NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

Aalto University

Avalanches in Dislocation Plasticity

Mikko Alava (Aalto, FI; NOMATEN, PL)

Particular thanks to A. Lehtinen and H. Salmenjoki; Lasse Laurson (TUNI); A. Esfandiarpour and S. Papanikolaou; various supercomputers

Contents today:

Bit of motivation

3D DDD and “disorder”

What is the yield stress and why?

Using Machine Learning to understand

Move on to complex alloys

Outlook

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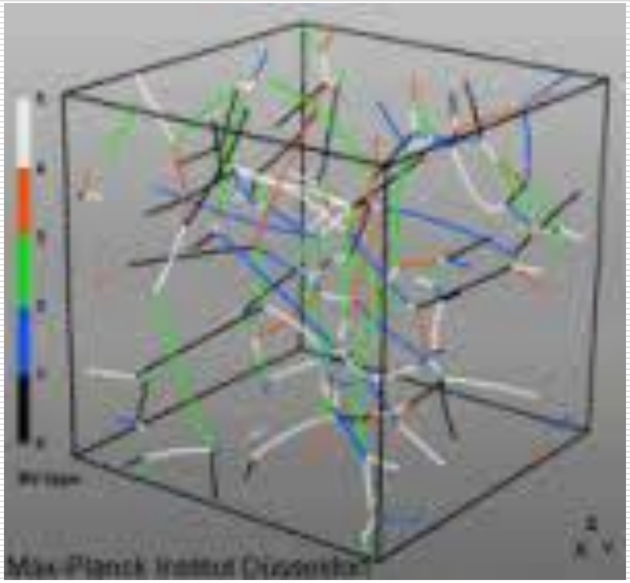
Needed: 3D dislocations

3D: DDD – integrate the response of a set of dislocation lines.

How to do that? ParaDis (Livermore)

Caveats: ε_{max}, dislocation density ρ

(I skip mostly 2D DDD)



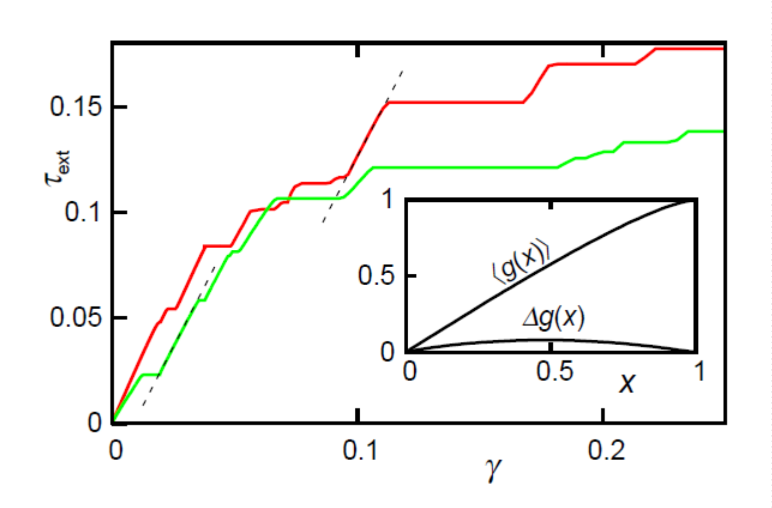
What is the deal?

Macroscopic effects of complexity: yield stress τ, finite size effects.

Dependence on microscopics: ”A”. On history: ρ.

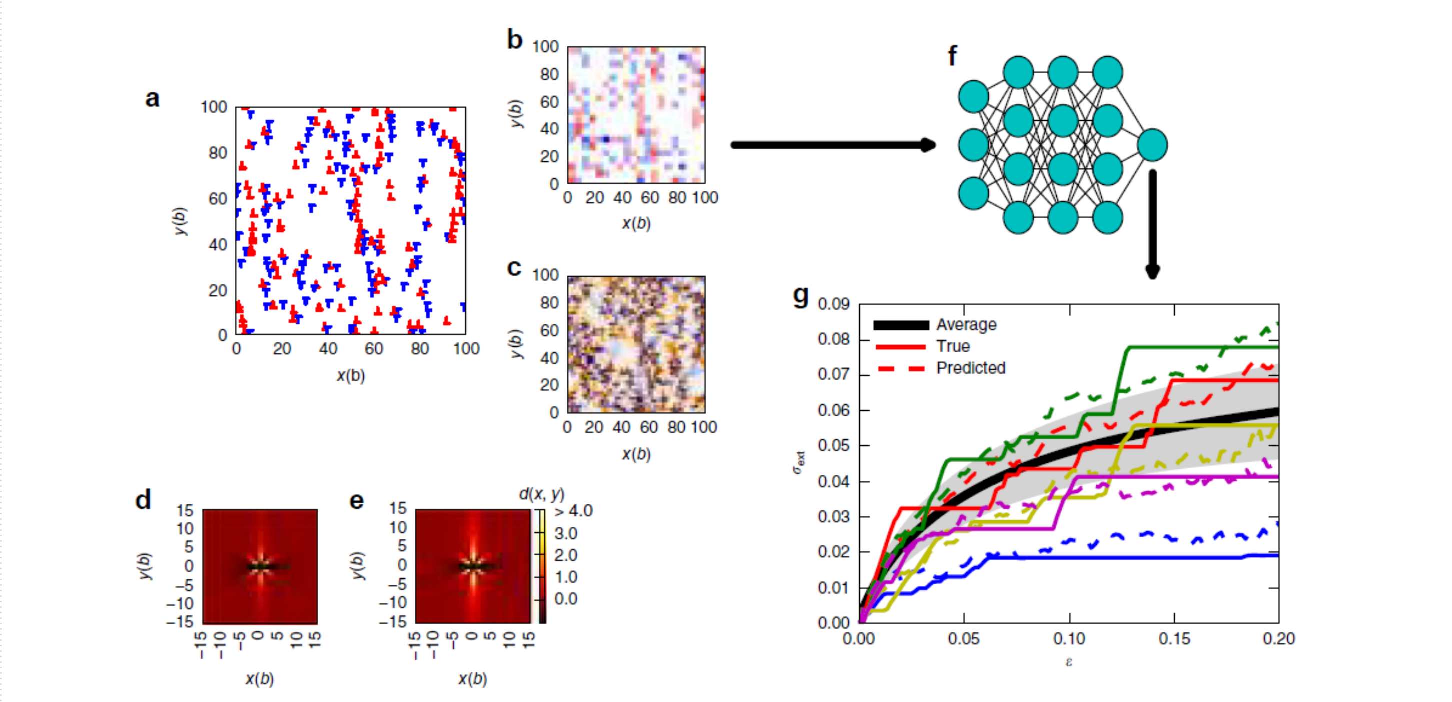
In other words, impact on stress-strain curves.

$$\tau = \tau_0 + A\sqrt{\rho}$$



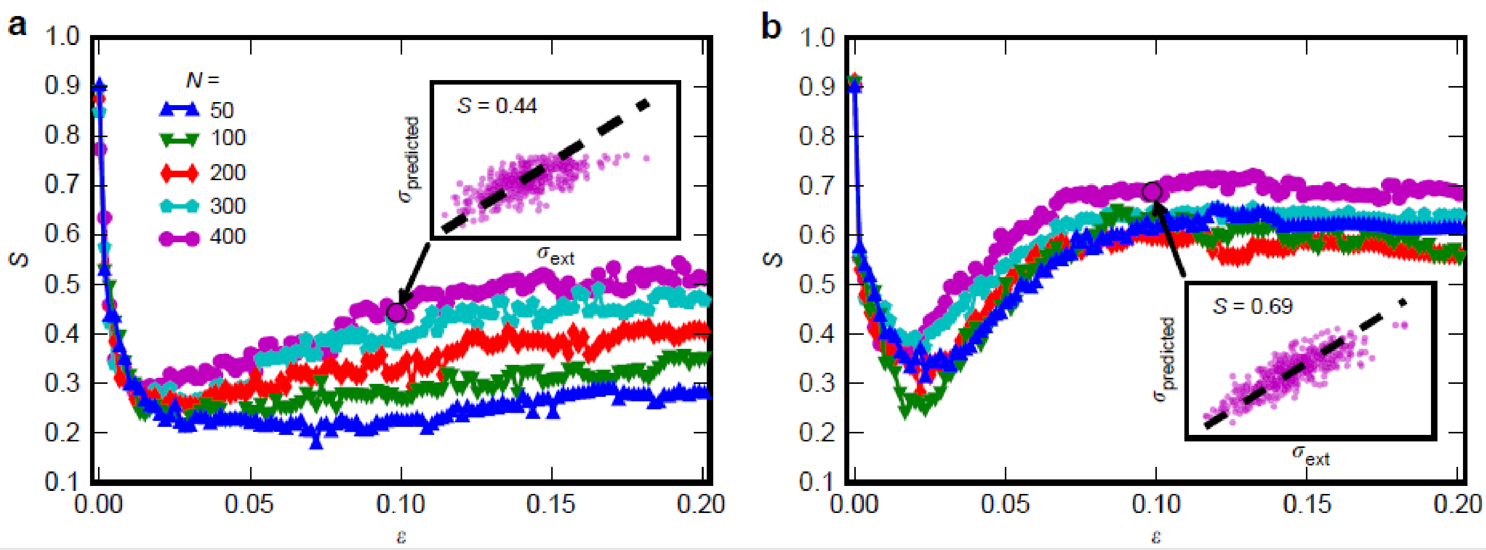
Szabo et al.
PRB 2015

Predicting (2d) DDD ss-curves

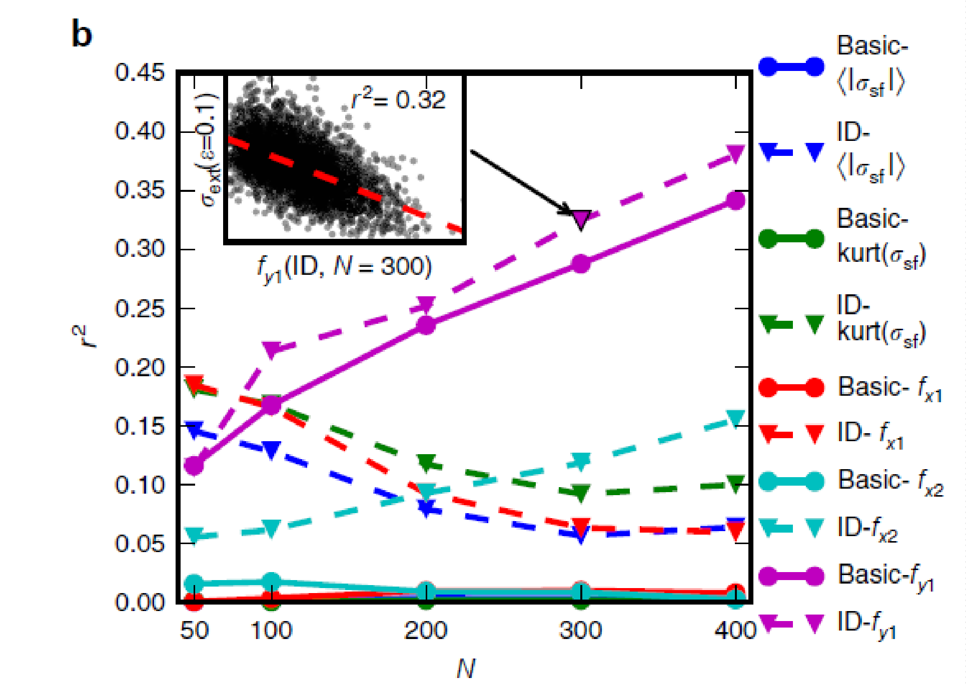


Salmenjoki 2018: since 2D is not depinning, can we predict it?

Error/Predictability vs. strain, N



Impact of descriptors



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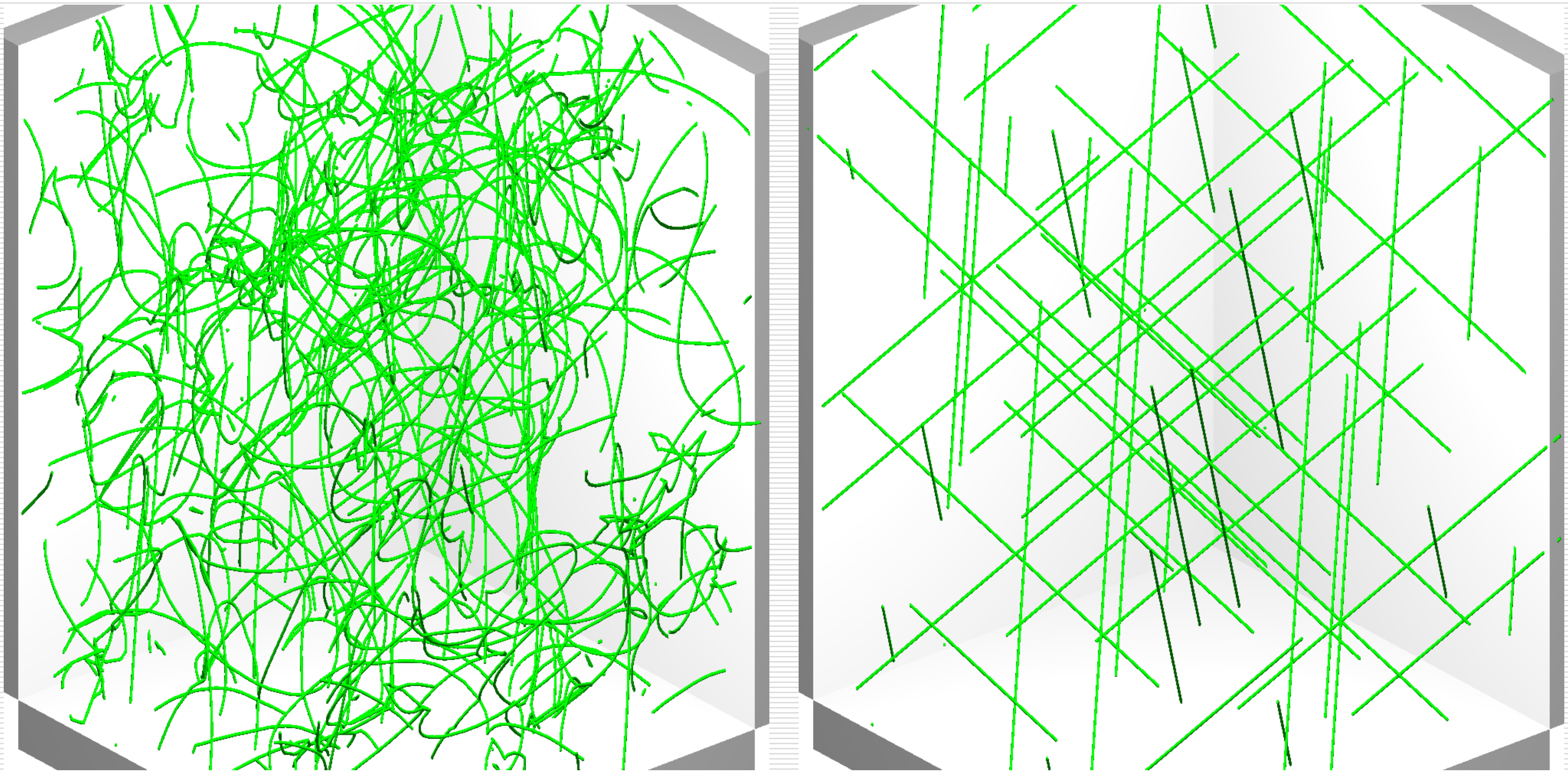
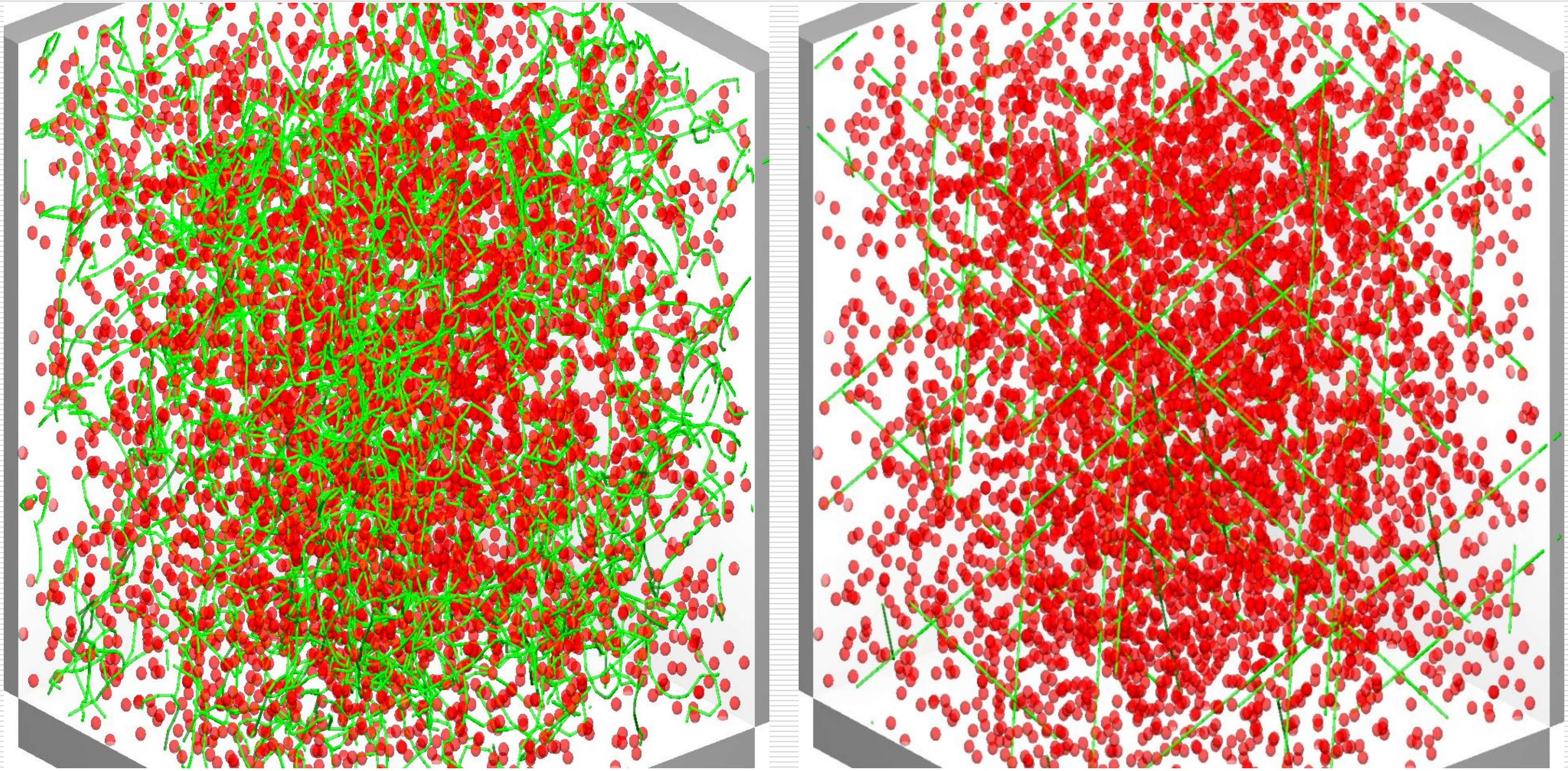
Move to 3D: dislocations… (left: after loading)



Dislocations… and precipitates



3D background

2D results predict “extended criticality”

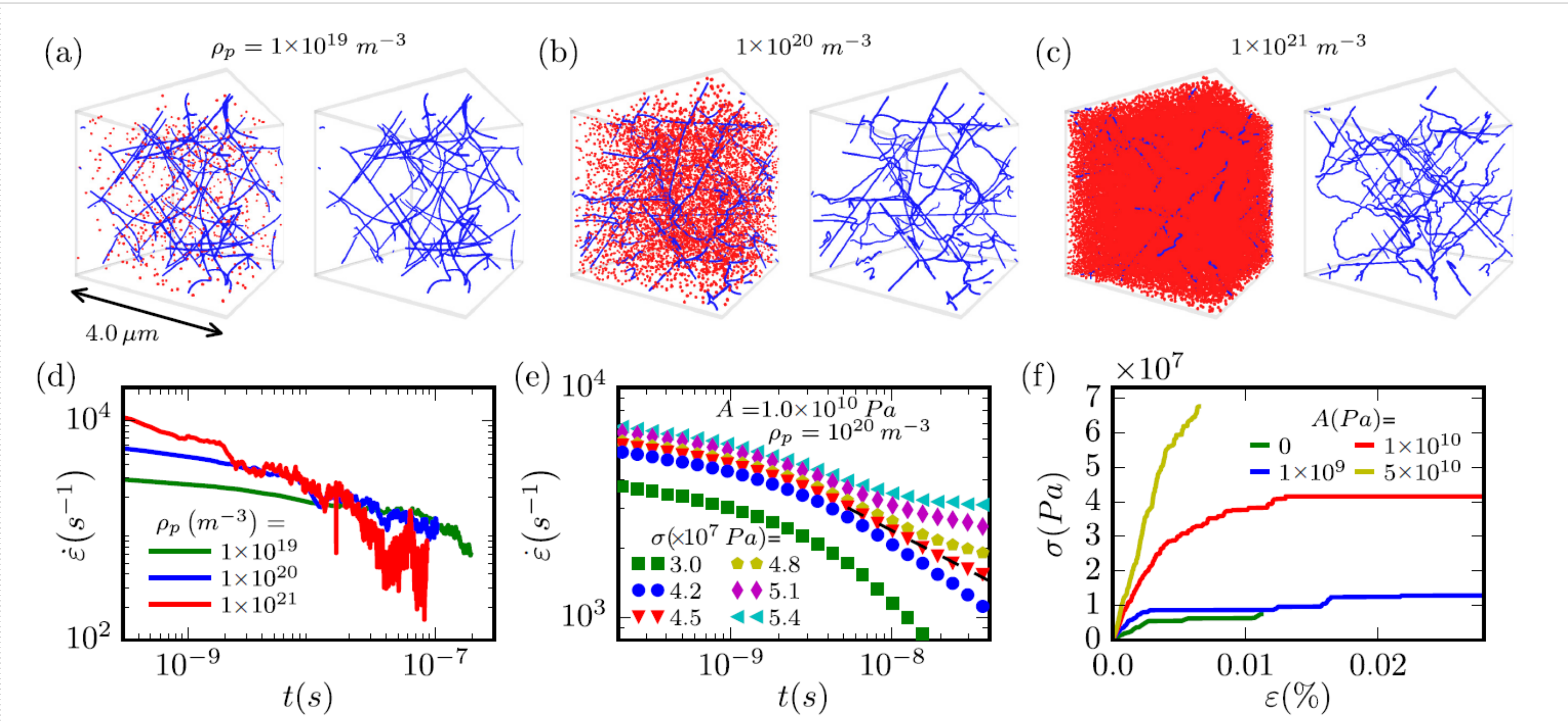
3D DDD (FCC parameters): the same (Lehtinen 2018 PRB) and a broad excitation spectrum (Lehtinen 2018 PRL).

2D shows that extra pinning is important (Ovaska 2015).

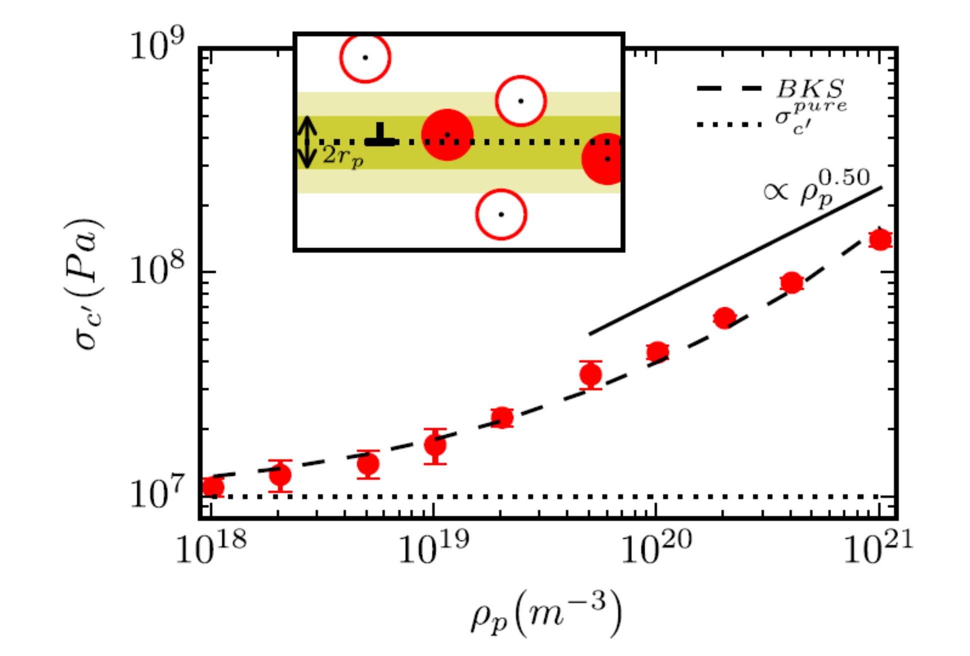
[Weiss, Truskinovsky, Groma et al, Zaiser…]

Precipitates and depinning

- Phys. Rev. Mat. 2020

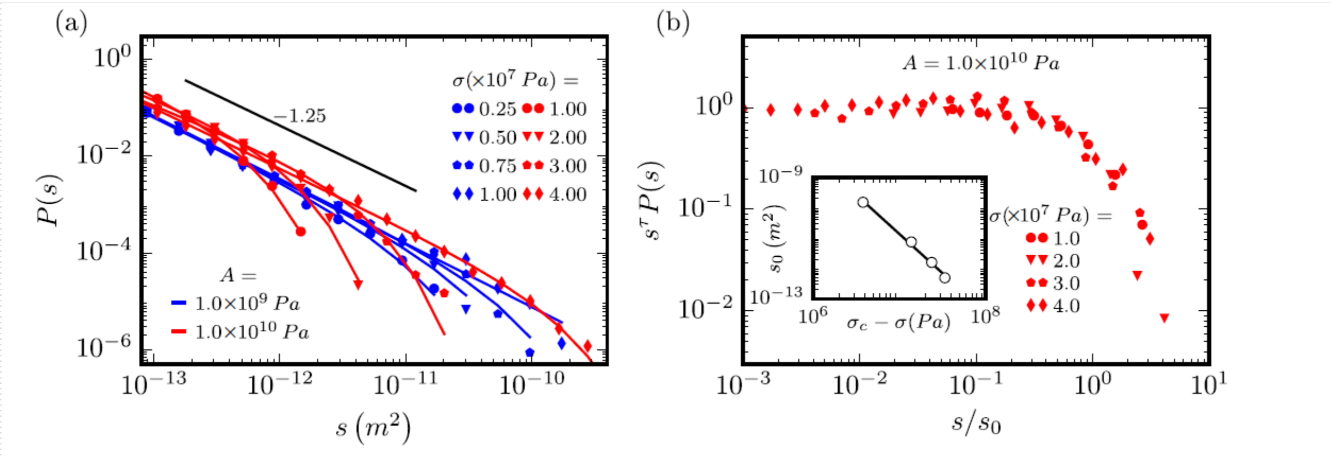


Strengthening effect

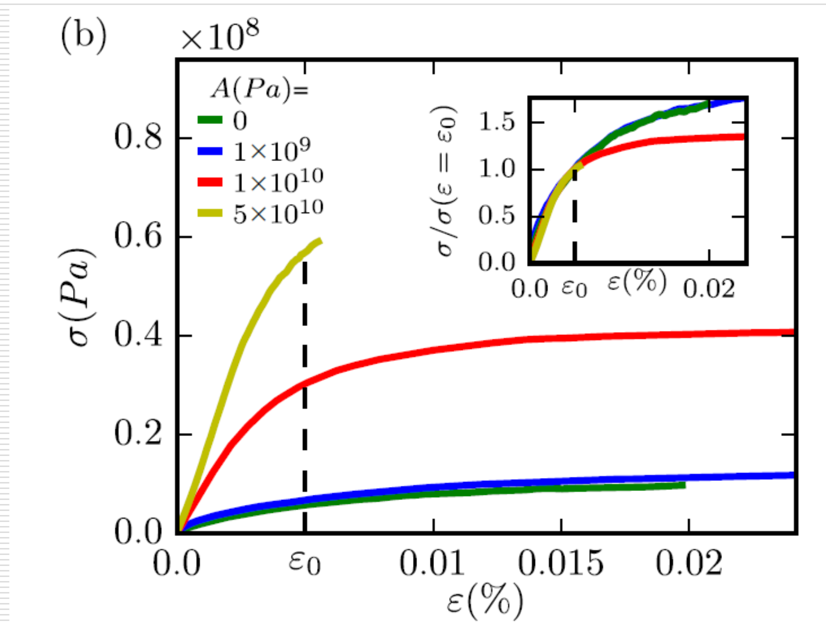


$$\sigma_{c'}(\rho_p) = \sigma_{c'}^{\text{pure}} + \frac{1}{2\pi} \frac{Gb}{\alpha\left[(2r_p\rho_p)^{-1/2} - 2r_p\right]} \times \left[\ln \frac{(2r_p\rho_p)^{-1/2}}{r_{\text{core}}}\right]^{-1/2} \left[\ln\left(\frac{\overline{D}}{r_{\text{core}}}\right) + 0.7\right]^{3/2},$$

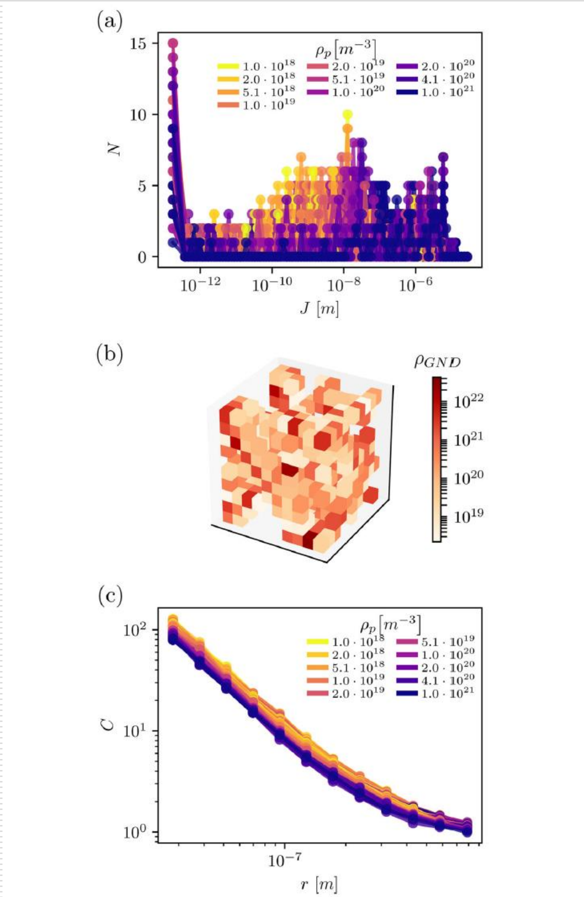
Bursts and ss-curves

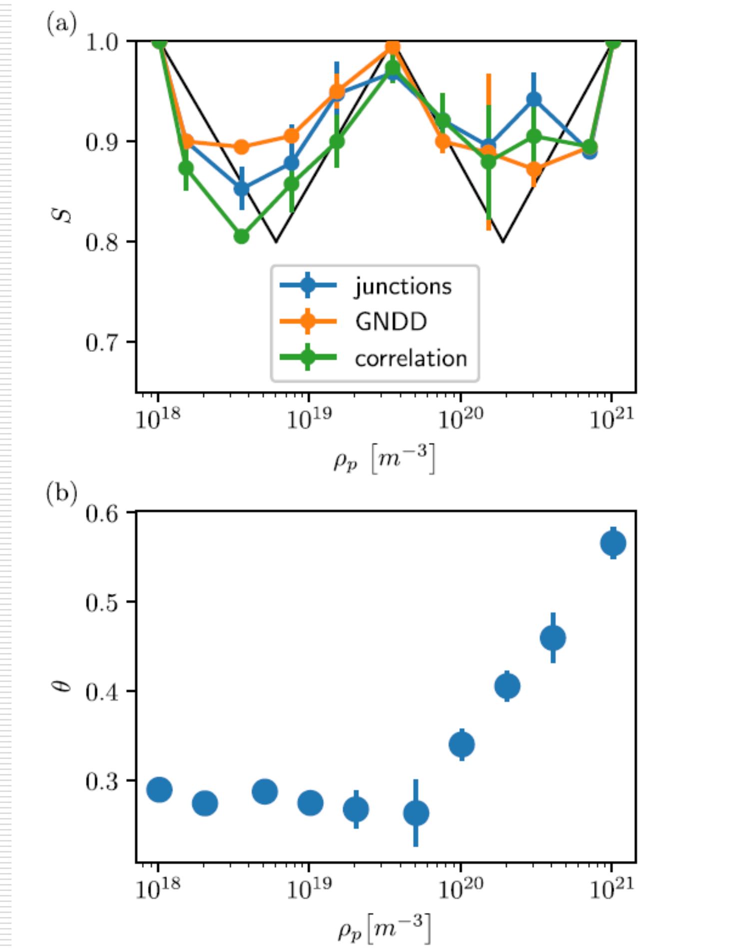


Large precipitate fraction: "real yield point".



Side-note: predicting phases





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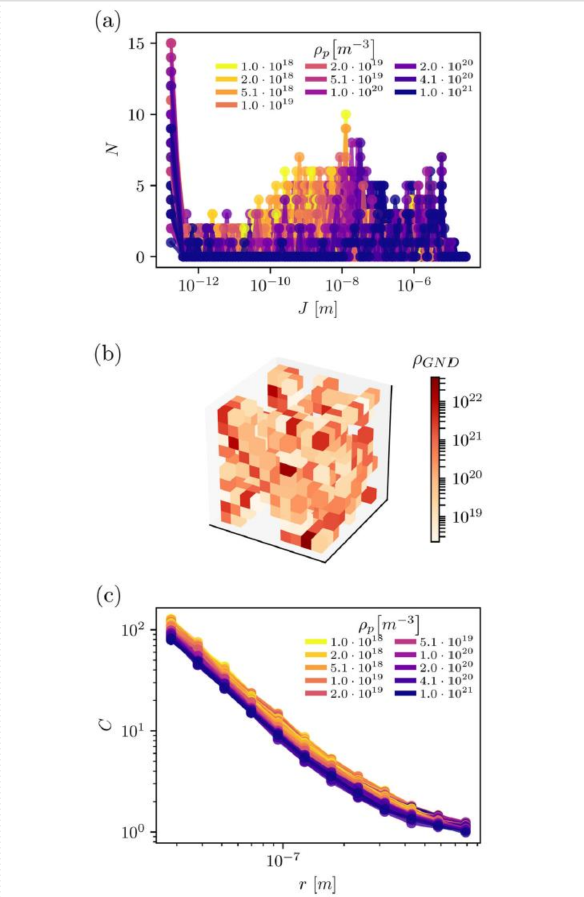
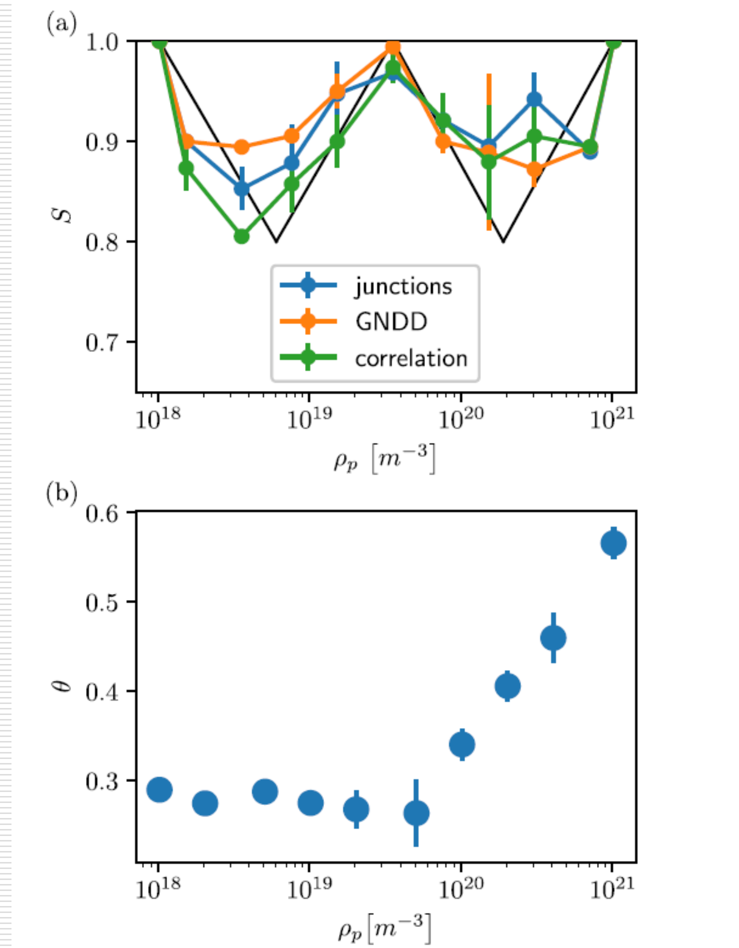
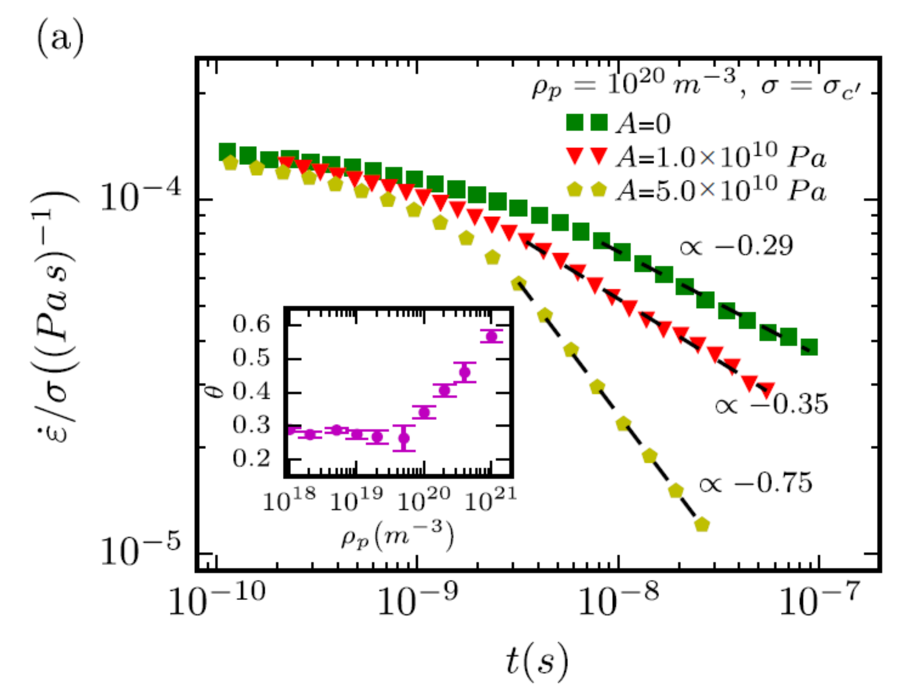
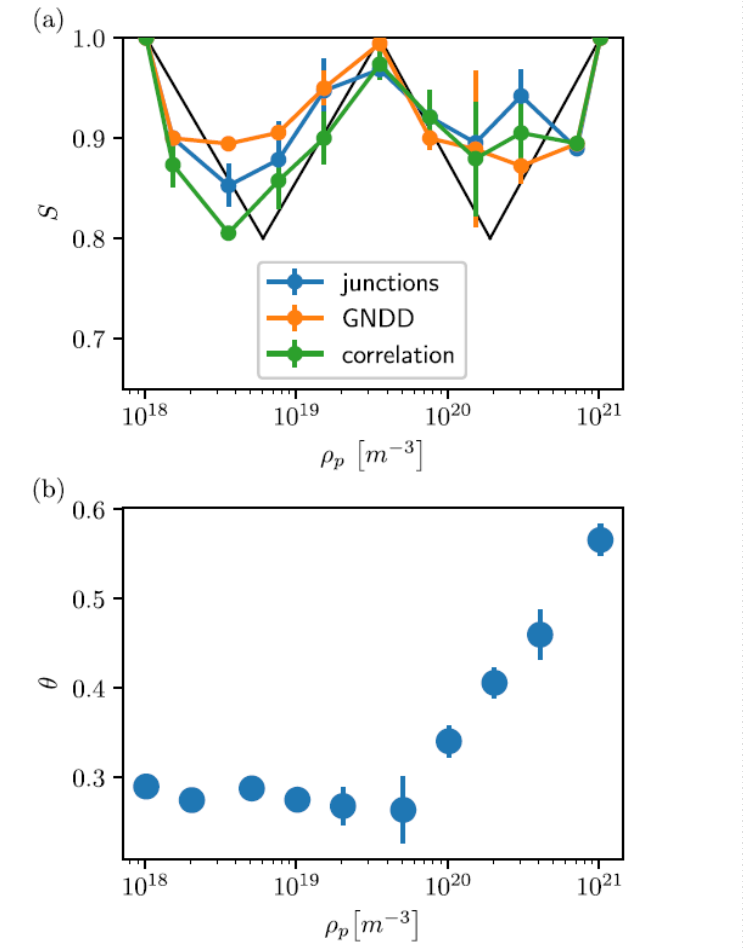


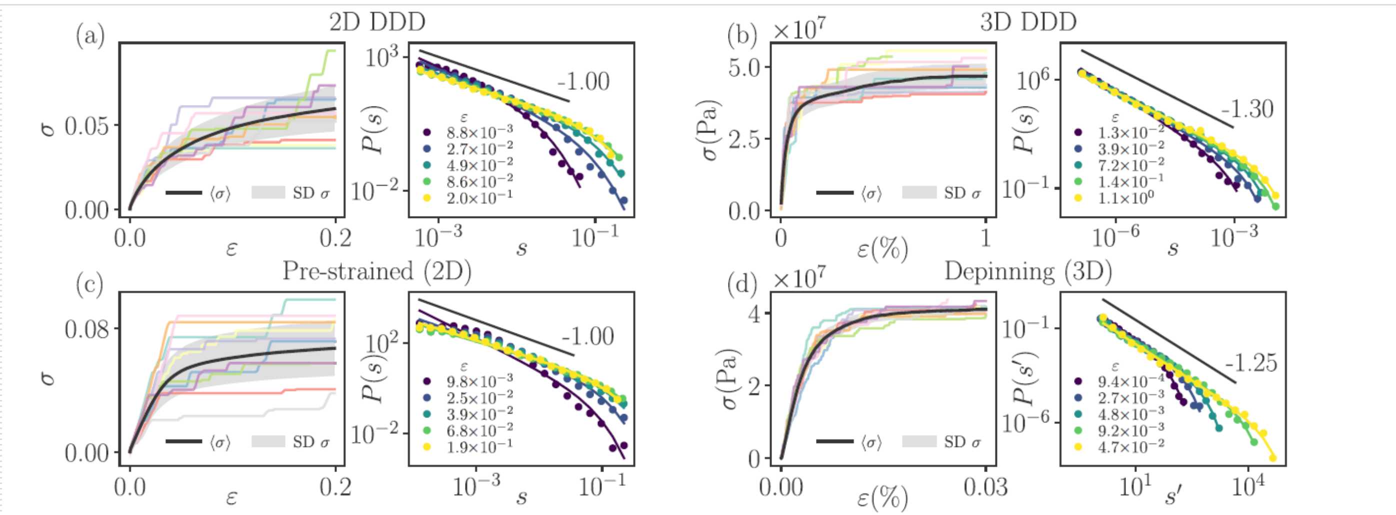


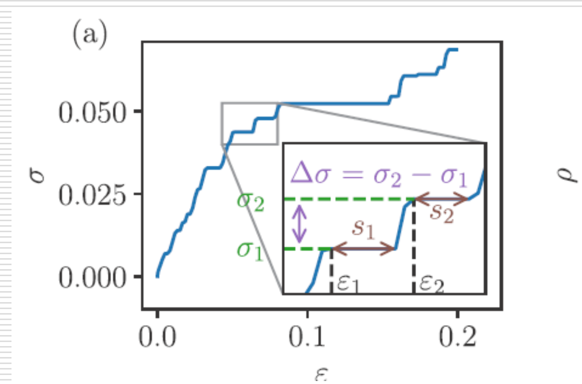
Side-note: predicting phases



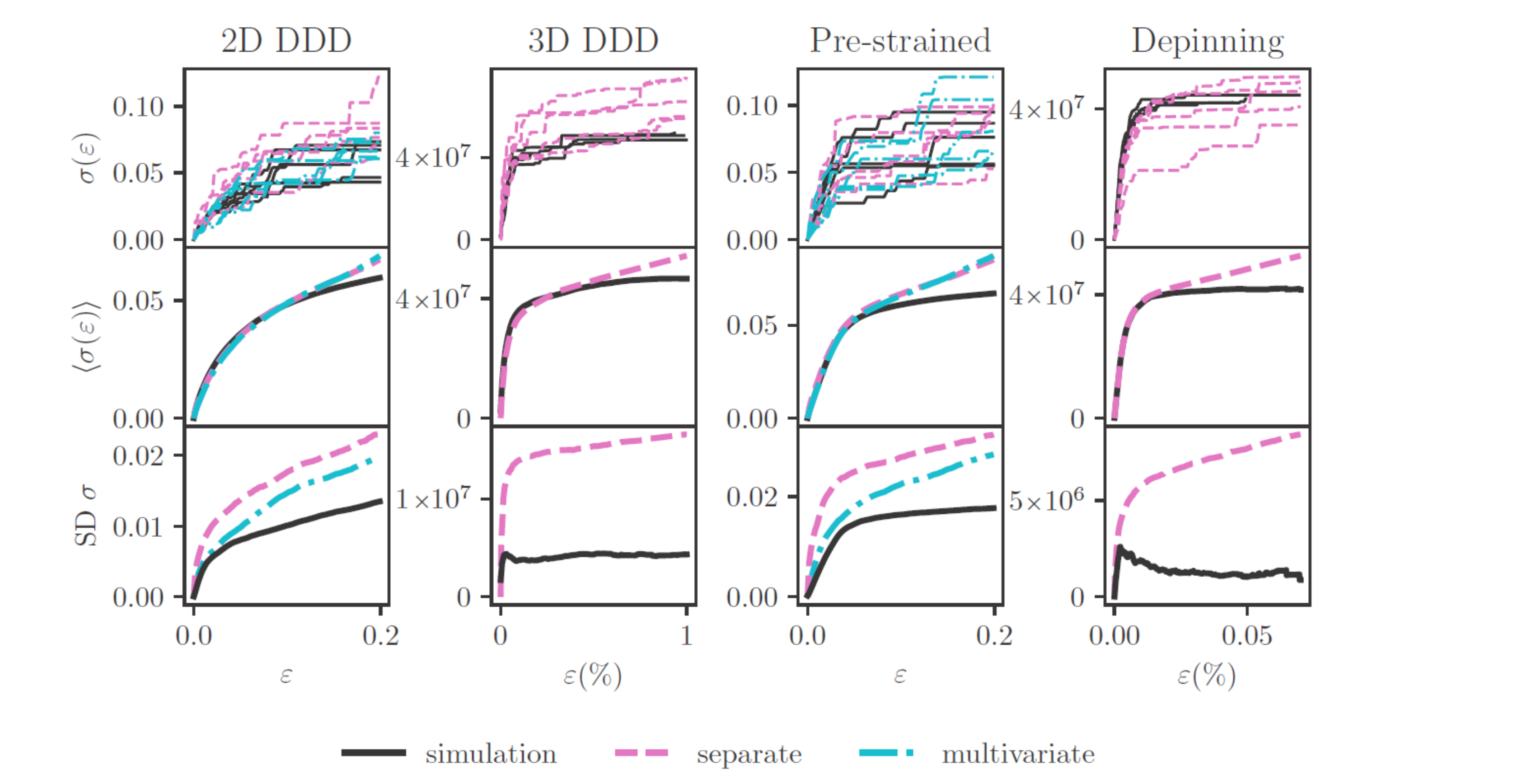


Avalanche correlations and stress-strain curves in discrete dislocation plasticity

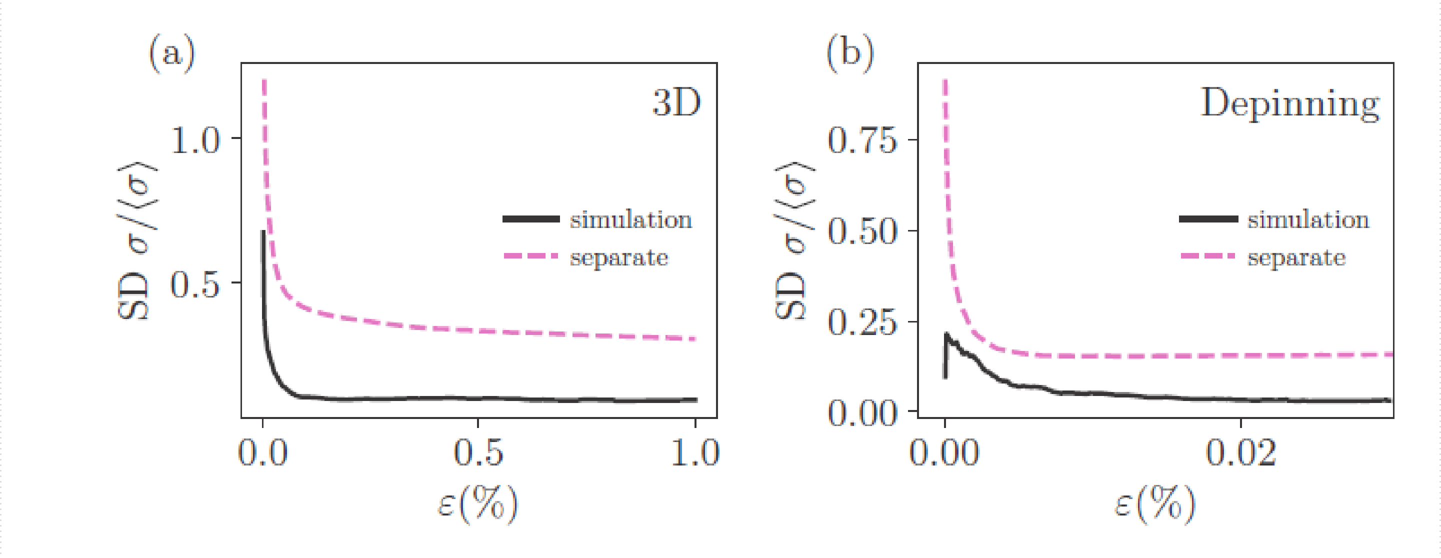




Predicting stress-strain curves



Effect of pinning centers on the stress-strain curve



Edge dislocations in multicomponent solid solution alloys: Beyond traditional elastic depinning

A. Esfandiarpour,[1] S. Papanikolaou,[1] and M. Alava[1,2]

[1]NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Soltana 7, 05-400 Swierk/Otwock, Poland

[2]Department of Applied Physics, Aalto University, PO Box 11000, 00076 Aalto, Finland

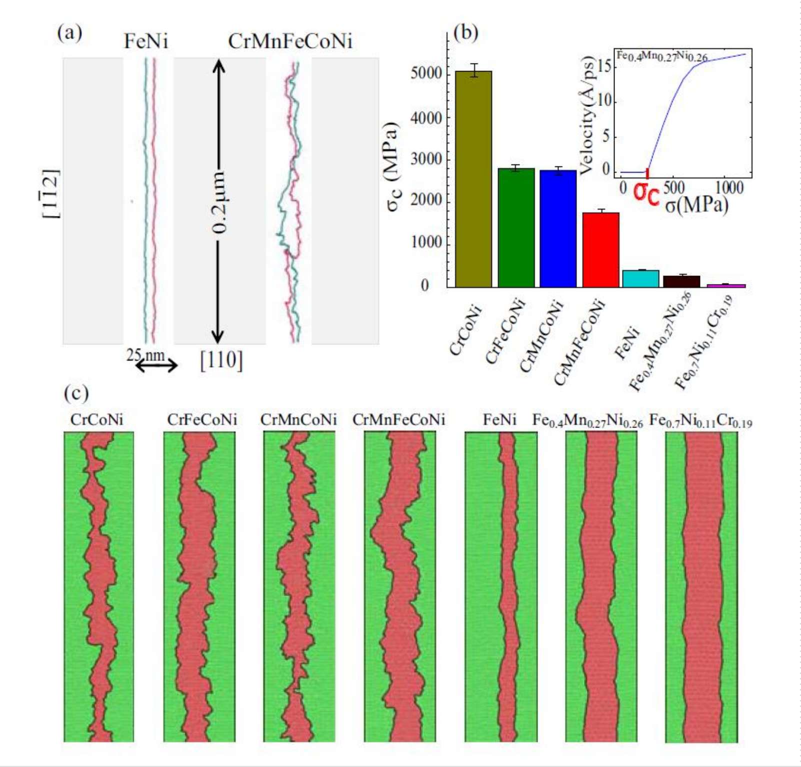
PHYSICAL REVIEW RESEARCH **4**, L022043 (2022)

Main question: does MF depinning theory work for FCC dislocations – two partials and Stacking Fault width/energy?

Playground complex alloys (HEA)

Theory by Varvenne & Curtin

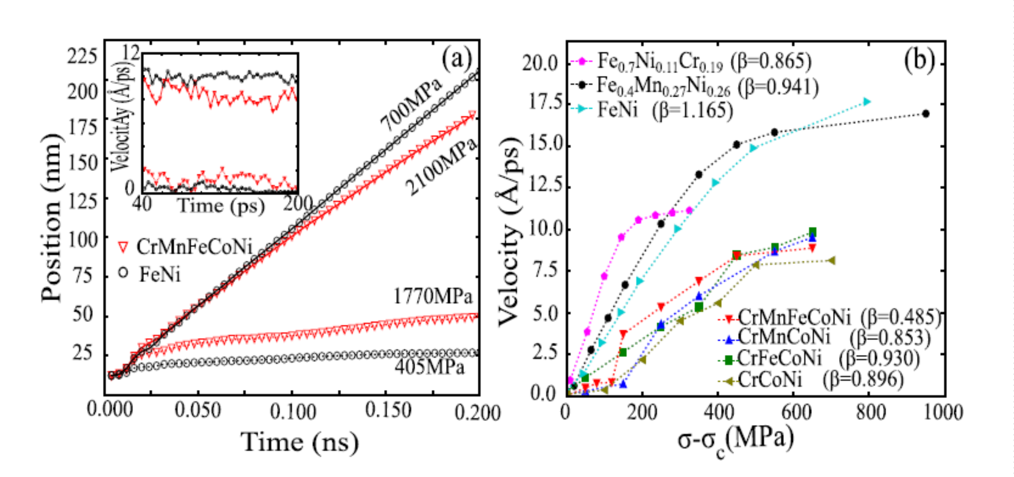
Recent work by Zaiser

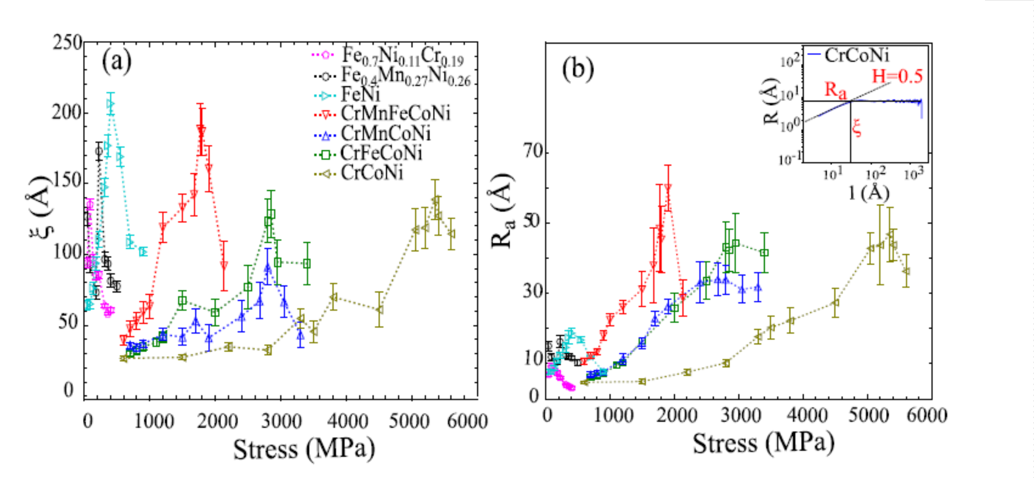


Grab the sword (MD)

What we want to find out:
Depinning stress
Critical properties

Velocity exponent case dependent (Laurson, 2022)



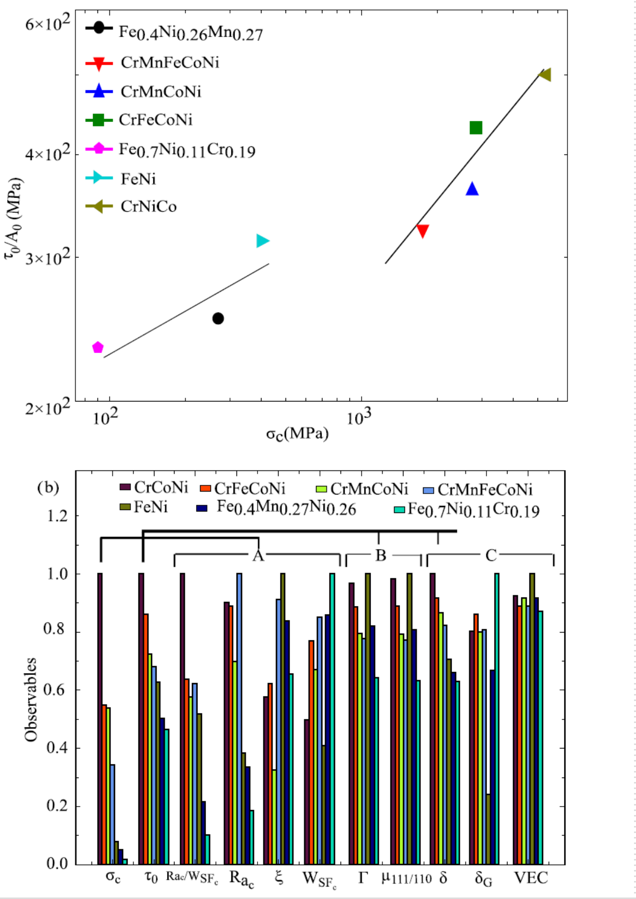


Complex depinning

$$\tau_0 \sim \left(\frac{1}{\Gamma}\right)^{\frac{1}{3}} \left(\mu \frac{1+\nu}{1-\nu}\right)^{\frac{4}{3}} (\delta)^{\frac{4}{3}},$$

MF would say "one parameter" (elastic mismatch) enough.

In reality, collective depinning increases depinning stress.



Conclusions

DDD: we can match depinning ideas to metallurgy (and vice versa).

Use of ML in describing (computational) samples to predict their behavior.

Much more work to do in real materials… non-universal exponents?