Link Statistics of Dislocation Network during Strain Hardening

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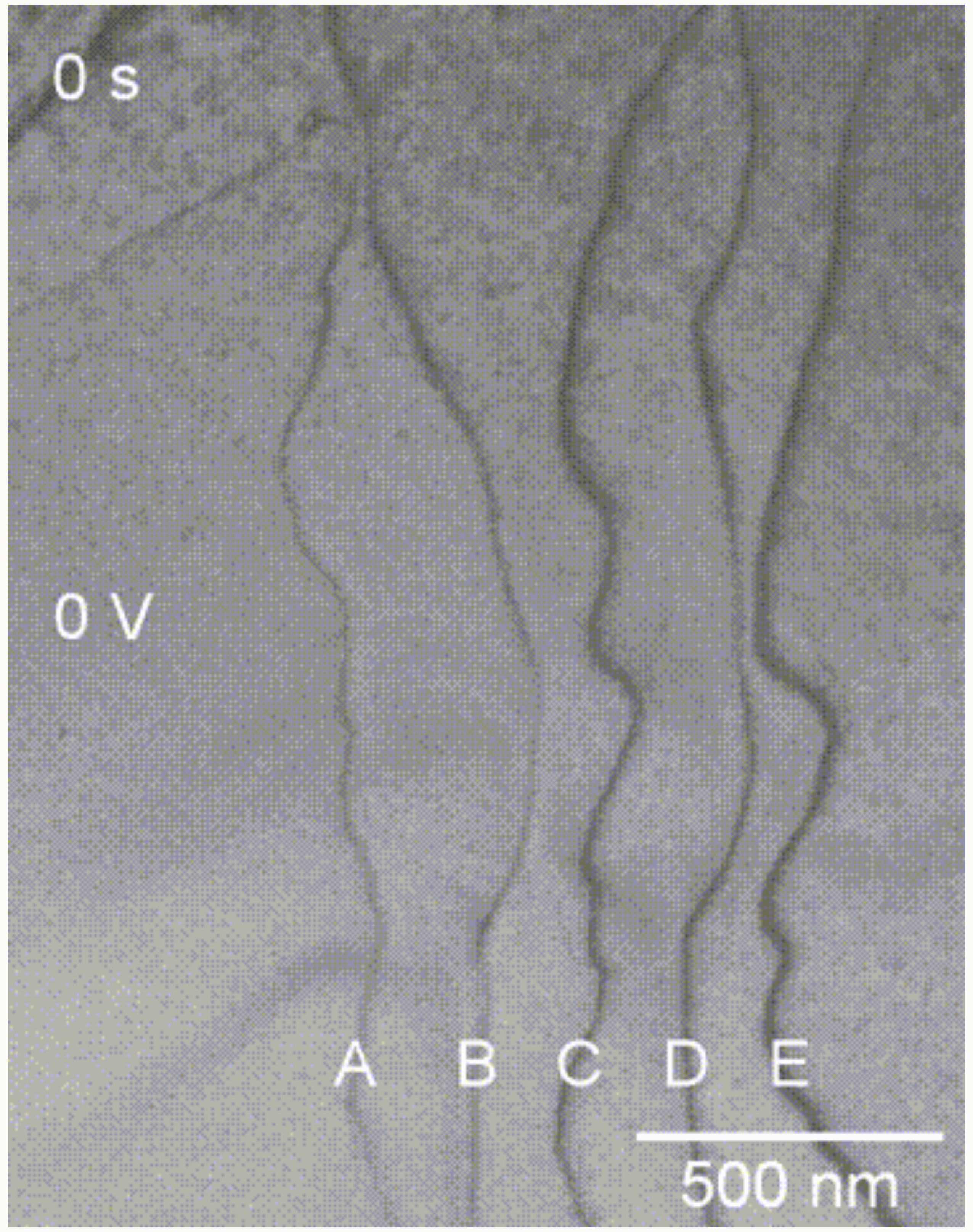
Alloys & Nuclear Materials:

Understanding evolution of ***defects***

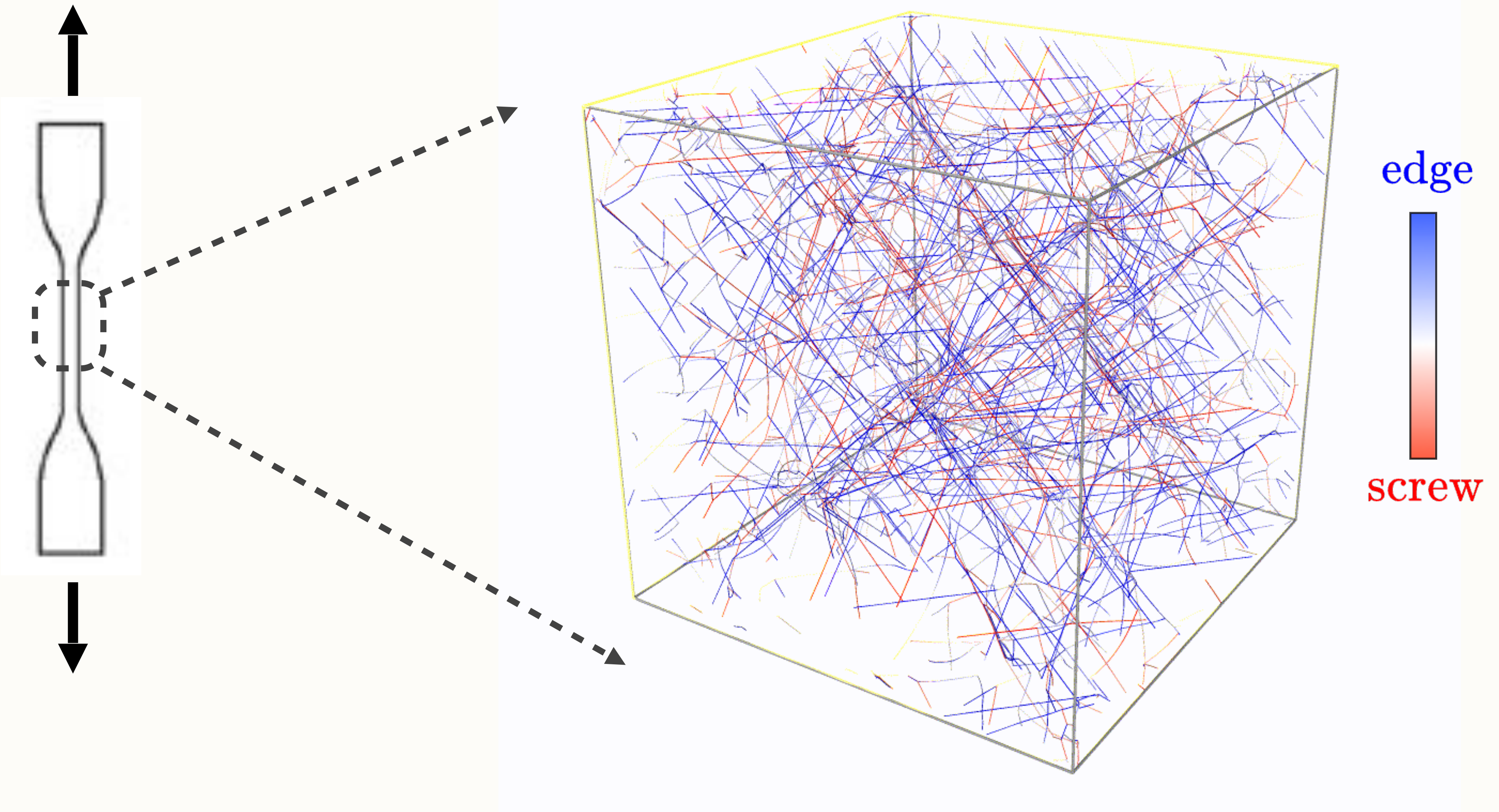
Dislocation dynamics controls plasticity

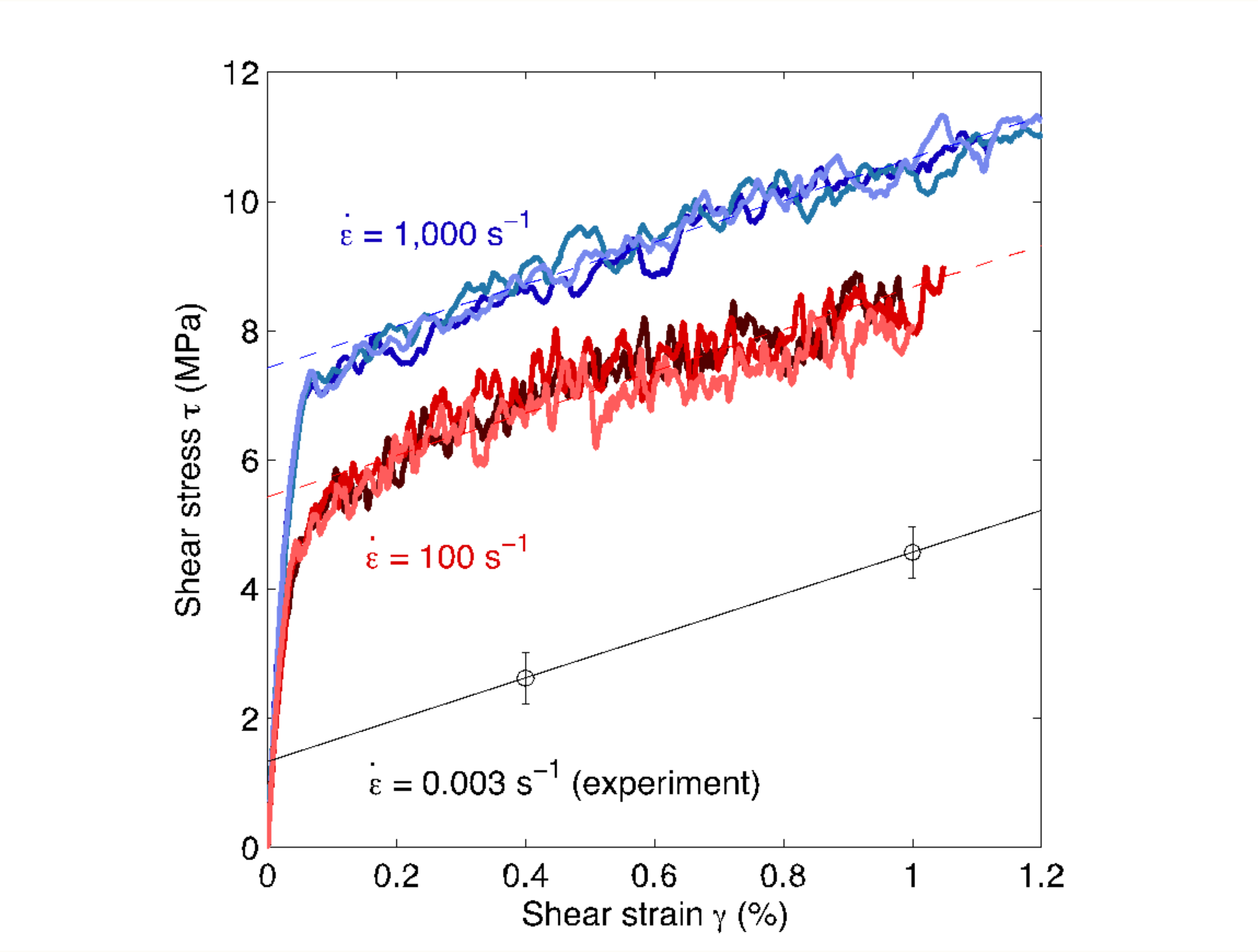
Dislocations are line **defects** in crystals

(Figure from experiment)



Li et al., *Nature Materials*, 2023



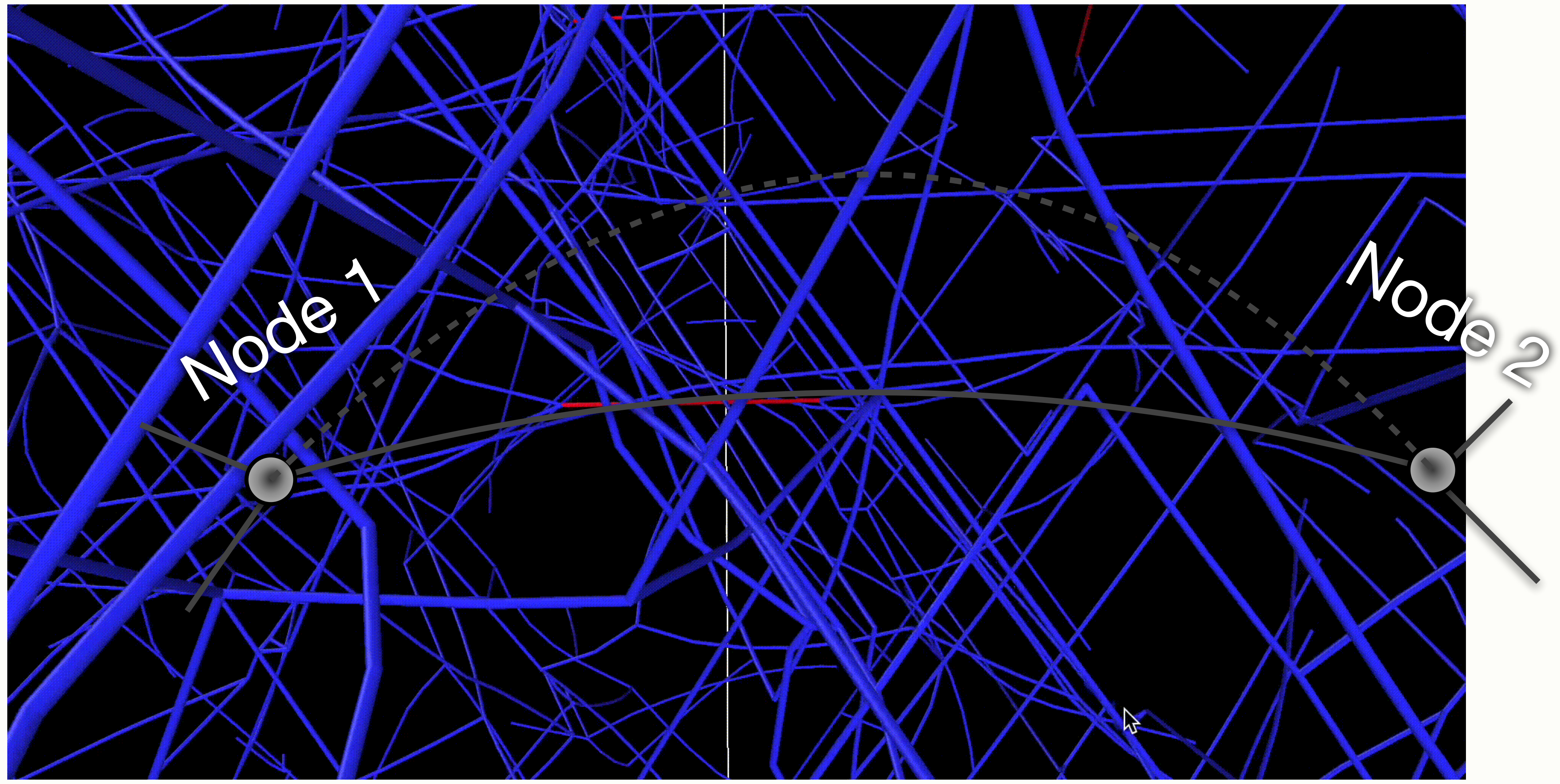


Sills et al., *Phys. Rev. Lett.*, 2018

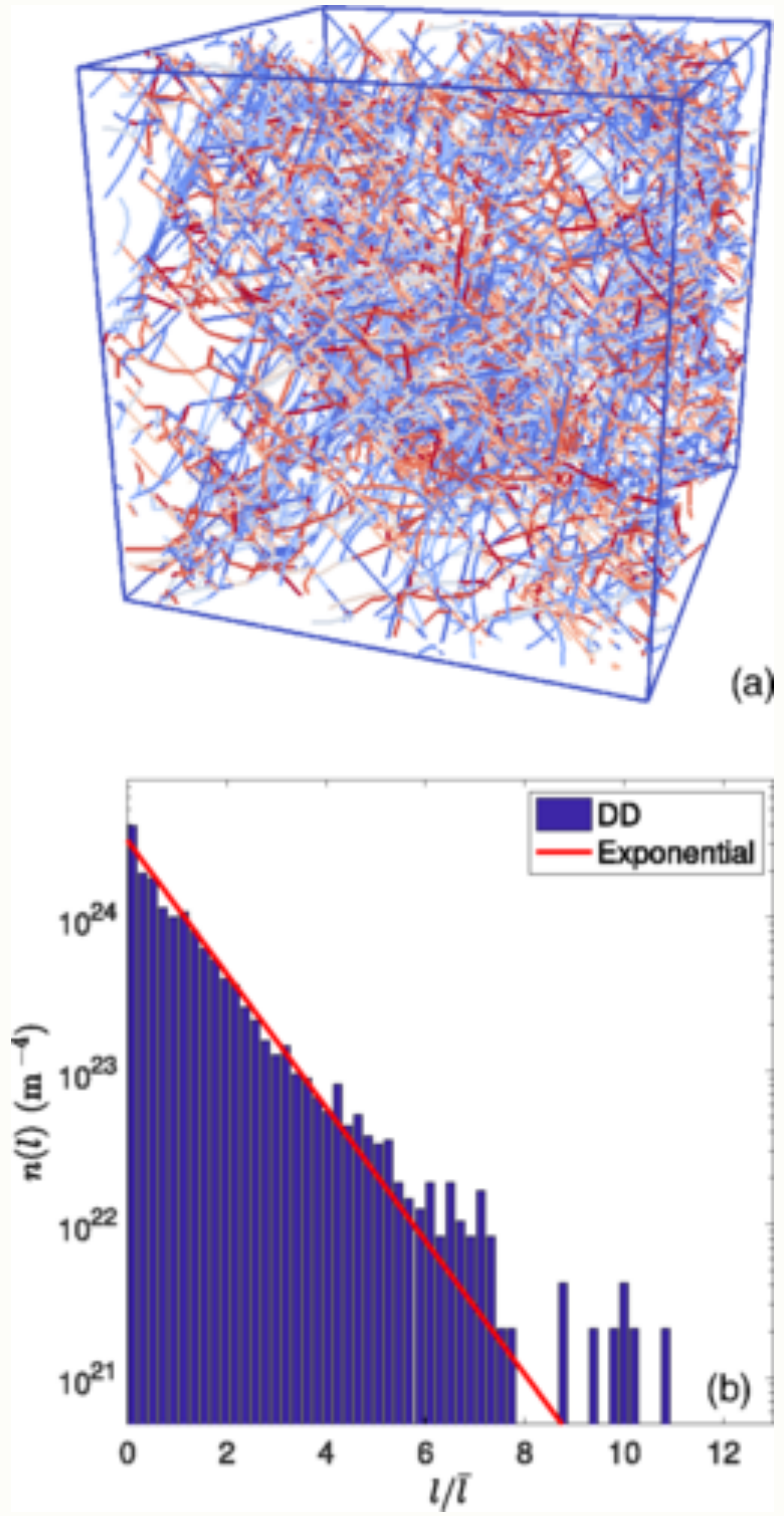
P: Lack of understanding of the **interactions** of the network (↔ mechanical properties)!

Dislocation link lengths statistics: from *link* to *network*

[001] Loading on Cu



What is a link?



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Dislocation Networks and the Microstructural Origin of Strain Hardening

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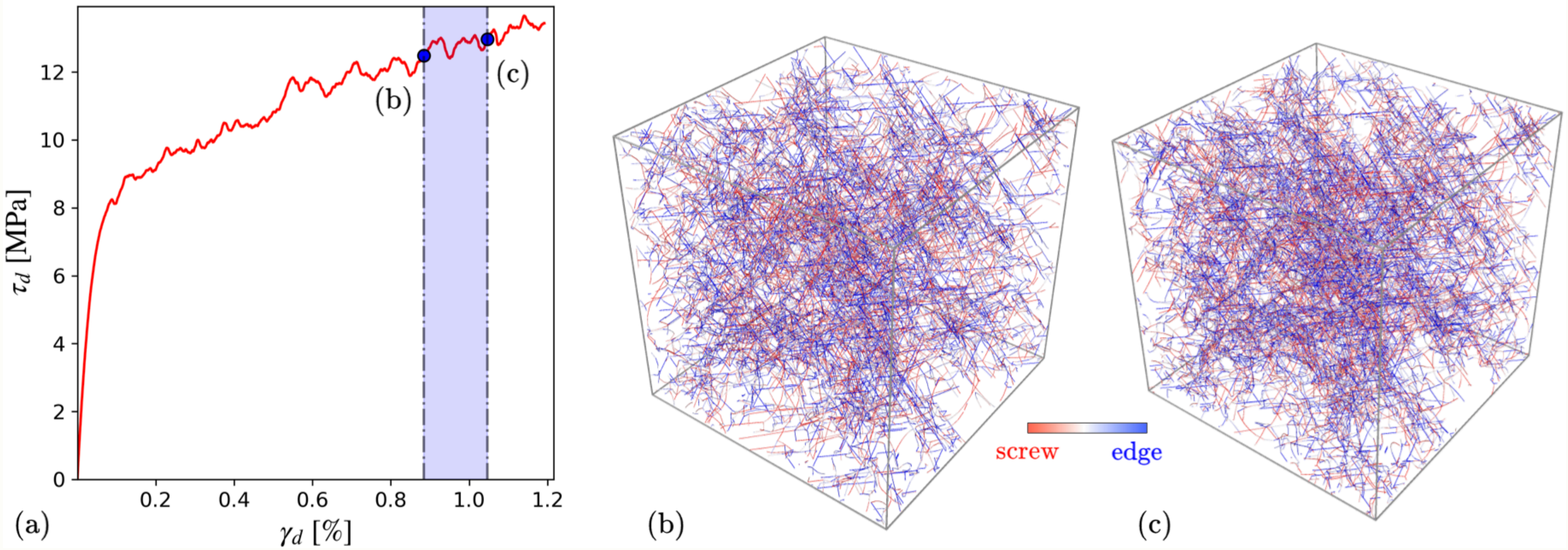
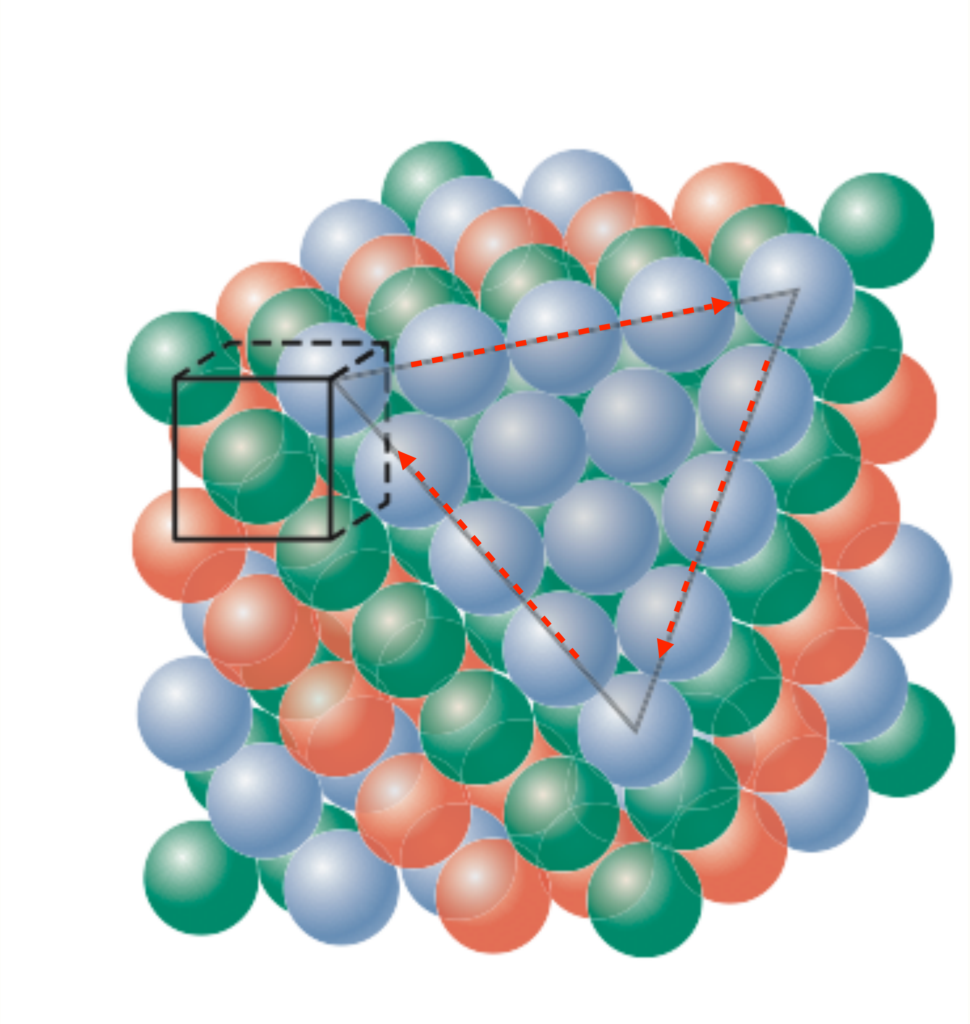
Dislocation link lengths are exponentially distributed

Dislocation link lengths are analyzed across different loadings

Loading orientation near $[001]$

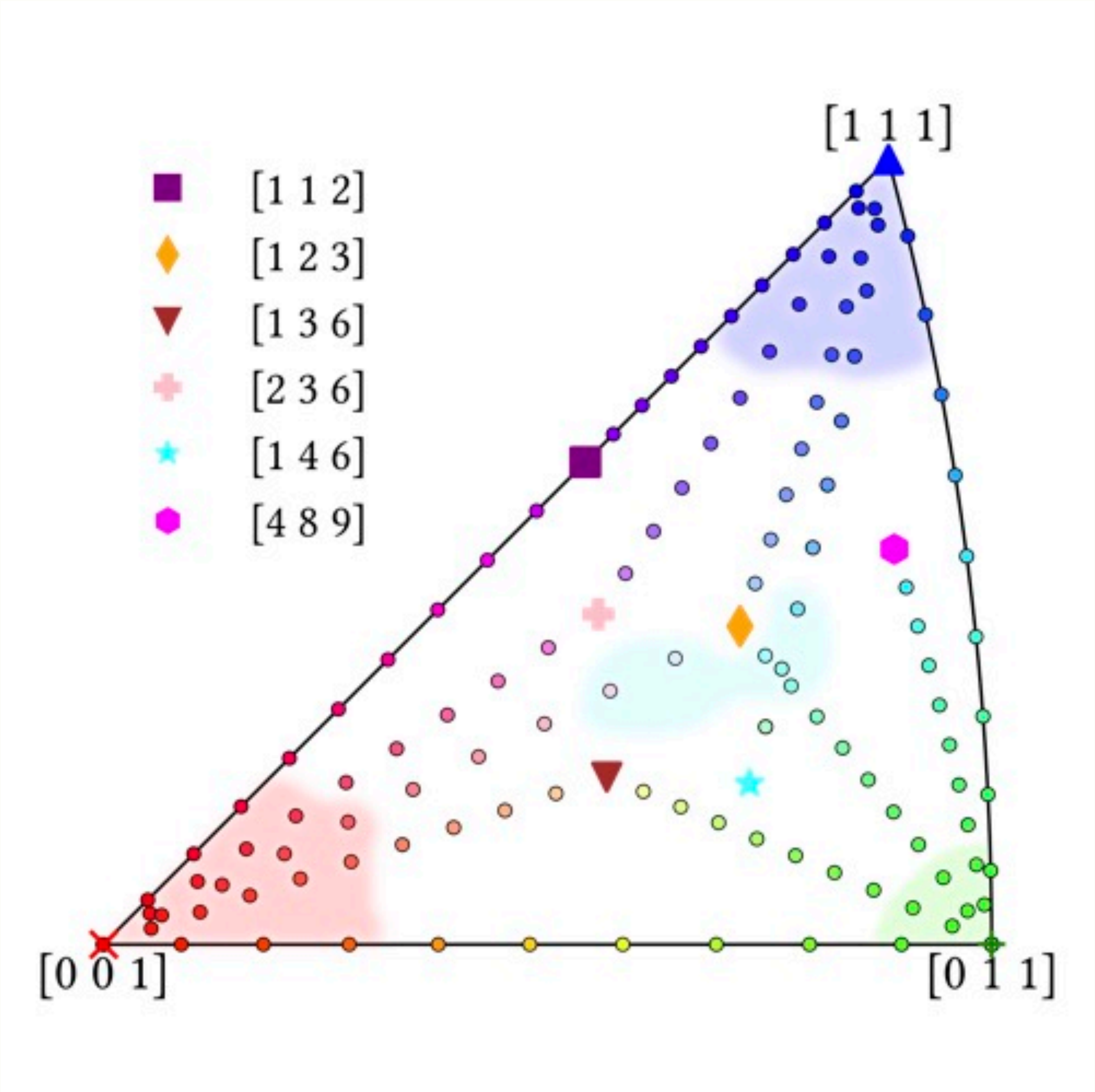




FCC (Cu) has 12 slip systems.

Q1: What about link length distribution on individual slip systems?

Q2: … link length distribution under general loading orientations?



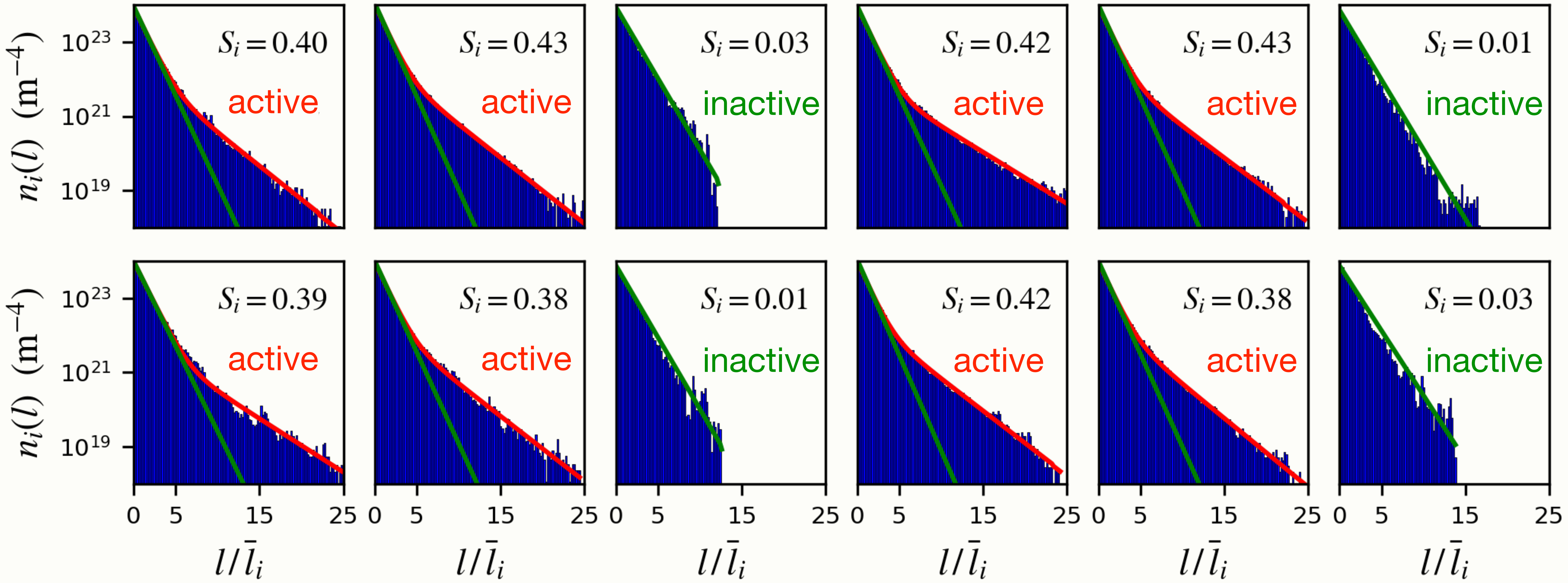
Link statistics were analyzed over 118 loading orientations, on individual slip systems.

Key features of link distributions

Different distributions on
active & inactive slip systems

Link statistics near $[001]$: double exponential for active slip systems

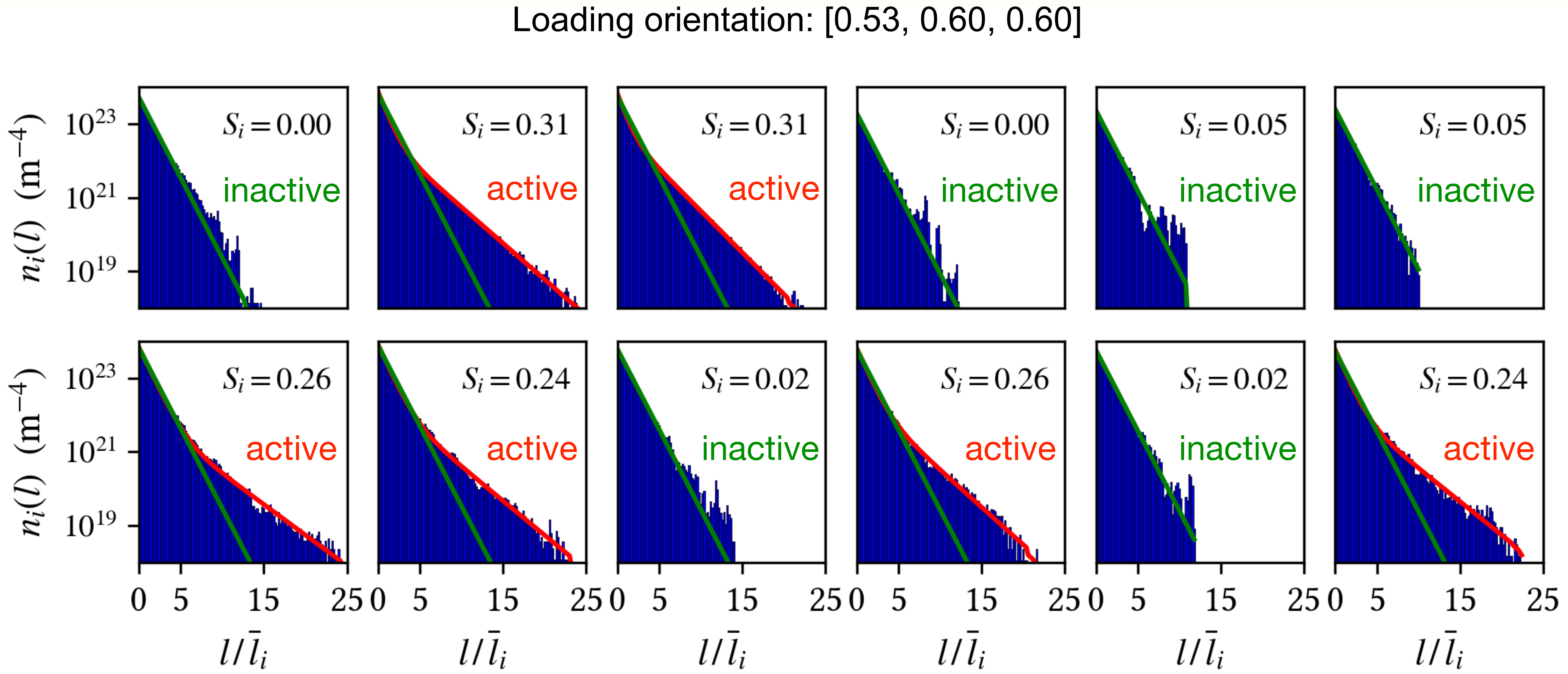
Loading orientation: [0.03, 0.05, 0.99]



Single exponential: $n_i(l) = \frac{N_i}{\bar{l}_i} e^{-l/\bar{l}_i}$

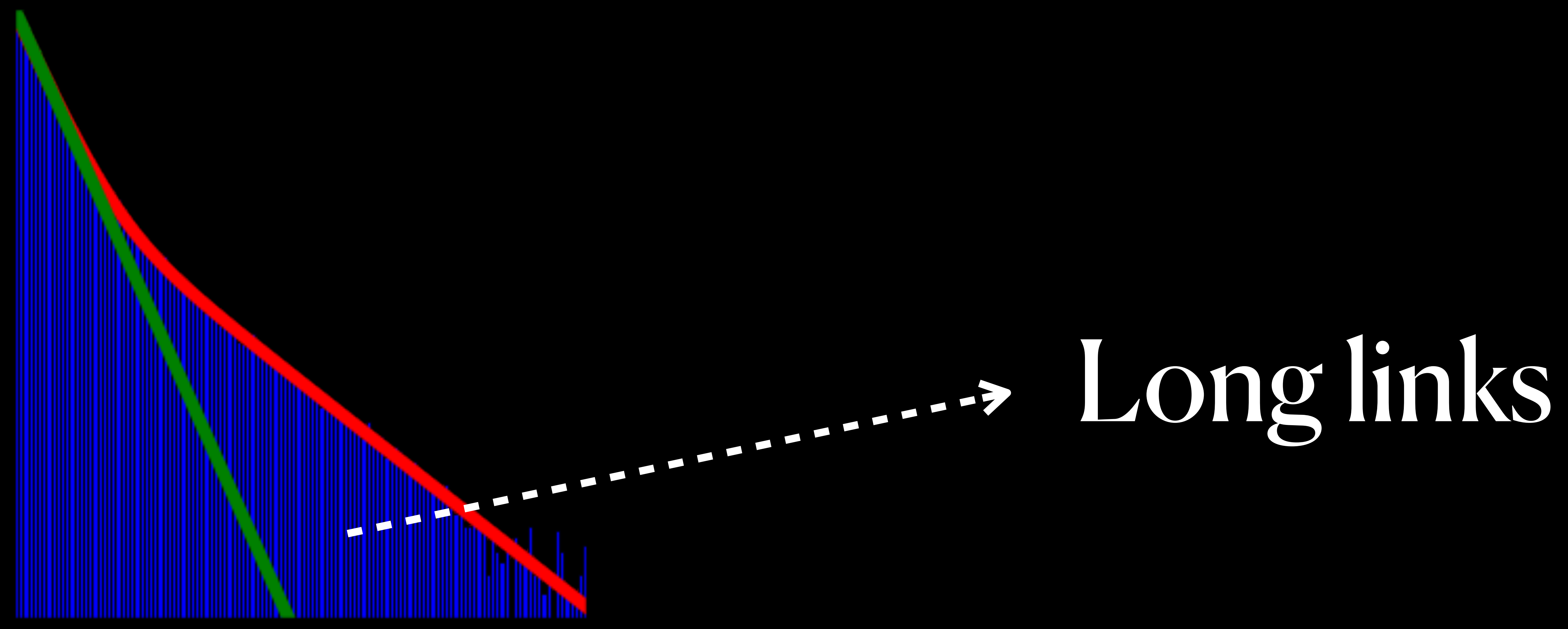
Double exponential: $n_i(l) = \frac{N_i^{(1)}}{\bar{l}_i^{(1)}} e^{-l/\bar{l}_i^{(1)}} + \frac{N_i^{(2)}}{\bar{l}_i^{(2)}} e^{-l/\bar{l}_i^{(2)}}$

Link statistics near $[111]$: double exponential for active slip systems



Single exponential: $n_i(l) = \frac{N_i}{\bar{l}_i} e^{-l/\bar{l}_i}$

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

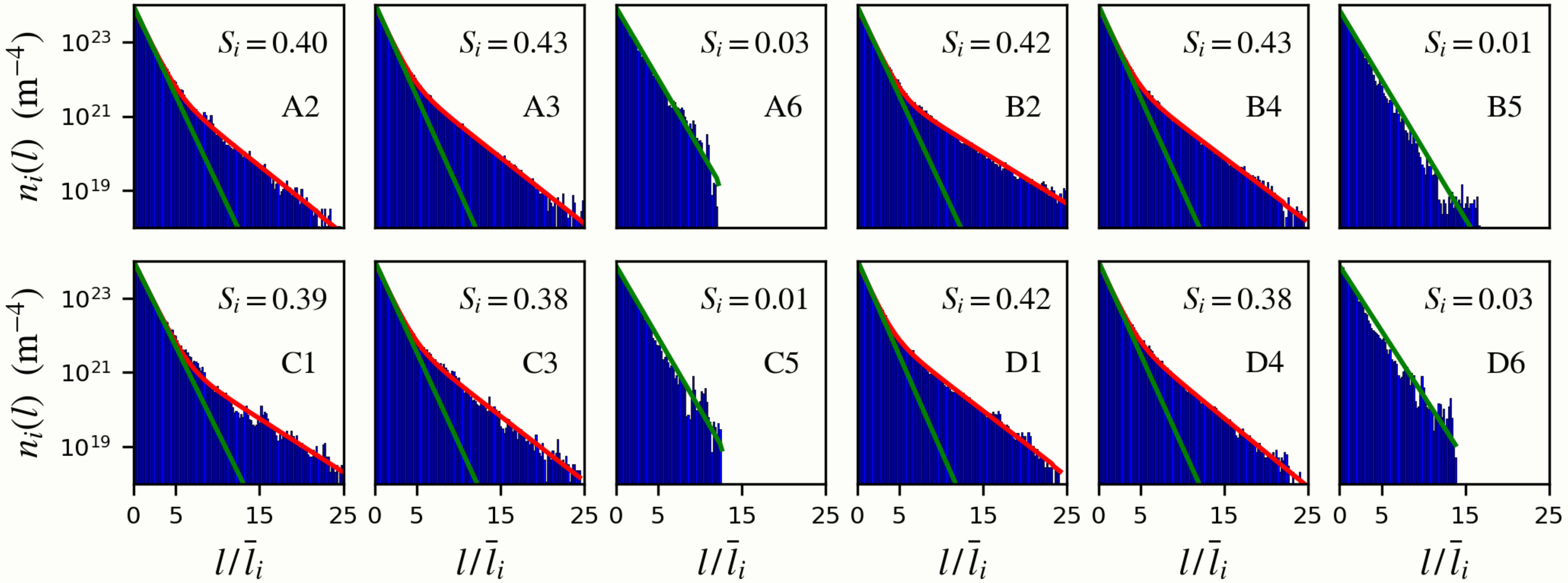


What caused longer links?

Hypothesis: *applied stress* → *plastic flow*

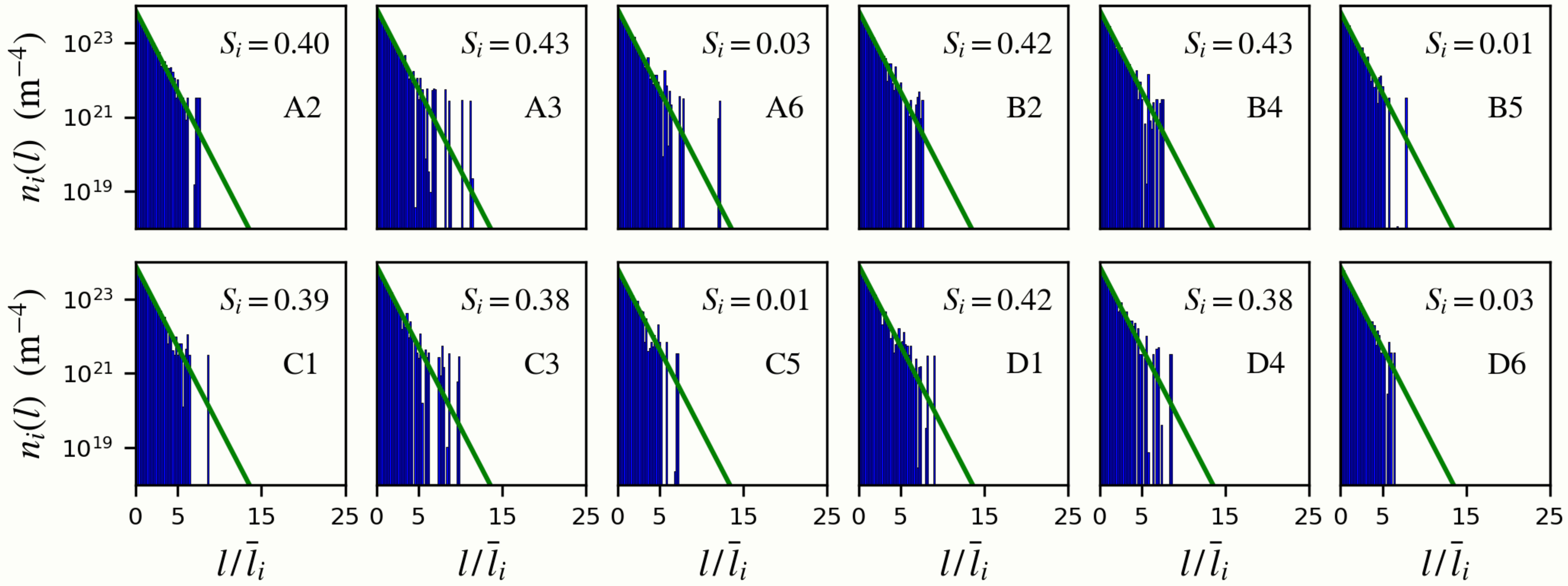
Link statistics near $[001]$: double exponential for active slip systems

Loading orientation: [0.03, 0.05, 0.99]



Testing the hypothesis: **remove applied stress!**

Link statistics near $[001]$: relaxed to a single exponential distribution

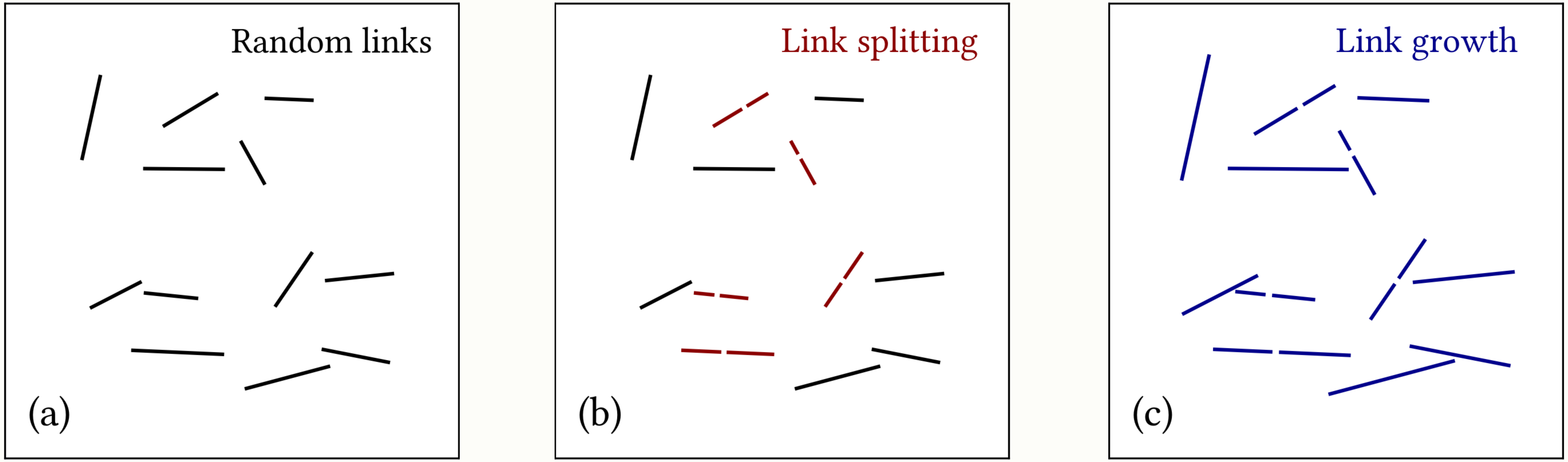


Loading orientation: [0.03, 0.05, 0.99] (relaxed at 0.9% $\dot{\gamma}_d$)

Why double exponential?

Generalized Poisson process models explains link distributions

A mathematical model inspired by dislocation behavior during plastic deformation



Split probability rate is proportional to the link length:

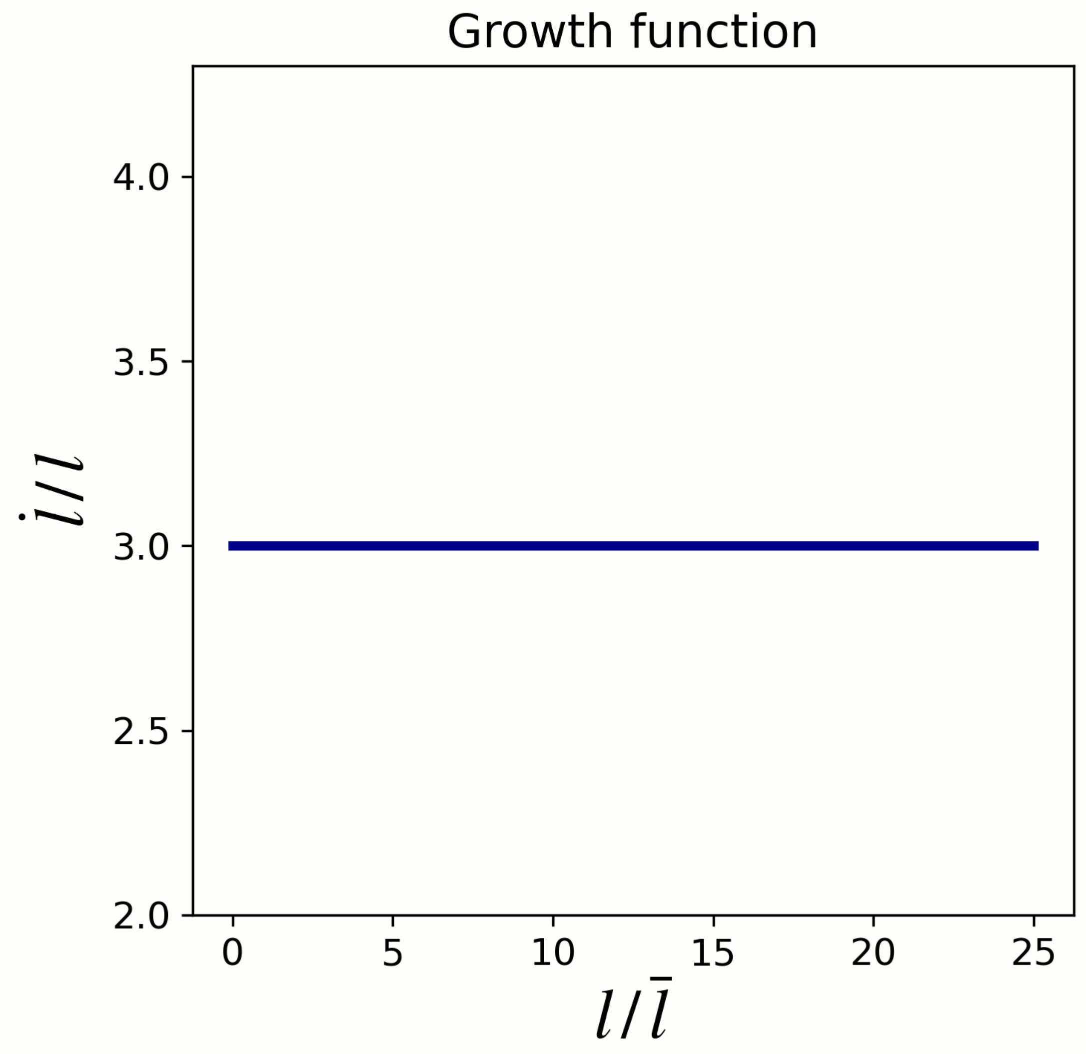
$$r_k = A \cdot \frac{l_k}{\bar{l}}$$

Link growth follows a growth function (of the normalized link length):

$$\dot{l}_k / l_k = G\left(l_k / \bar{l}\right)$$

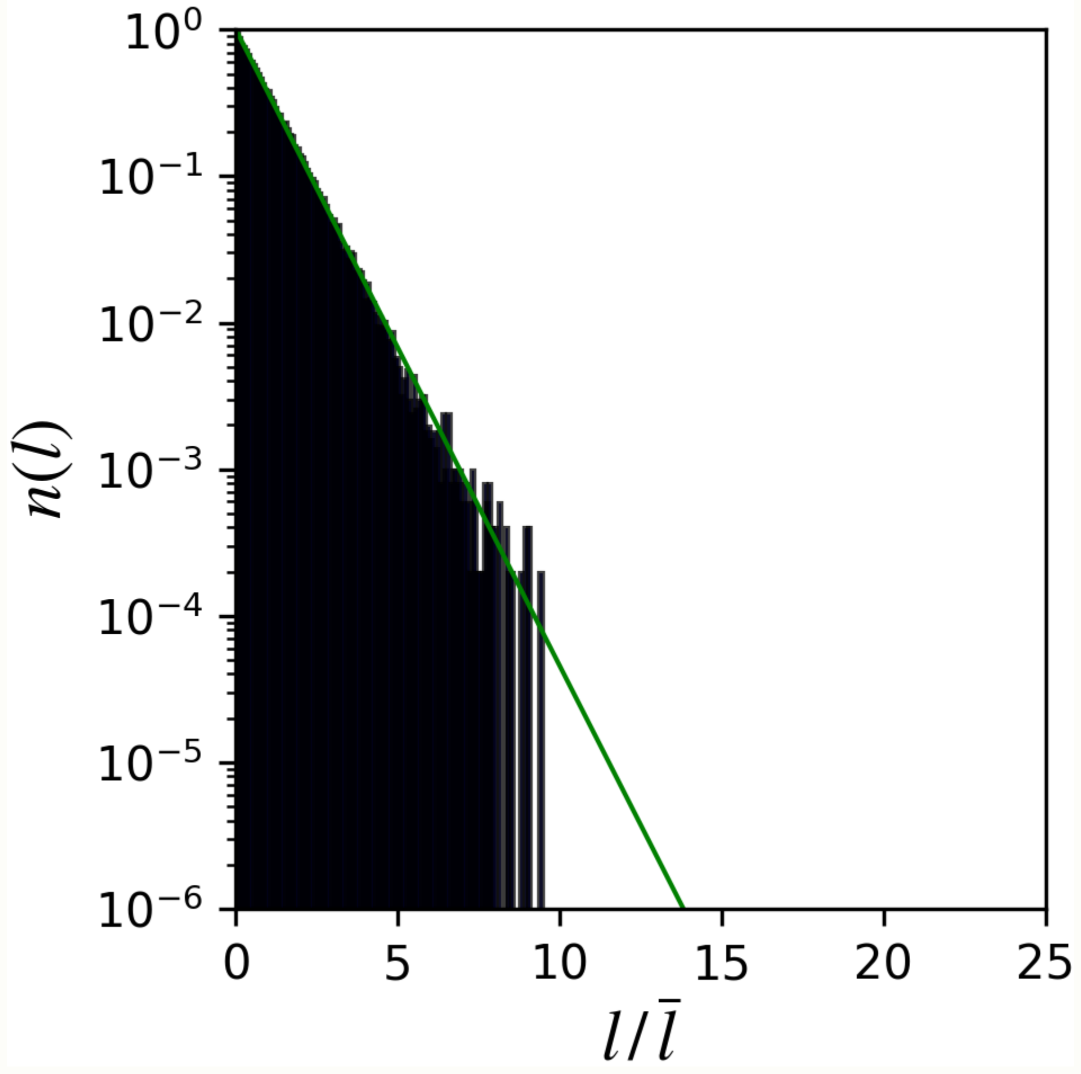
Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

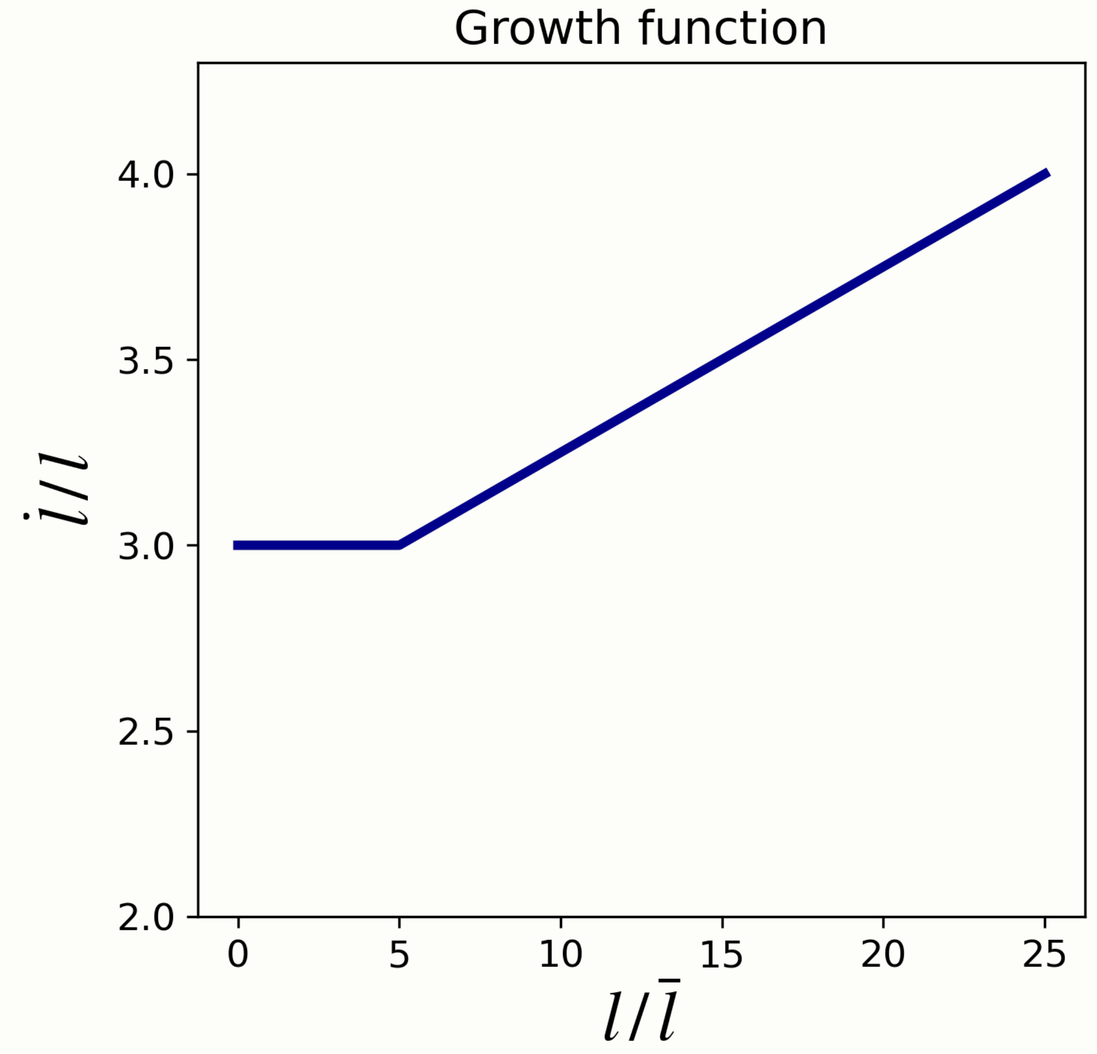
Generalized Poisson process models explains link distributions



Constant growth of $\dot{l}/l$ leads to single exponential distribution.

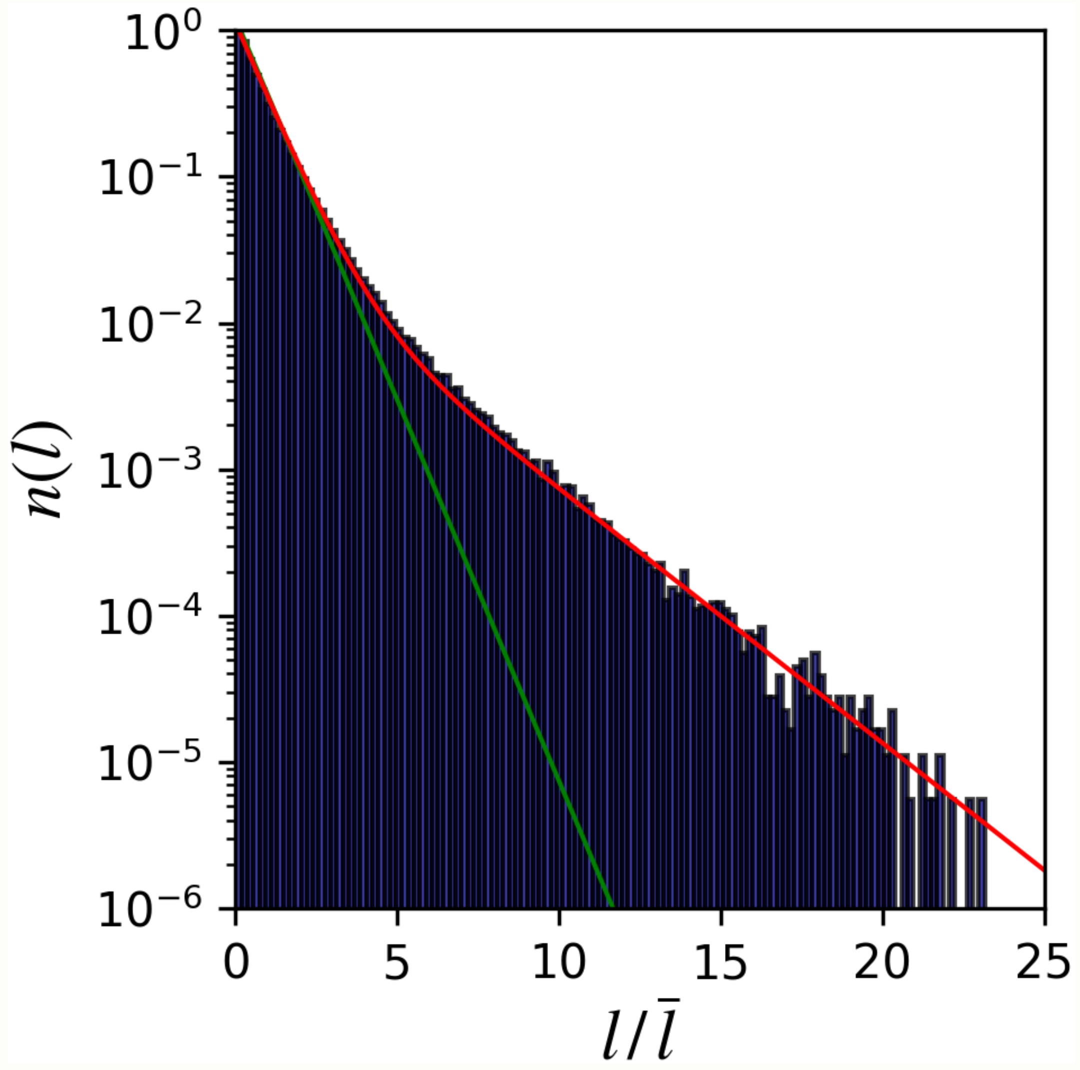
(Equivalent with no growth)





Piecewise linear growth of $\dot{l}/l$ leads to double exponential distribution.

(Or other functions that conform to a similar qualitative form)

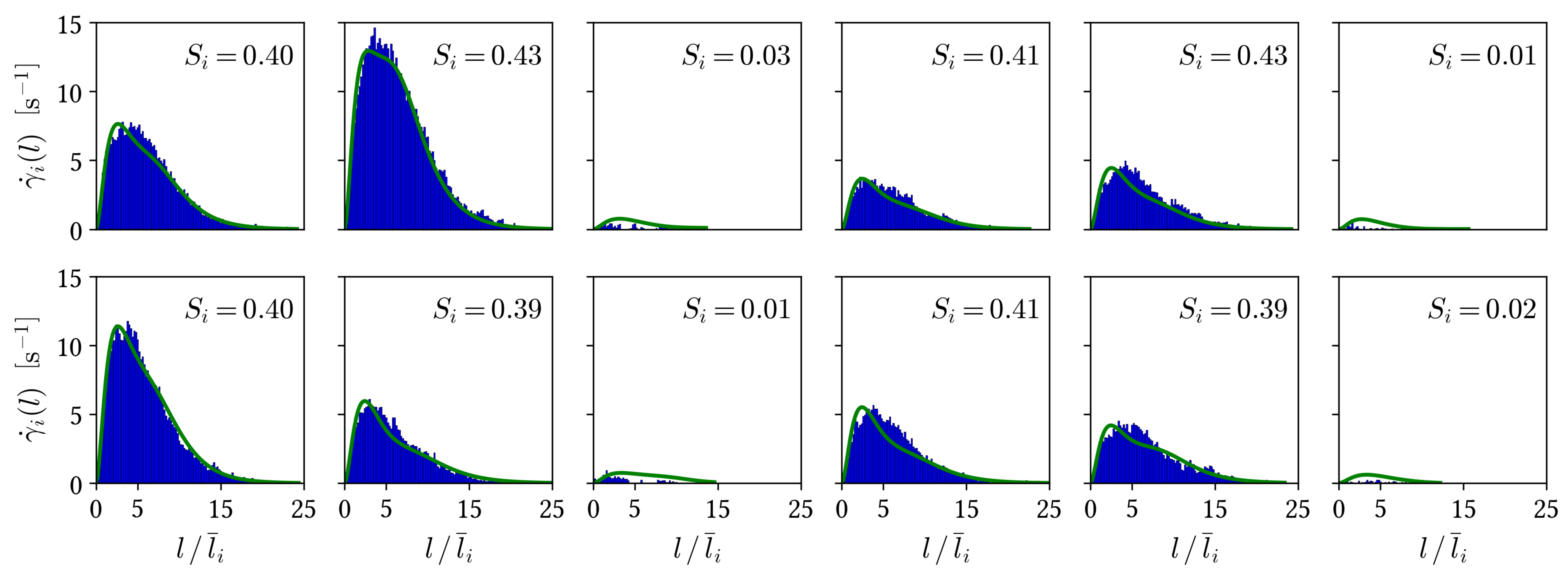


Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

Crystal plasticity: *link length → shear rates*

Shear rates distributions as a function of link length

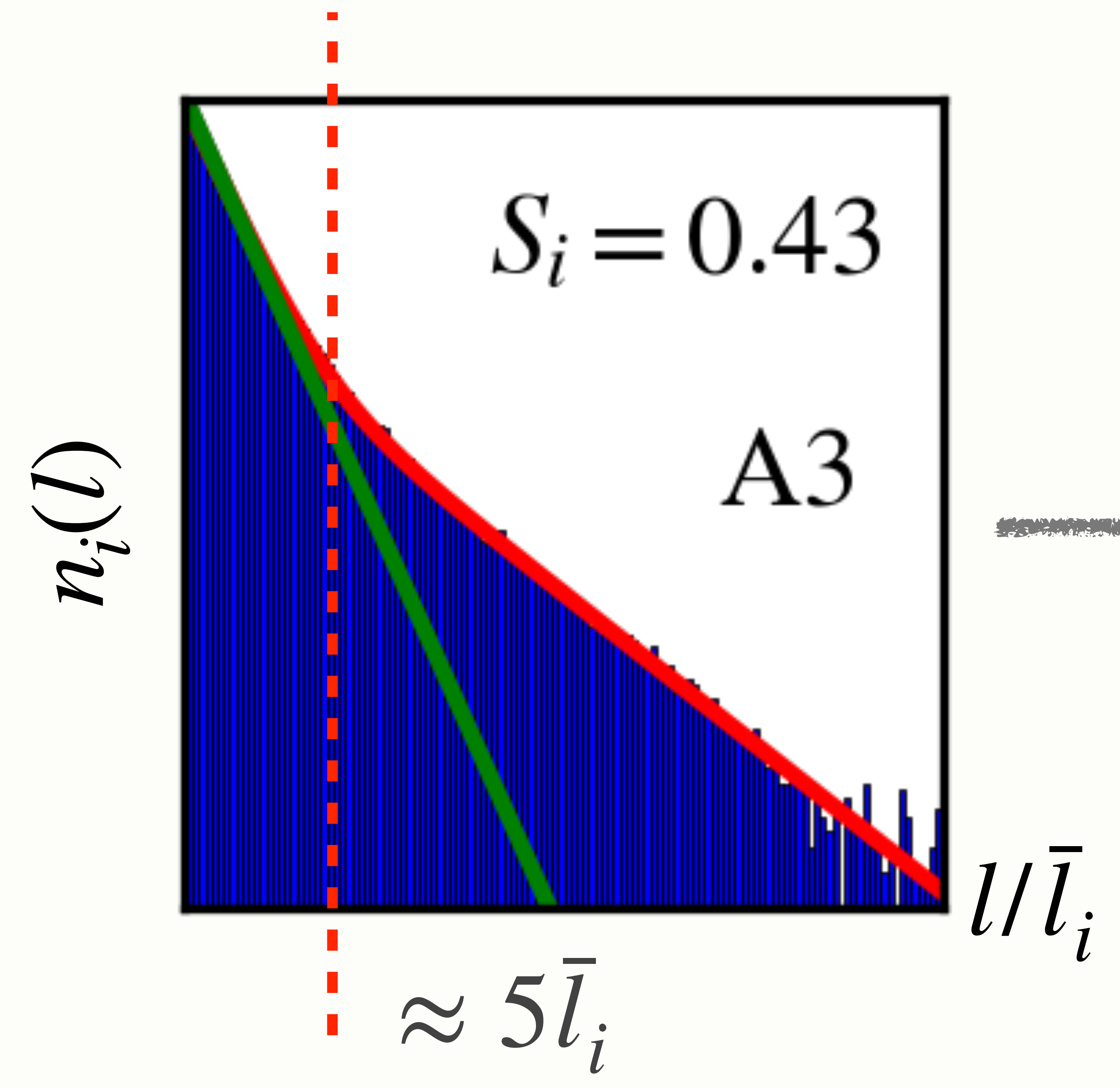
Loading orientation: [0.01, 0.04, 0.99]

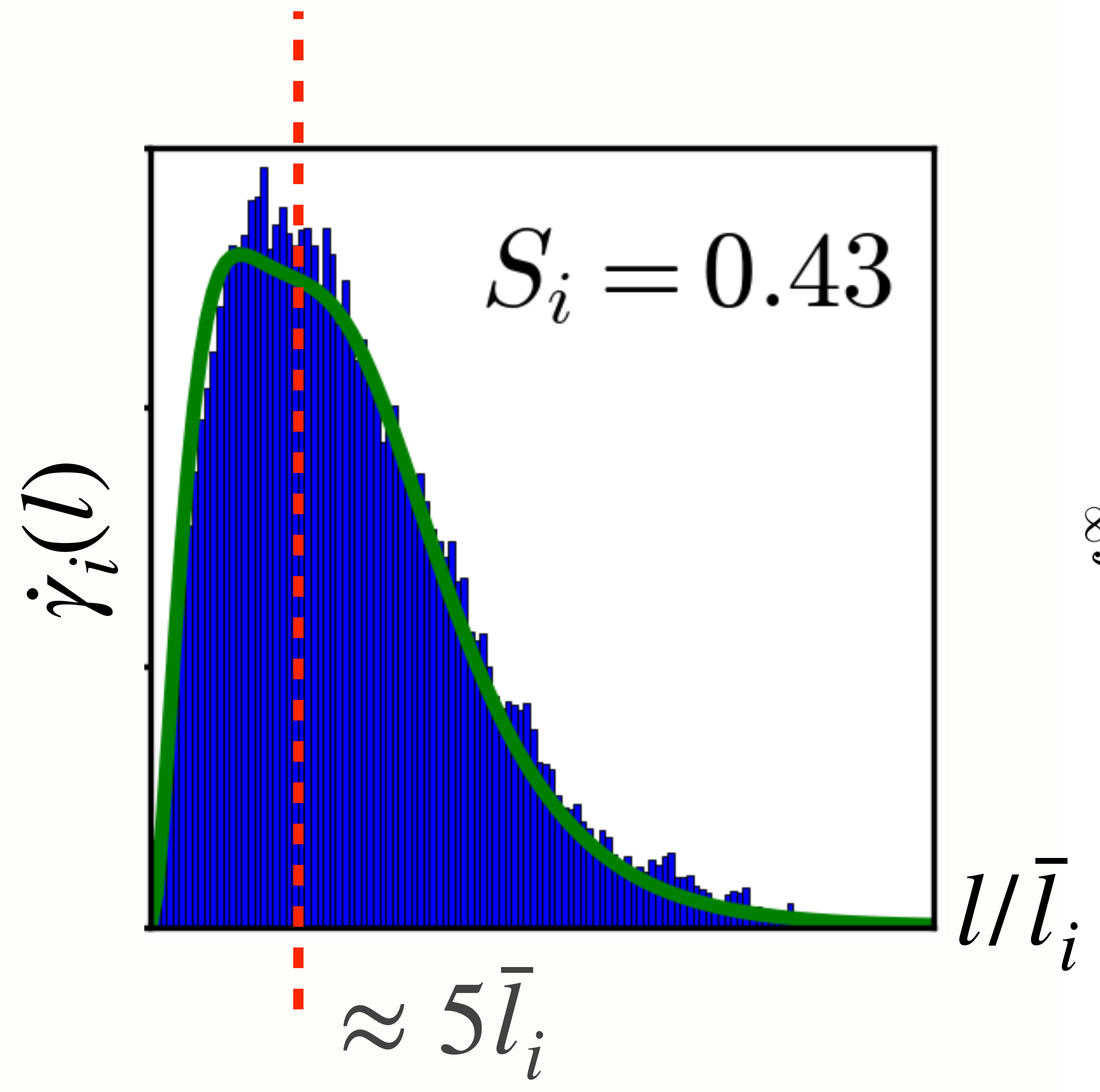


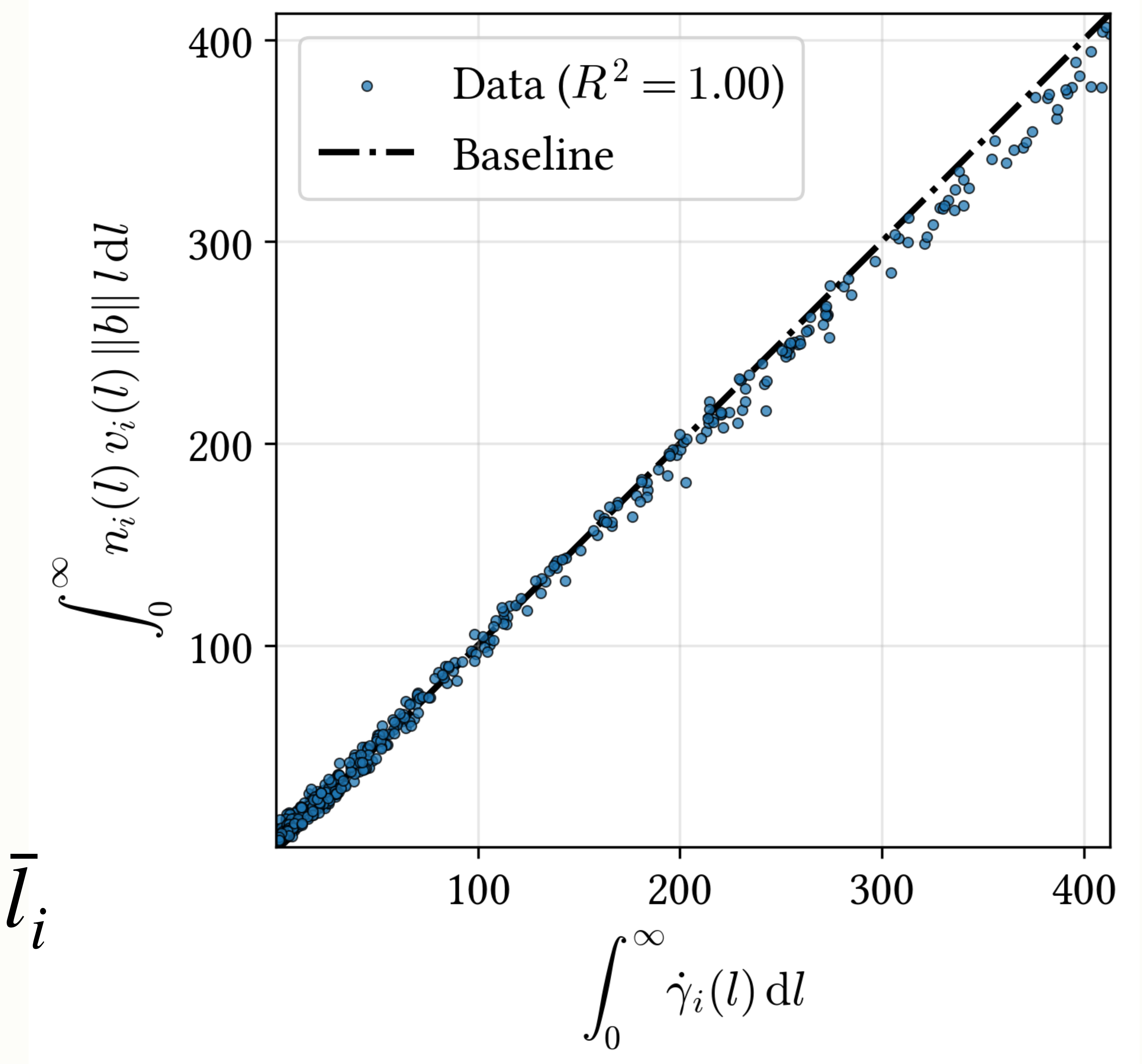
We postulate velocity function-based flow rule — can predict shear rates (as a function of link length) accurately on individual slip systems across different loading orientations.

Shear rates distributions can be accurately predicted

Loading orientation near $[001]$







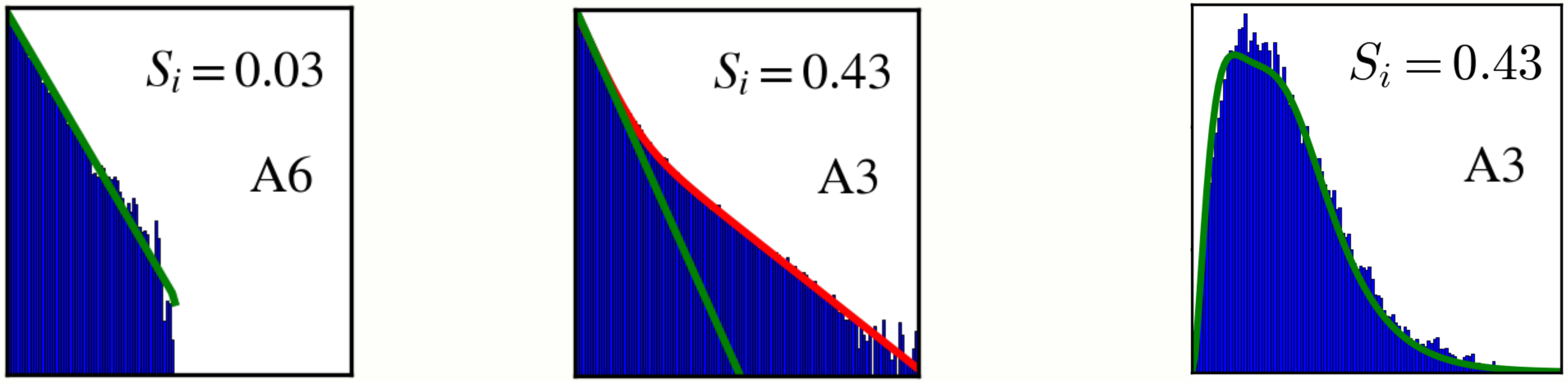
Shear rate (on individual slip system) as a function of link length peaks at around $l \approx 5\bar{l}_i$.

Longer links ($\geq 5\bar{l}_i$) contribute significantly to the shear rates (as a function of l).

Overall shear strain rates can be predicted accurately.

Summary

- Inactive slip systems follow a **single-exponential distribution**.
- Active slip systems follow a **double-exponential distribution** with a long tail.
- A **generalized Poisson process** with growth rules explains both single- & double-exponentials.
- Longer links **contribute significantly** to shear rates; one can predict strain rates from link statistics.



Q & A

Paper

J. Mech. Phys. Solids, 210, 106533 (2026).
DOI:10.1016/j.jmps.2026.106533

OpenDiS

Open source DDD code. (Python & C++)
https://github.com/OpenDiS/OpenDiS

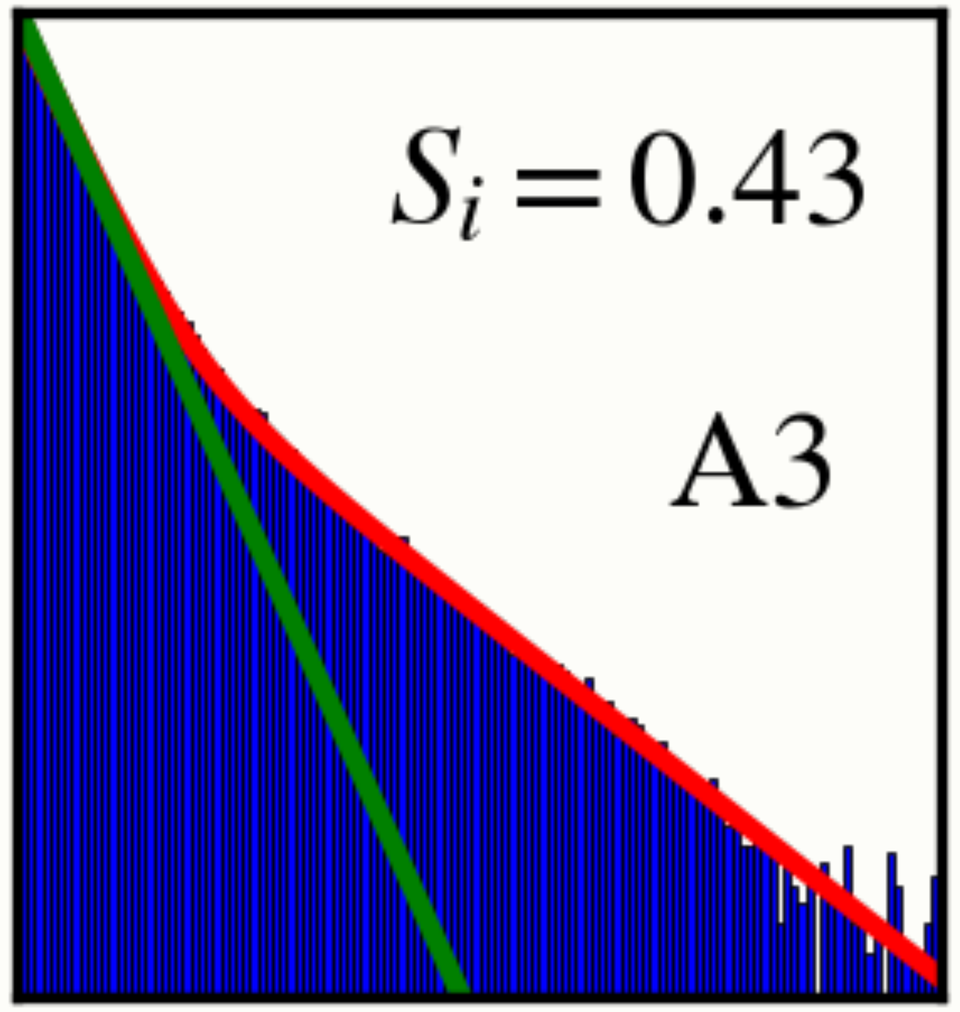
Contact: hzhai@stanford.edu (H.Z.); caiwei@stanford.edu (W.C.)

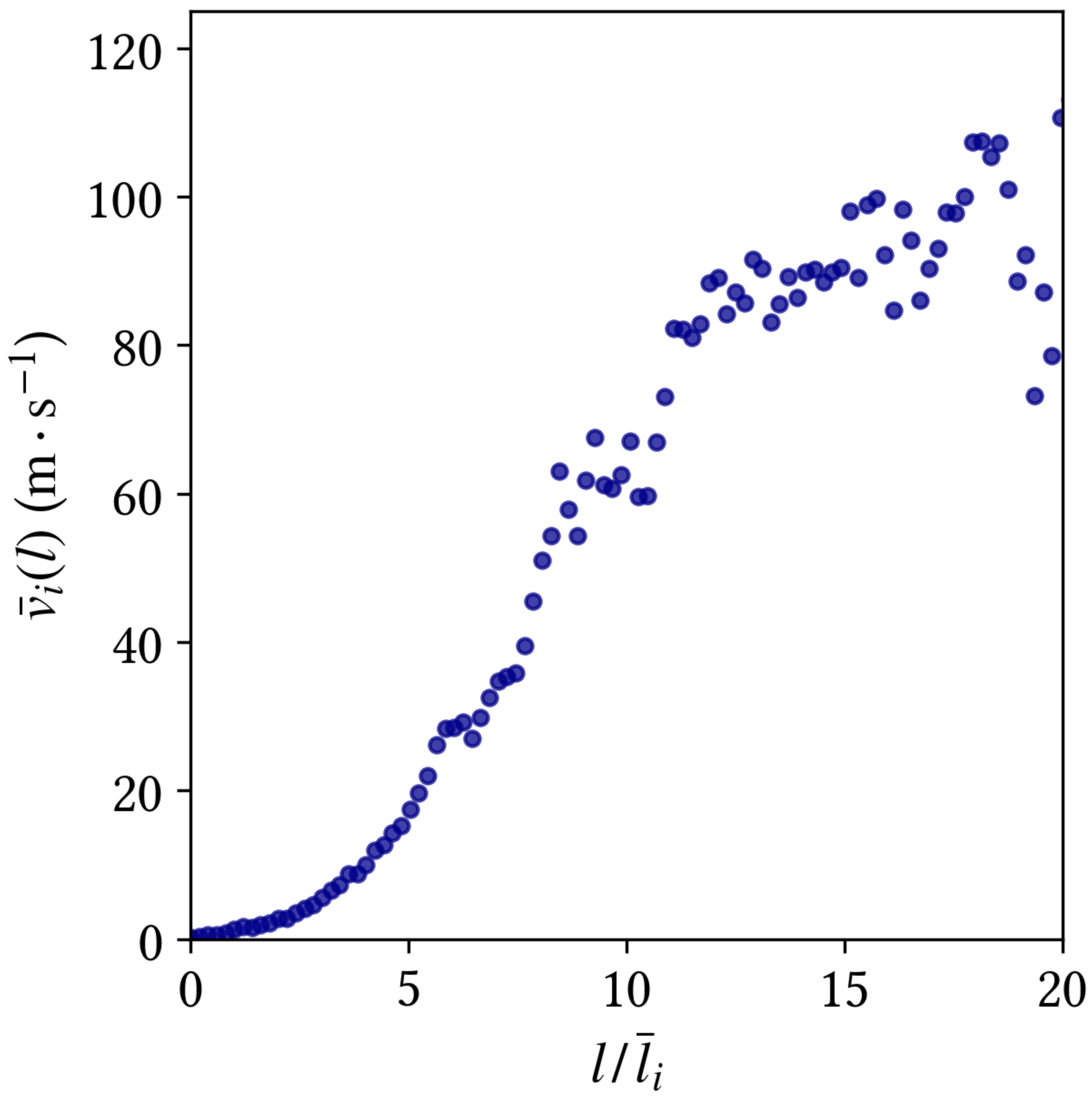
Supplementary Slides

Mobility of dislocation links

Link velocity is defined as shear rates divided by link length distributions times link length:

$$\bar{v}_i(l) = \dot{\gamma}_i(l) / \left(l\, b\, n_i(l) \right)$$

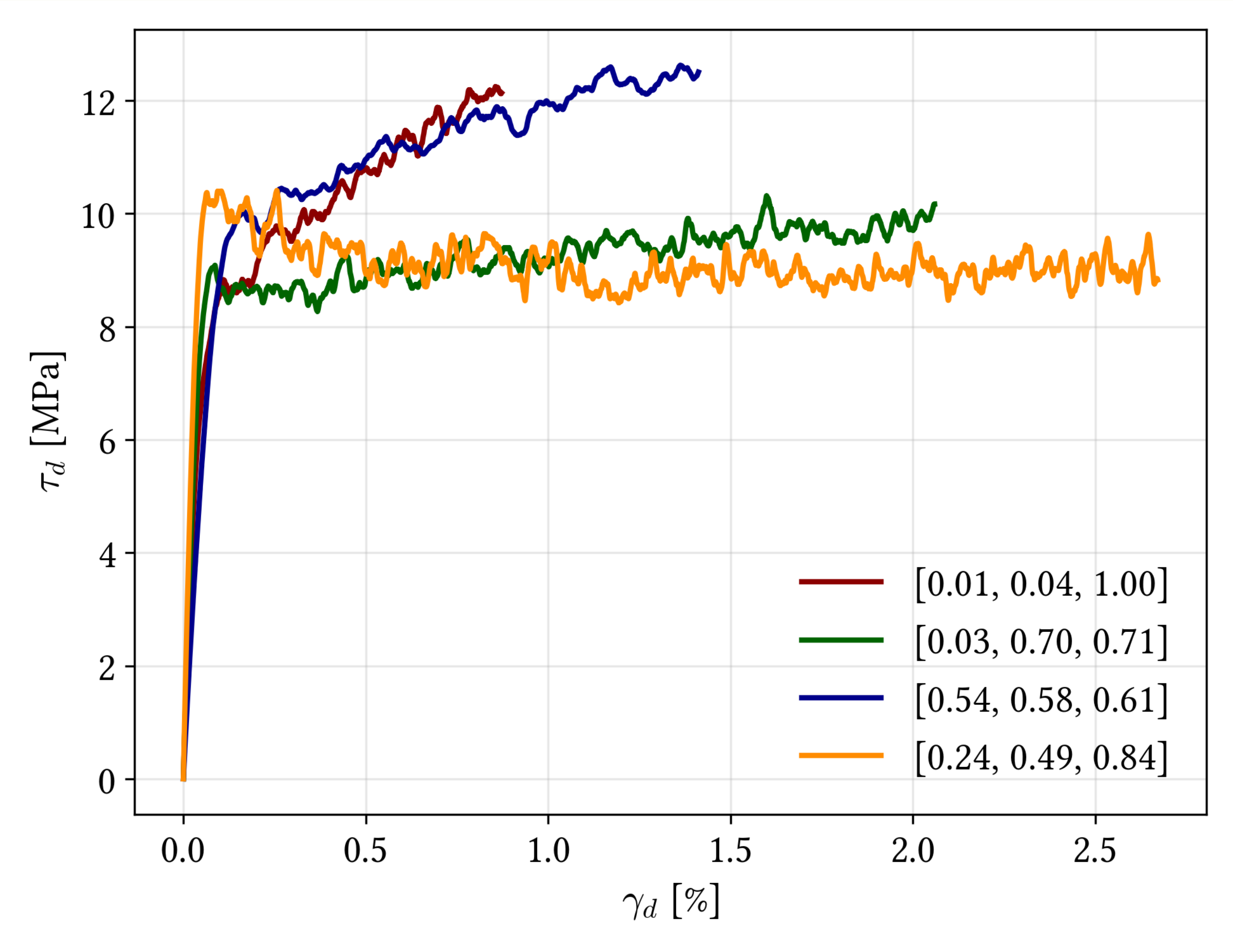




Longer links are highly mobile (higher velocity) during strain hardening.

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

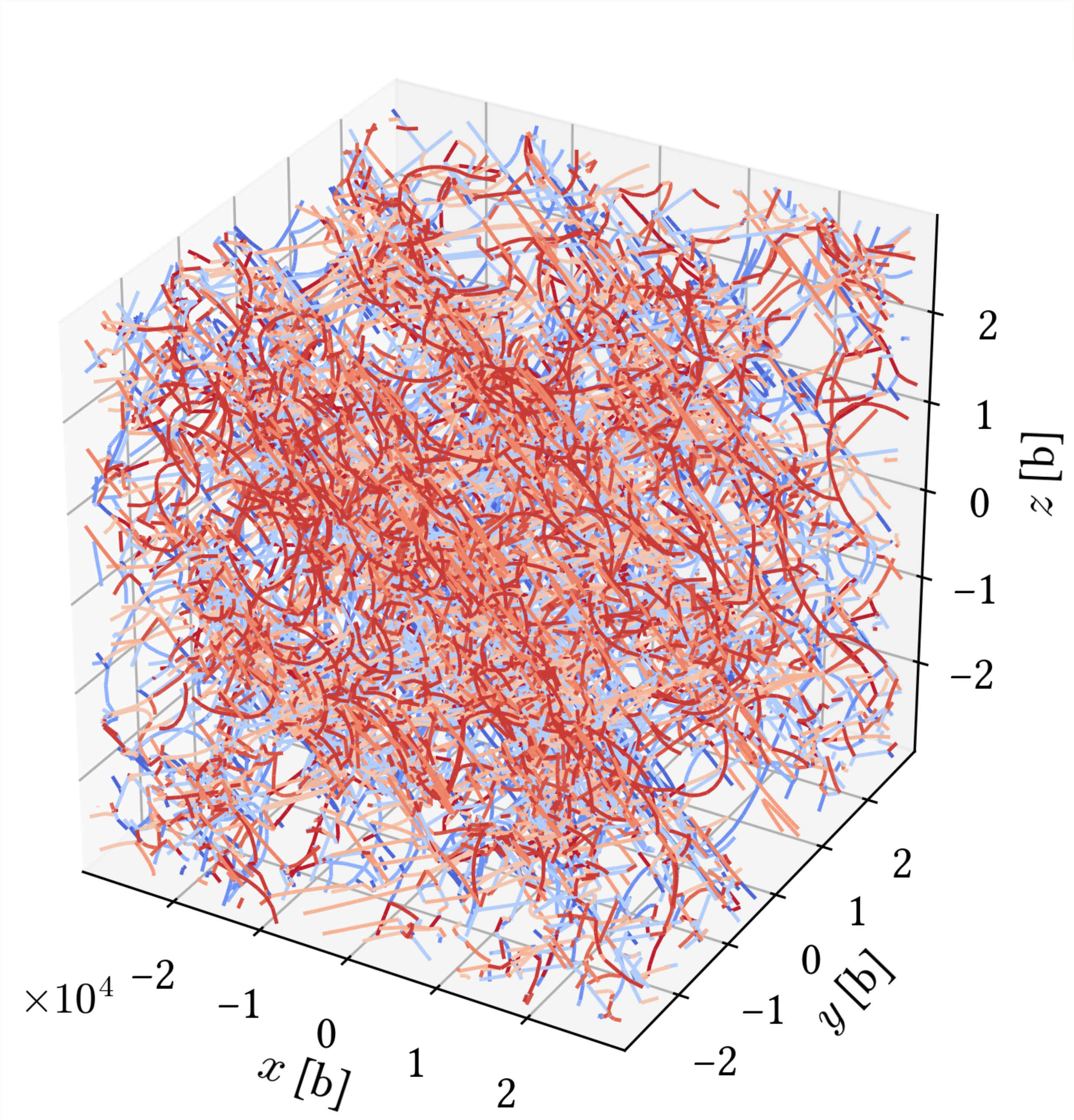
From link statistics to flow rule

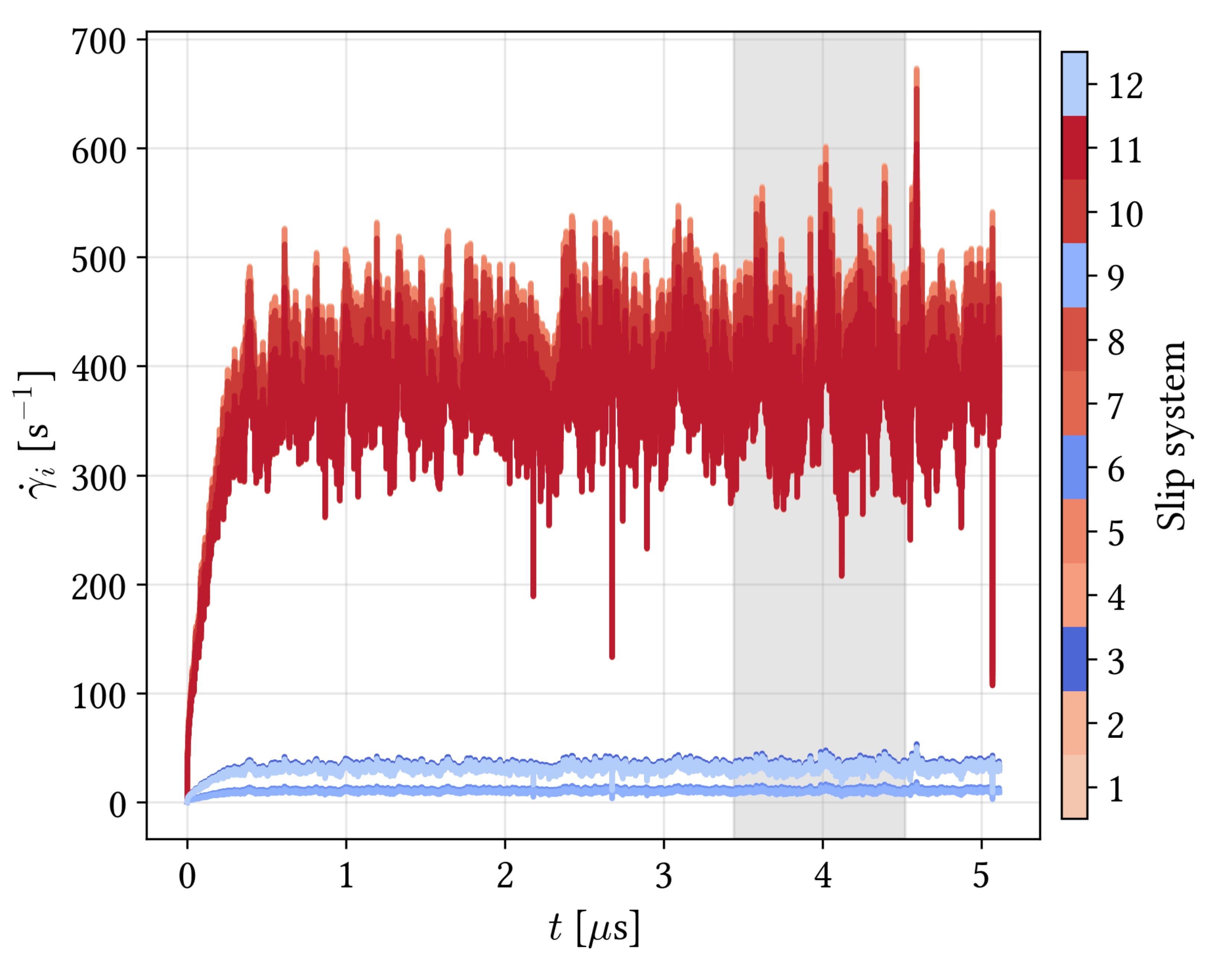


Stress-strain curves behave differently (different hardening rates) under different loading orientations.

Q: Can you predict strain rates from link length statistics (on individual slip systems)?

Link length distribution $n_i(l)$ relates to shear rates $\dot{\gamma}_i$ via dislocation line motion, i.e., the velocity v_i.



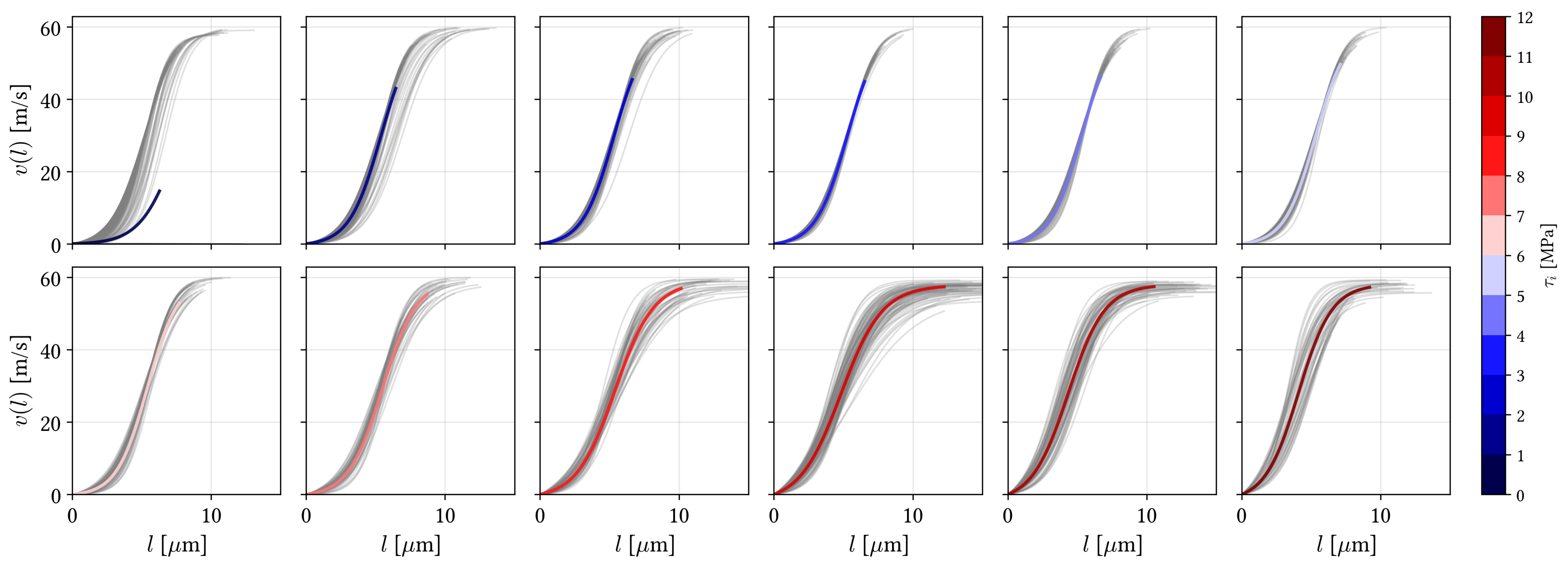


Loading orientation: [0.01, 0.04, 0.99]

Zhai[1], Akhondzadeh[1], et al., *to be submitted*, 2026.

Flow rule from link statistics

We hypothesize there exists a velocity function $v_i(l)$ that can describe the motion of dislocation lines during strain hardening.



We postulate that this velocity function takes the form a sigmoid function.

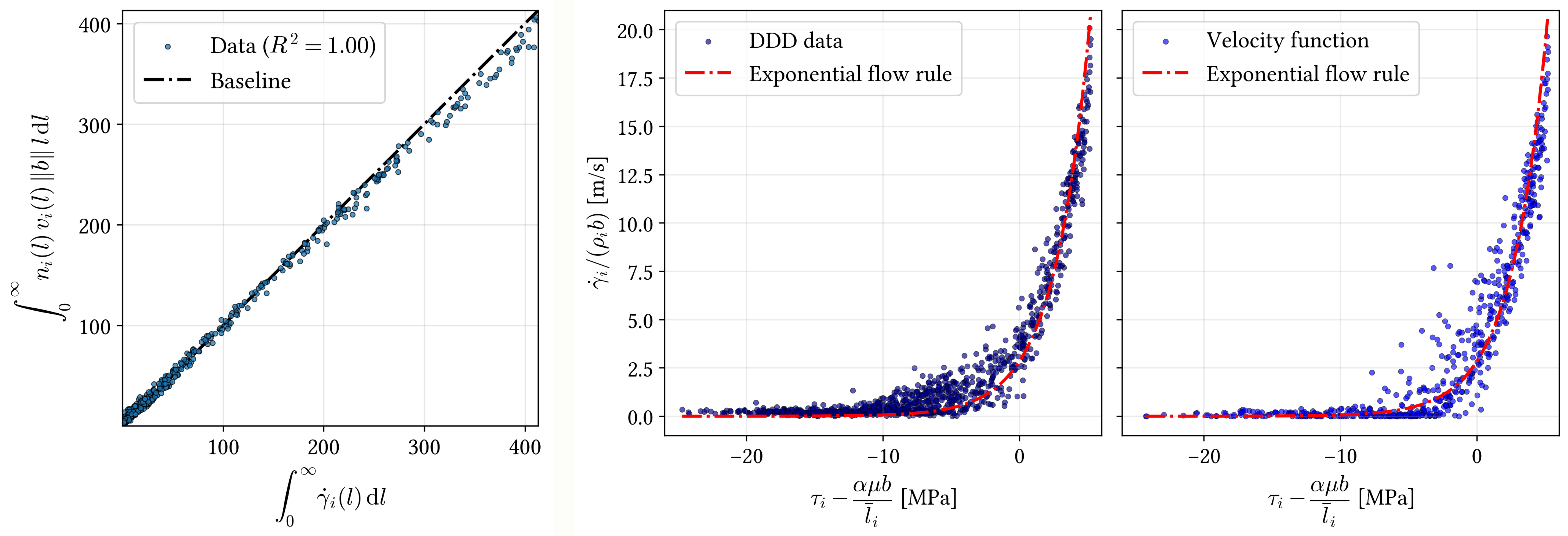
This function captures an asymptotic behavior and "activation effects" w.r.t. link length.

Zhai[1], Akhondzadeh[1], et al., *to be submitted*, 2026.

Flow rule from link statistics

Previous work reported density-based flow rule (Akhondzadeh et al., *JMPS*, 2020):

$$\frac{\dot{\gamma}_i}{\rho_i b} = v_0 \exp\left[\frac{1}{s_0}\left(\tau_i - \left(\mu b\sqrt{a'_{ij}\rho_j} - \tau_0\right)\right)\right]$$

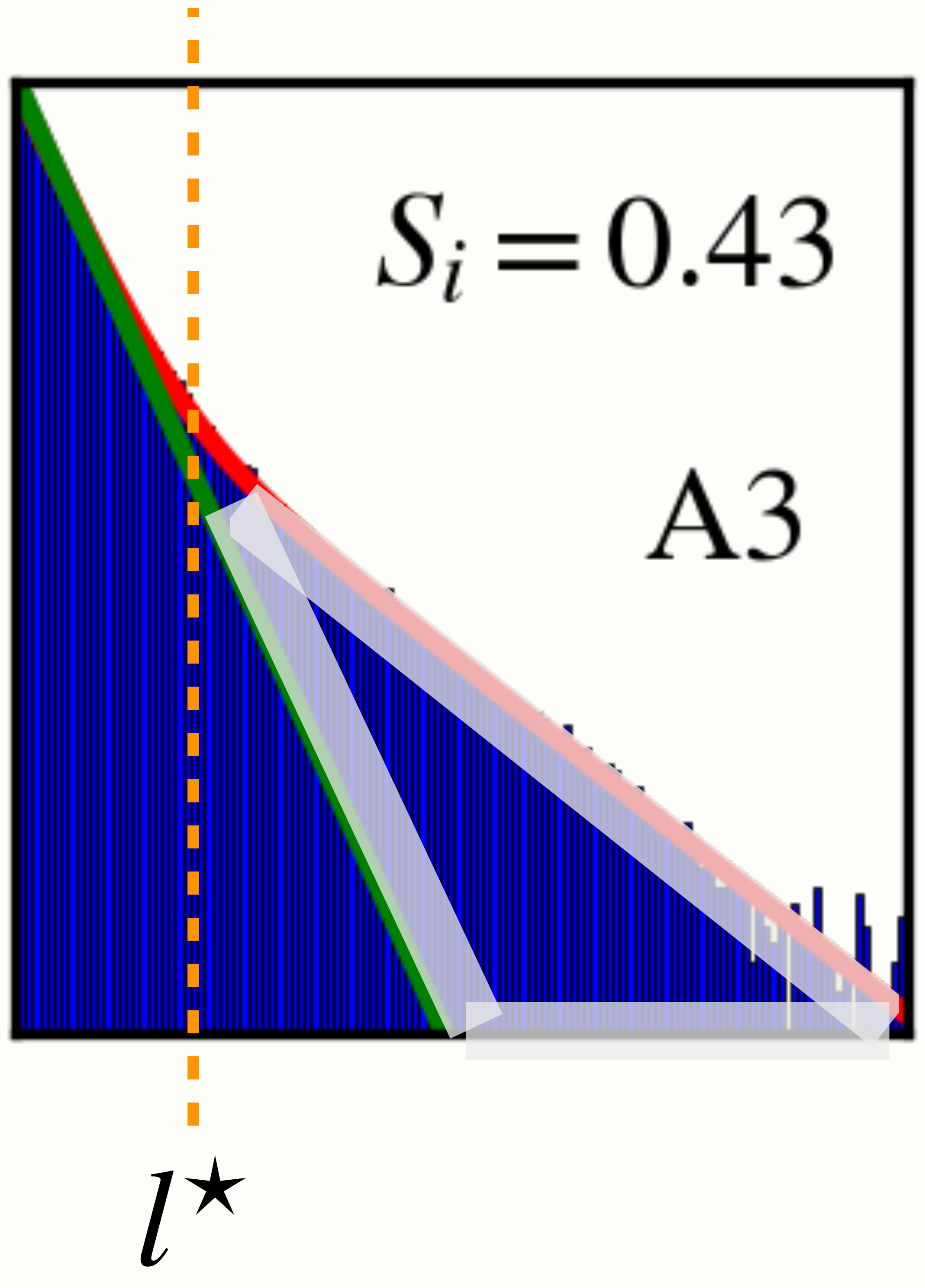


The proposed model can predict the overall strain rates pretty accurately. It also captures the spread of the shear rates when plotted against the applied stress.

Zhai[1], Akhondzadeh[1], et al., *to be submitted*, 2026.

Statistical characteristics of long links

Statistical characteristics



"Transition length" from single → double exponential distribution:

$$l^\star = \ln\left(\frac{N_i^{(1)}}{l_i^{(1)}} \cdot \frac{l_i^{(2)}}{N_i^{(2)}}\right) \Big/ \left(\frac{1}{l_i^{(1)}} - \frac{1}{l_i^{(2)}}\right)$$

Fraction of longer links (2nd exponential) in the full distribution:

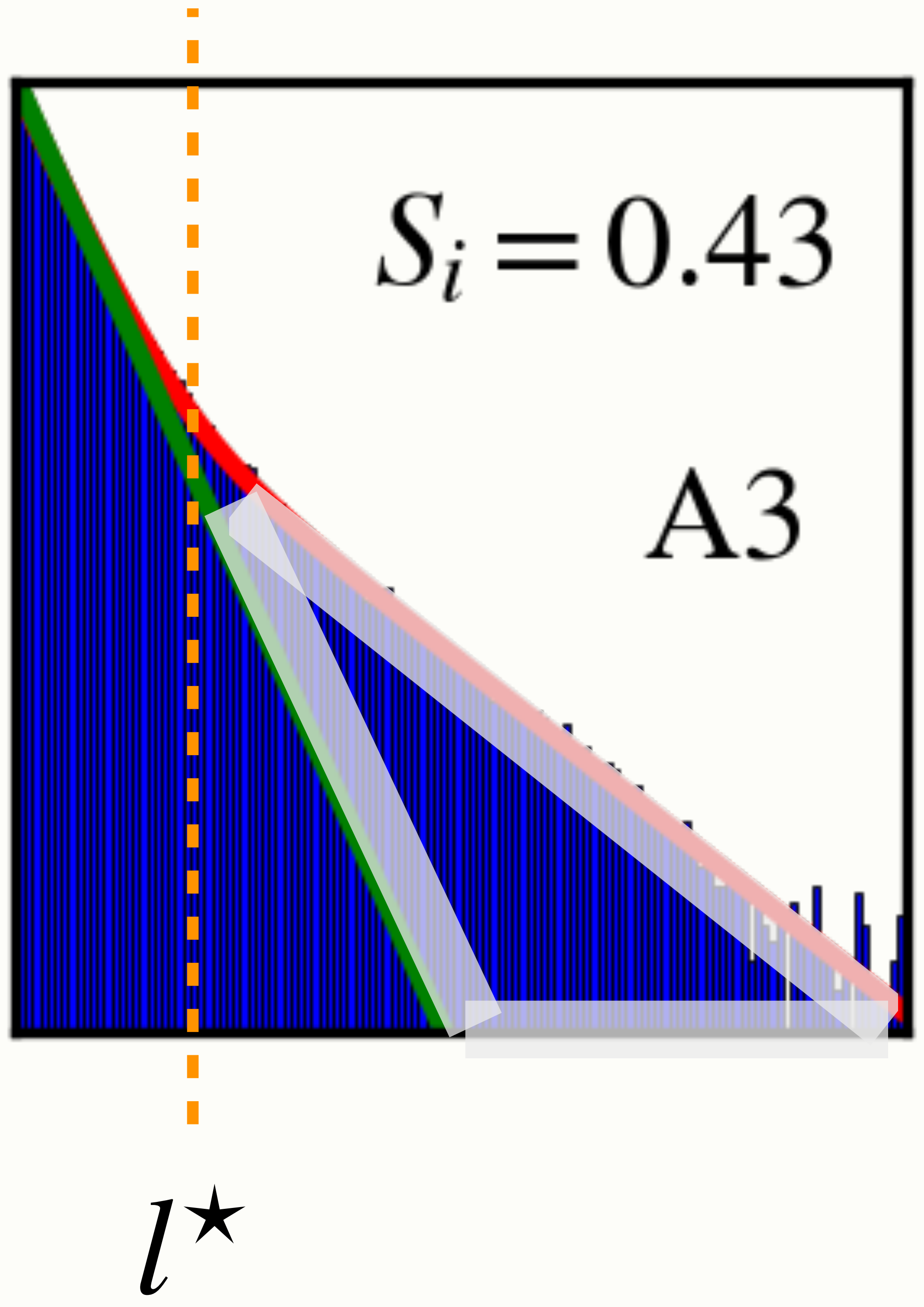
$$f_i^{(2)} \equiv \frac{1}{N_i}\int_{l^\star}^{\infty} \frac{N_i^{(2)}}{\bar{l}_i^{(2)}} e^{-l/\bar{l}_i^{(2)}}\, dl$$

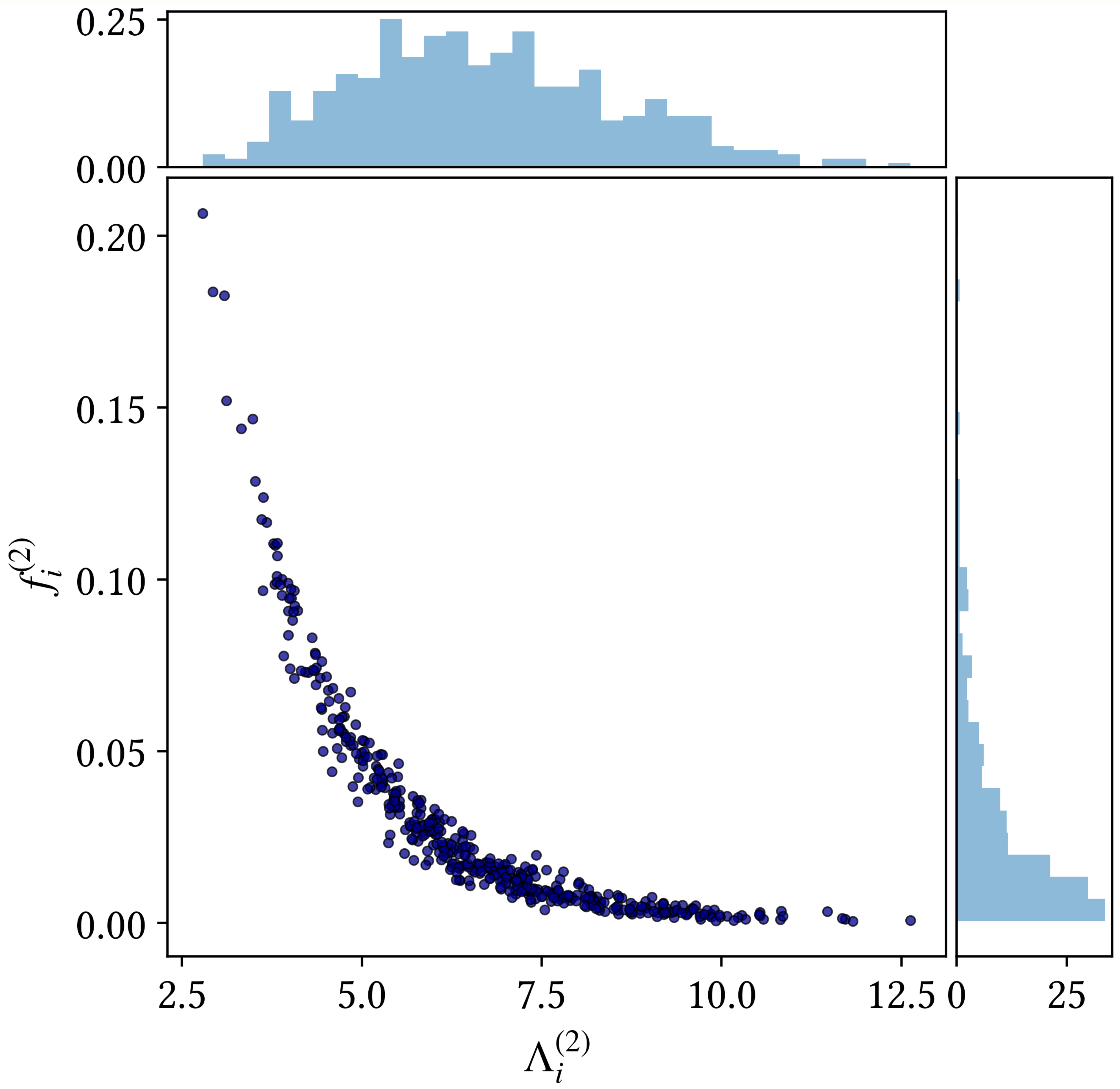
Average link length of the tail (of the 2nd exponential):

$$\Lambda_i^{(2)} \equiv \frac{1}{\bar{l}_i} \frac{1}{f_i^{(2)} N_i} \int_{l^\star}^{\infty} l\, \frac{N_i^{(2)}}{\bar{l}_i^{(2)}} e^{-l/\bar{l}_i^{(2)}}\, dl = \frac{l^\star + \bar{l}_i^{(2)}}{\bar{l}_i} = \frac{l^\star}{\bar{l}_i} + \lambda_i^{(2)} = \lambda_i^{(2)}\left(1 + \frac{l^\star}{\bar{l}_i^{(2)}}\right).$$

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. [10.1016/j.jmps.2026.106533](https://doi.org/10.1016/j.jmps.2026.106533)

Statistical characteristics





Long-tail links typically constitute less than 5% of all links but are 5–10 times longer than the system average $\bar{l}_i$, with a clear negative correlation between tail fraction $f_i^{(2)}$ and characteristic length $\Lambda_i^{(2)}$.

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

Double exponential distributions

Single exponential distribution (no fitting parameters):

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

Double exponential distribution (summation of two exponential distributions):

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

Fitting parameters (for the double exponentials):

$$\lambda_i^{(1)} \equiv \bar{l}_i^{(1)} / \bar{l}_i \qquad \lambda_i^{(2)} \equiv \bar{l}_i^{(2)} / \bar{l}_i$$

Fitting constrains (for the double exponentials):

$$N_i^{(1)} + N_i^{(2)} = N_i \qquad N_i^{(1)}\, \bar{l}_i^{(1)} + N_i^{(2)}\, \bar{l}_i^{(1)} = N_i\, \bar{l}_i$$

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. [10.1016/j.jmps.2026.106533](https://doi.org/10.1016/j.jmps.2026.106533)

Double exponential distributions

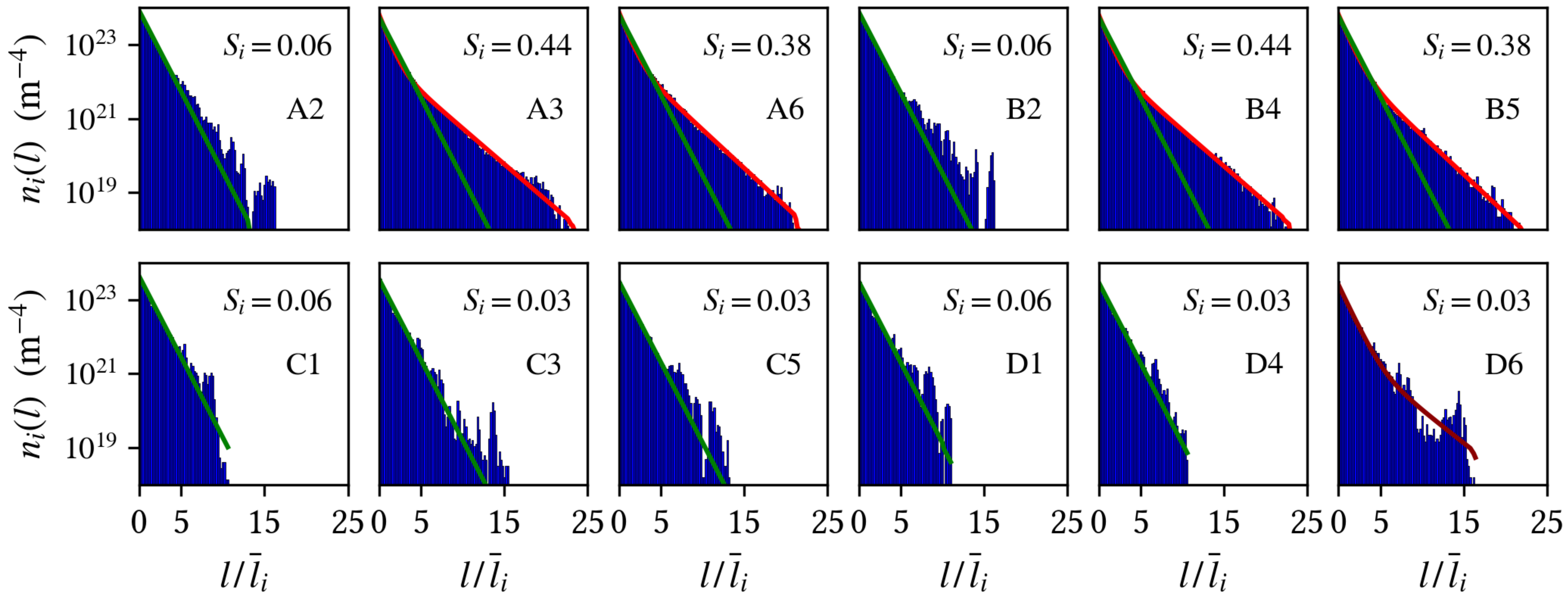
Index i	$\mathbf{n}_i$	$\mathbf{b}_i$	SB index	S_i	N_i	$N_i^{(1)}$	$N_i^{(2)}$	$\bar{l}_i$	$\lambda_i^{(1)}$	$\lambda_i^{(2)}$	ρ_i
1	$(\bar{1}11)$	$\frac{1}{2}[0\bar{1}1]$	A2	0.40	4.15	3.89	0.26	4.53	0.91	2.42	1.88
2	$(\bar{1}11)$	$\frac{1}{2}[101]$	A3	0.43	5.64	5.15	0.48	5.32	0.86	2.44	3.00
3	$(\bar{1}11)$	$\frac{1}{2}[110]$	A6	0.03	4.17	—	—	3.94	—	—	1.64
4	(111)	$\frac{1}{2}[0\bar{1}1]$	B2	0.42	5.06	4.83	0.23	5.43	0.90	3.13	2.75
5	(111)	$\frac{1}{2}[\bar{1}01]$	B4	0.43	4.95	4.57	0.37	5.16	0.87	2.55	2.55
6	(111)	$\frac{1}{2}[\bar{1}10]$	B5	0.01	3.83	—	—	4.26	—	—	1.63
7	$(\bar{1}\bar{1}1)$	$\frac{1}{2}[011]$	C1	0.39	4.86	4.74	0.12	4.63	0.95	3.01	2.25
8	$(\bar{1}\bar{1}1)$	$\frac{1}{2}[101]$	C3	0.38	4.25	3.94	0.31	4.29	0.88	2.48	1.83
9	$(\bar{1}\bar{1}1)$	$\frac{1}{2}[\bar{1}10]$	C5	0.01	3.72	—	—	4.01	—	—	1.49
10	$(1\bar{1}1)$	$\frac{1}{2}[011]$	D1	0.42	5.38	4.87	0.50	5.17	0.85	2.50	2.78
11	$(1\bar{1}1)$	$\frac{1}{2}[\bar{1}01]$	D4	0.38	4.57	4.16	0.40	4.68	0.87	2.35	2.14
12	$(1\bar{1}1)$	$\frac{1}{2}[110]$	D6	0.03	3.89	—	—	3.88	—	—	1.51

Loading orientation: [0.03, 0.05, 0.99]

The first exponential takes up most of the links in the distribution.

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

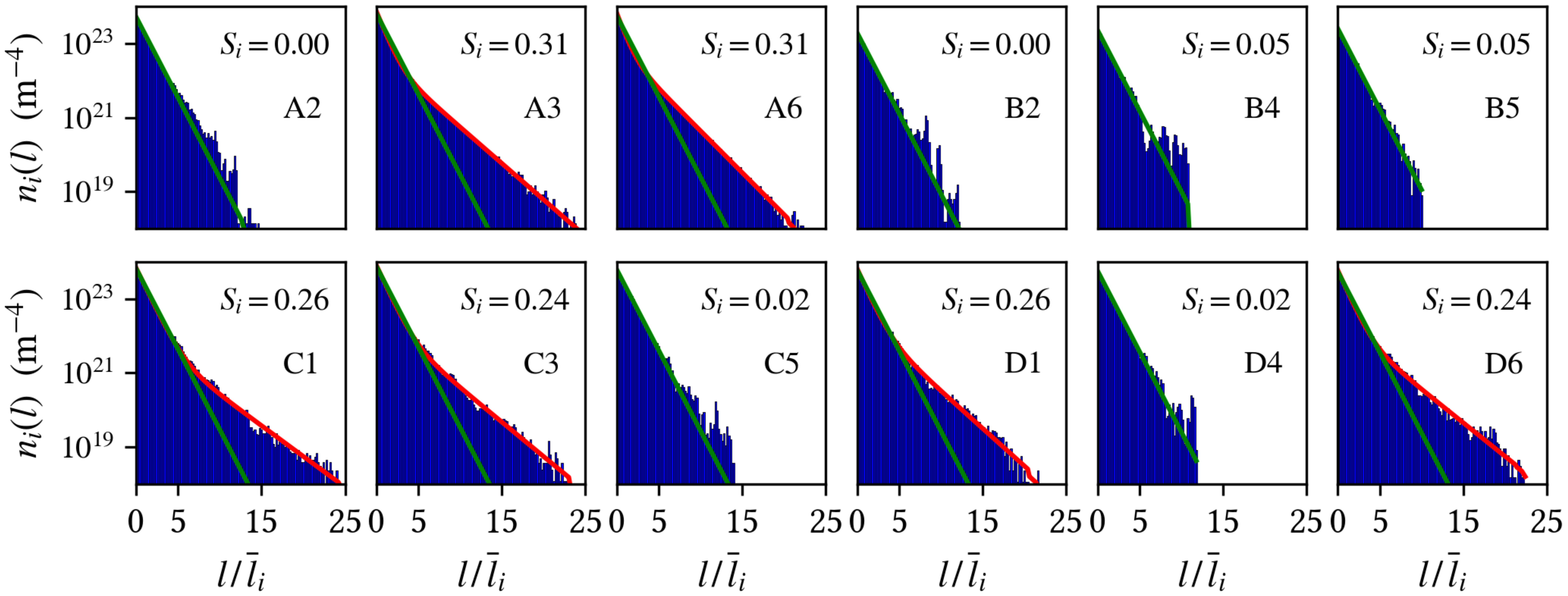
Link statistics near $[0\ 1\ 1]$



Loading orientation: [0.00, 0.65, 0.76]

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

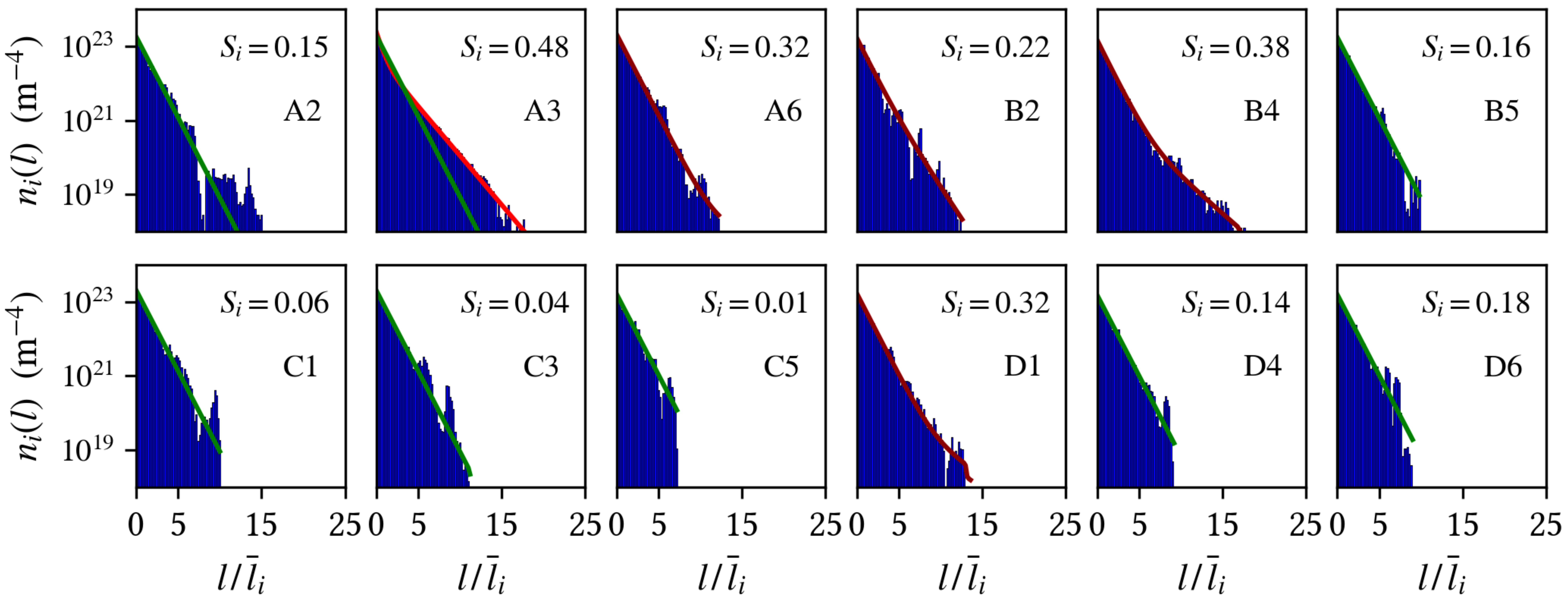
Link statistics near $[1\ 1\ 1]$



Loading orientation: [0.53, 0.60, 0.60]

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

Link statistics near $[1\,2\,3]$



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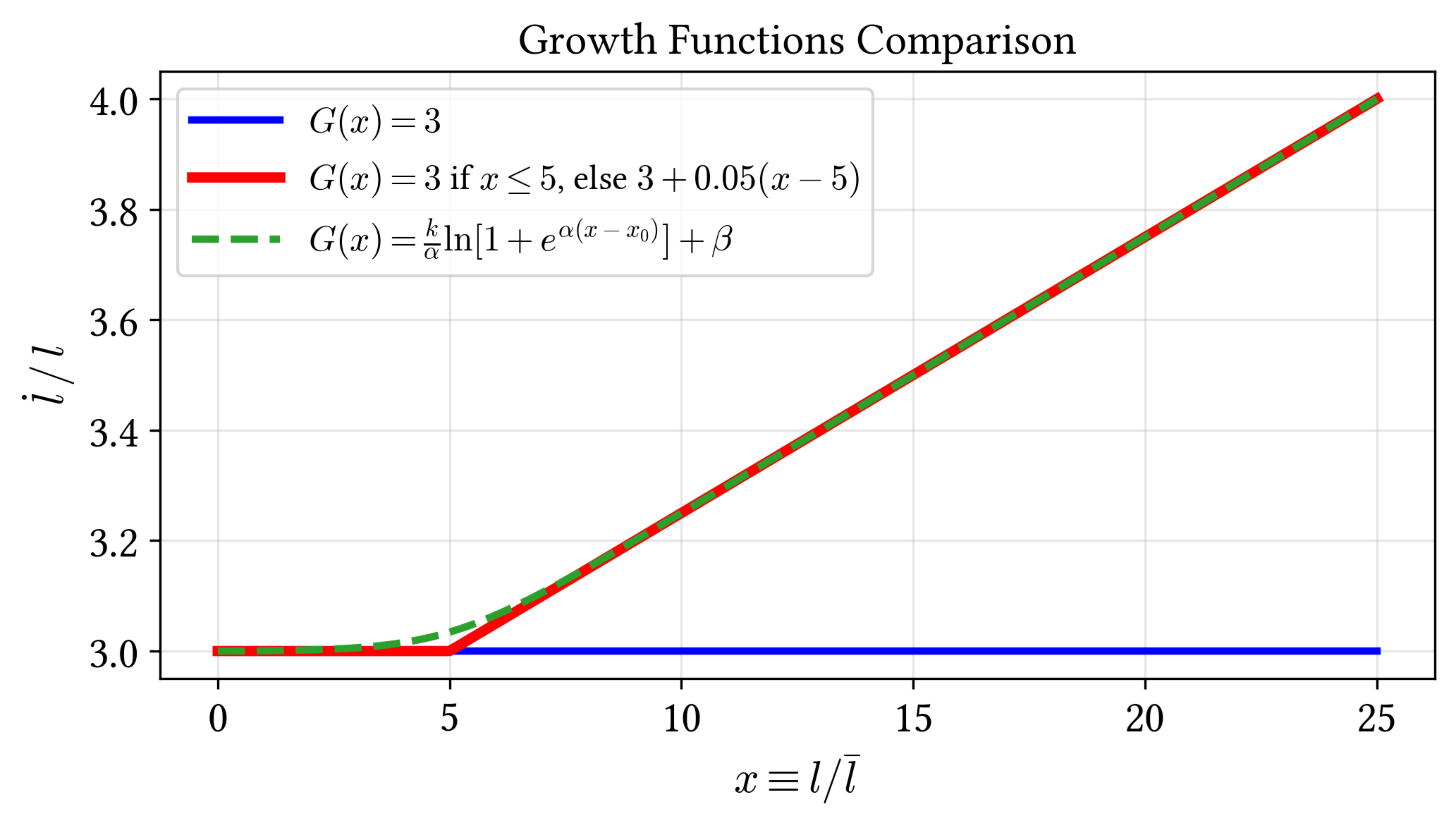
Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. 10.1016/j.jmps.2026.106533

Growth function comparison



Doesn’t have to be a bistep function!

Akhondzadeh[1], Zhai[1], et al., *J. Mech. Phys. Solids*, 2026. [10.1016/j.jmps.2026.106533](https://doi.org/10.1016/j.jmps.2026.106533)