal and the extraction region used for measuring dislocation link statistics.

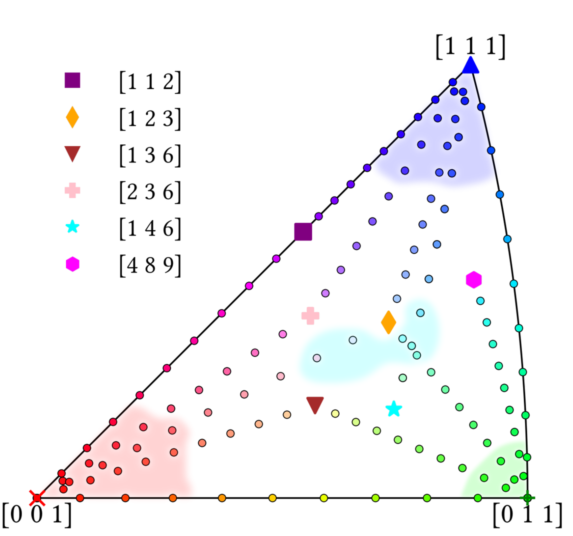

Figure 2: 118 loading orientations distributed over the stereographic triangle.

Each point represents a unique loading direction used in the simulations, covering the full crystallographic orientation space between [001], [011], and [111].

The link length distributions at a later stage of the strain hardening were collected based on the strain window shown in the schematic.

Link length distributions on individual slip systems

Earlier work [2] reported a **single-exponential** distribution:

$$n_i^{\mathrm{S}}(l) = \frac{N_i}{\bar{l}_i} e^{-l/\bar{l}_i}. \tag{1}$$

where N_i is the number of links for slip system i, and $\bar{l}_i$ is the average link length for slip system i.

We extend this to a **double exponential** form for active systems:

$$n_i(l) = \frac{N_i^{(1)}}{\bar{l}_i^{(1)}} e^{-l/\bar{l}_i^{(1)}} + \frac{N_i^{(2)}}{\bar{l}_i^{(2)}} e^{-l/\bar{l}_i^{(2)}}, \tag{2}$$

where $\bar{l}_i^{(2)} > \bar{l}_i^{(1)}$ and $N_i^{(2)} \ll N_i^{(1)}$. The first term dominates short links ($l < 5\bar{l}_i$), while the second forms a long tail ($l > 5\bar{l}_i$) corresponding to high-velocity links.

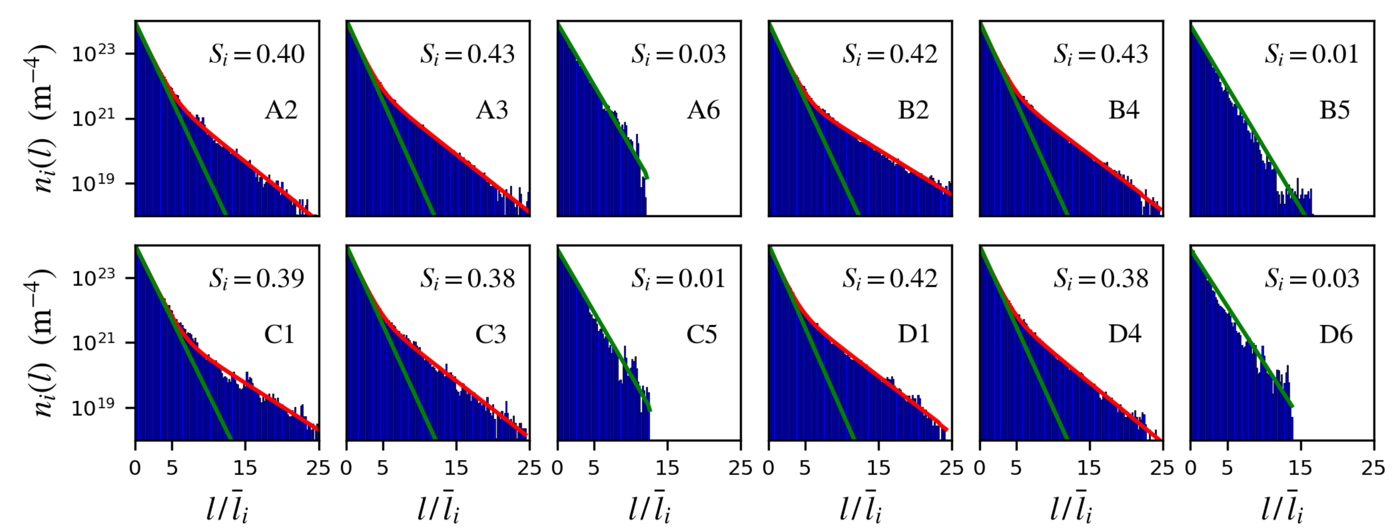

Figure 3: Double- and single-exponential link length distributions for [001] loading.

For [001] loading, inactive slip systems can be well described by a single exponential distribution (low Schmid factors). However, active systems' (high Schmid factors) distributions deviate from this form, showing a secondary, slower-decaying component.

This secondary exponential tail corresponds to a minority of longer dislocation links that experience bowing-out under applied stress.

This distinction highlights slip-system-level differences in strain hardening.

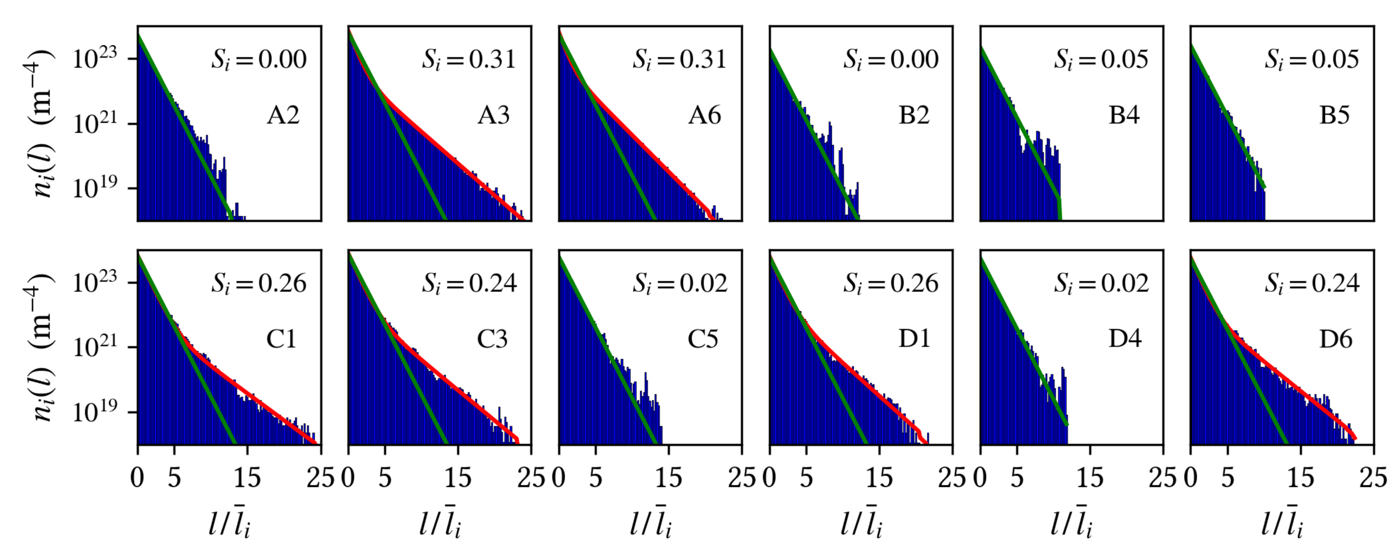

Figure 4: For [111] loading, double-exponential tails appear on active systems.

Under [111] loading, the distribution also exhibits long-tail behavior on active slip systems, consistent across most loading orientations in the stereographic triangle.

The pronounced tails at $S_i > 0.2$ confirm links "bowing-out" caused by higher resolved shear stress. In contrast, inactive slip systems (subjected to lower applied stress) retain single-exponential behavior.

This clear contrast implies the stress-activated nature of the long-link population.

Stress effects on link distributions

When the same configuration is relaxed to zero stress, all slip systems revert to a single exponential form:

$$n_i(l) \propto e^{-l/\bar{l}_i}.$$

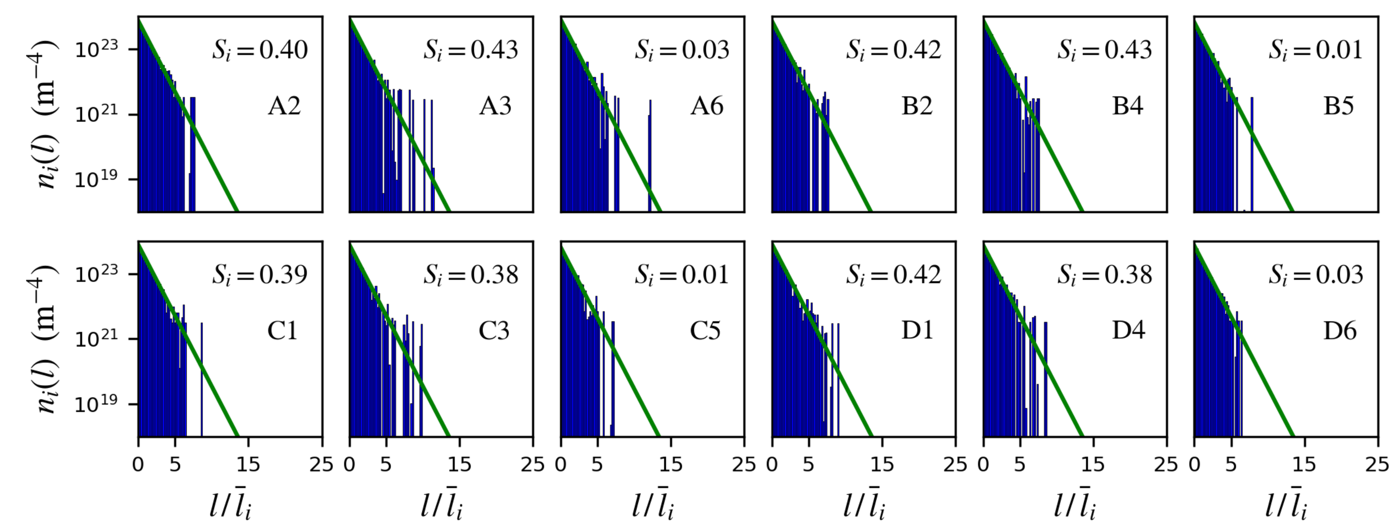

Figure 5: After stress removal, long tails vanish, confirming stress-induced bowing.

After stress relaxation, the double-exponential behavior disappears, leaving a single exponential distribution across all systems.

This verifies that the long tails originate from stress-induced dislocation bowing during the strain hardening process.

Statistical features of long links

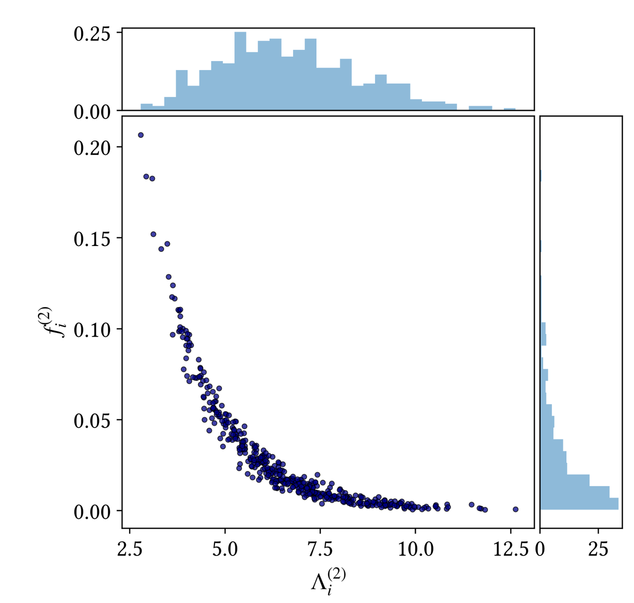

Figure 6: Correlation between long-link length and population fractions.

Figure 6 shows the correlation between the long-link fraction and its normalized length. Slip systems with longer normalized mean length $\Lambda_i^{(2)}$ (second exponential population) exhibit smaller populations $f^{(2)}$, indicating that long links are rare but influential.

The normalized mean length $\Lambda_i^{(2)}$ lies mostly within $[5, 10]$, suggesting that a few extended segments dominate the distribution tail and reflect stress-induced bowing.

References

[1] S. Akhondzadeh, R. B. Sills, N. Bertin, and W. Cai. Dislocation density-based plasticity model from massive discrete dislocation dynamics database. *Journal of the Mechanics and Physics of Solids*, 145:104152, 2020.

[2] R. B. Sills, N. Bertin, A. Aghaei, and W. Cai. Dislocation networks and the microstructural origin of strain hardening. *Physical review letters*, 121(8):085501, 2018.

Generalized Poisson process with growth

We extend the 1D Poisson link-splitting model [2] by allowing link growth:

$$r = A \cdot \frac{l}{\bar{l}}, \qquad \text{(split rate)} \tag{3}$$

$$\dot{l}\,/\,l = G(l\,/\,\bar{l}), \qquad \text{(growth function).} \tag{4}$$

If G is constant (linear growth), $\Rightarrow$ single exponential. If G becomes super-linear ($\dot{l} \propto l^2$ beyond threshold), $\Rightarrow$ double exponential.

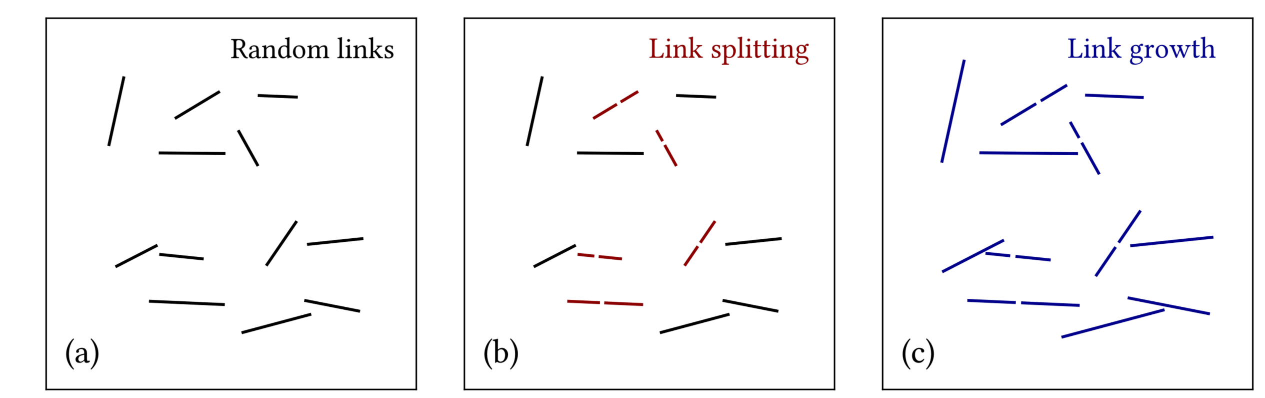

Figure 7: Extended Poisson process: random splitting & link growth.

The schematic illustrates a generalized point Poisson process, connecting dislocation links randomly split while simultaneously elongating under stress.

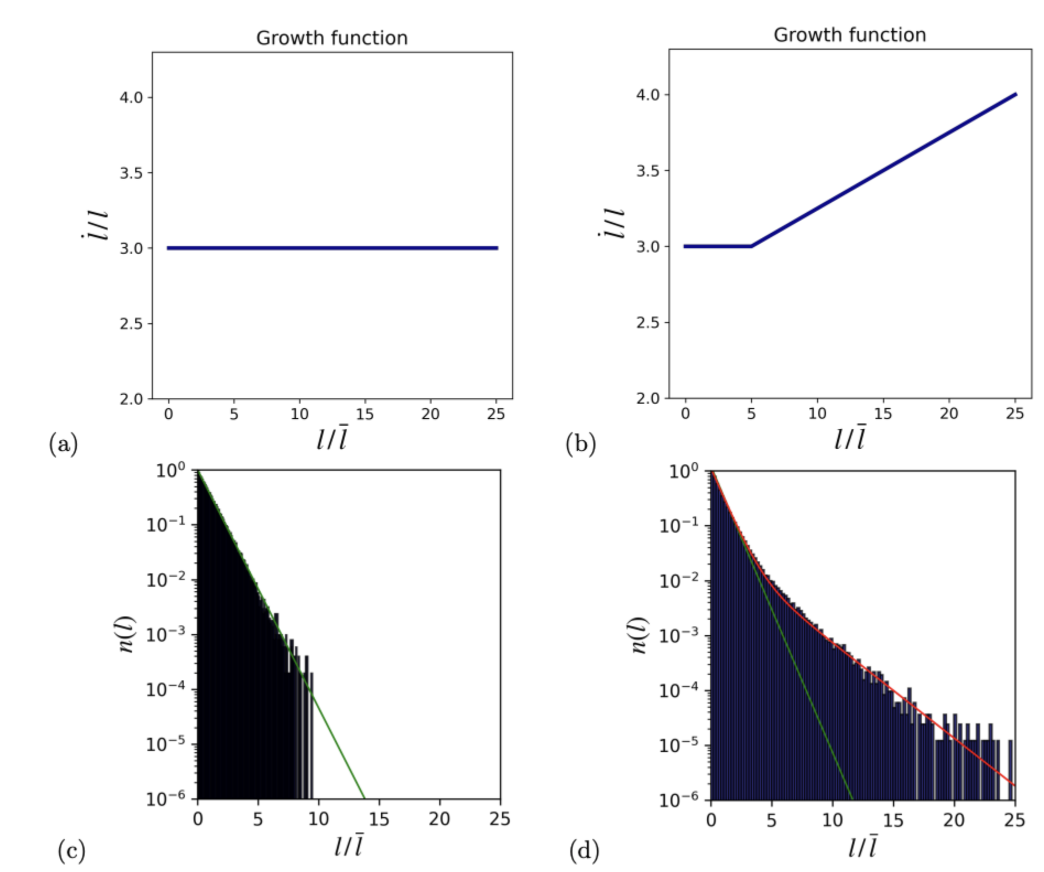

Figure 8: Numerical Poisson model reproducing single and double exponentials.

The numerical simulation confirms that linear growth yields a single-exponential link distribution, matching equilibrium DDD behavior.

Introducing super-linear growth reproduces the observed double-exponential form, with a sharp crossover at the critical length scale. This model links the emergence of long tails to stress-induced link bowing out.

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