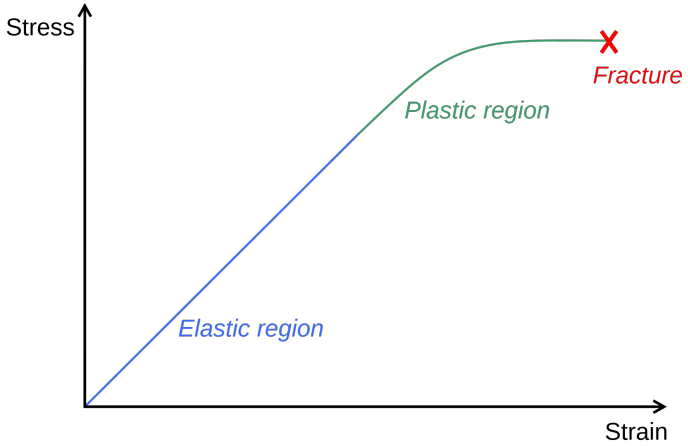
Modeling Plasticity in the DDD Framework

Dénes Berta ⬢ Bolyai Seminar ⬢ 24 April 2024

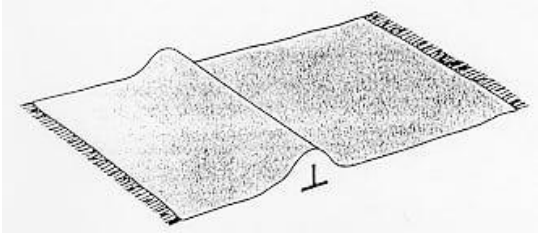
Plastic deformation of crystalline materials

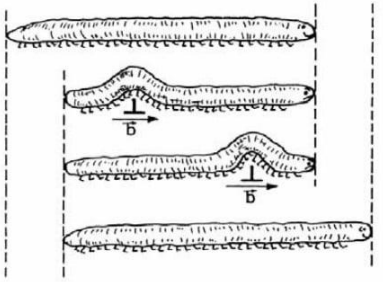


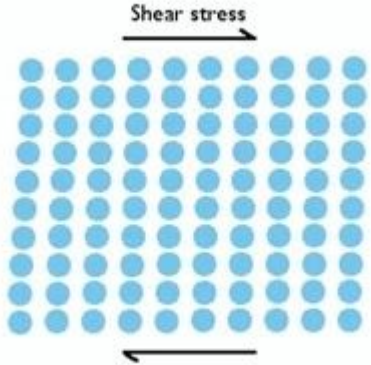
- Small strains: elastic deformation
- Large strains: elasto-plastic deformation

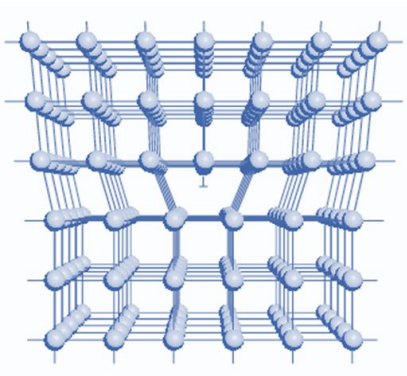
Conundrum of the critical stress

- Critical stress
  - Theory: ≈ 30 GPa
  - Experiment: ≈ 100 MPa
- Solution: **dislocations**
- Orován, Polányi, Taylor



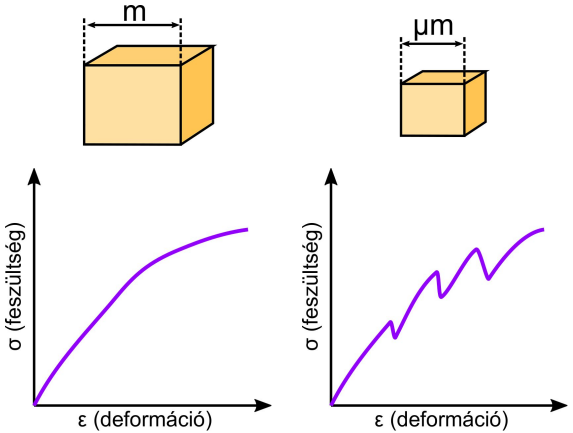


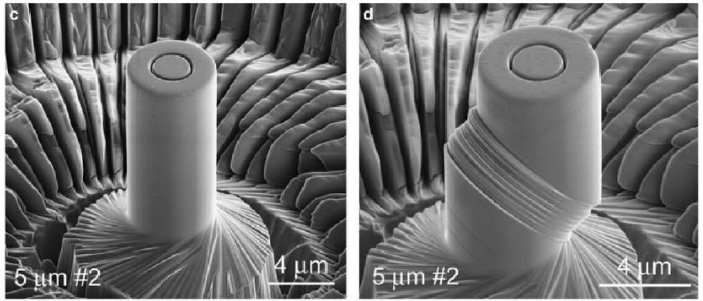




Plasticity at the (sub)micron scale

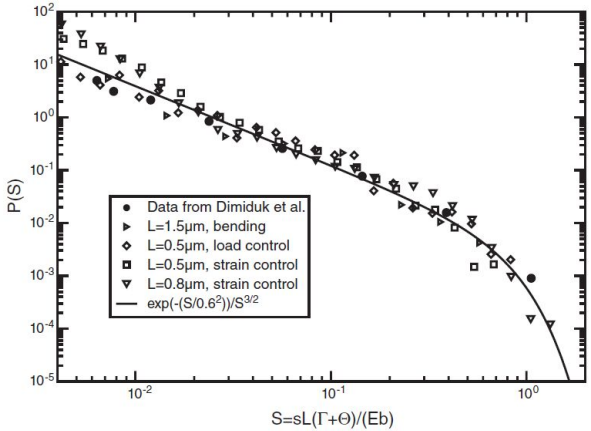
- Size-related hardening
- Sample-to-sample variation
- Random strain bursts (scale-free)
- Dislocation avalanches



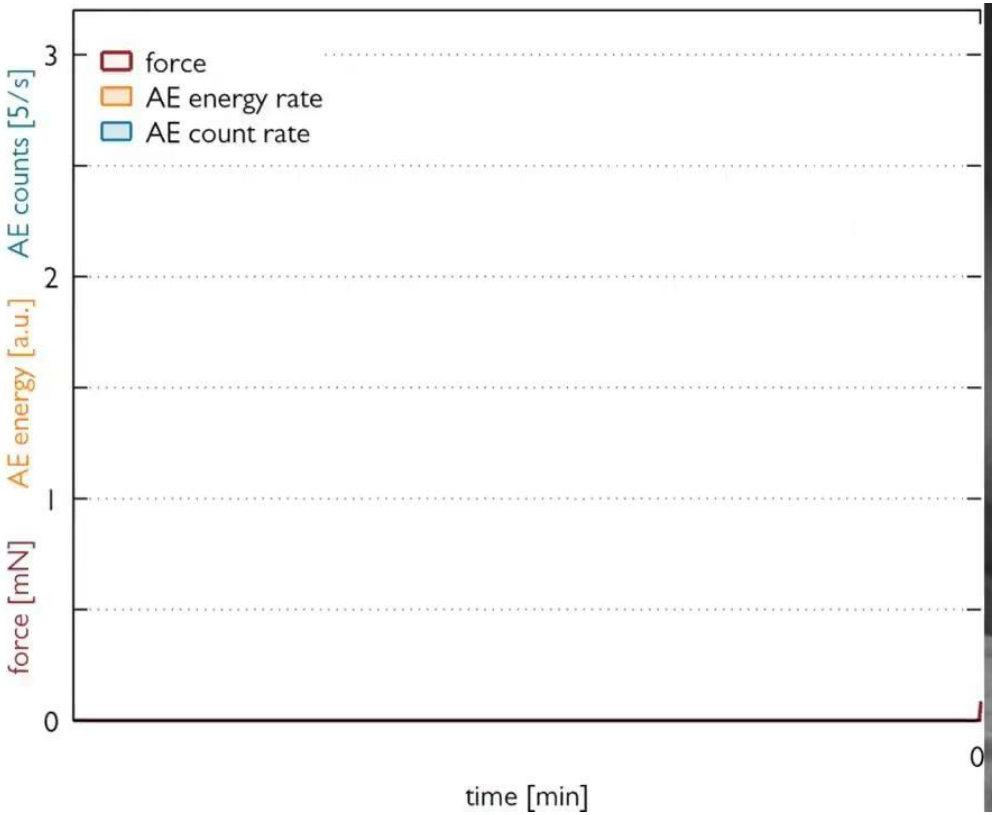


D. M. Dimiduk, C. Woodward, R. LeSar és M. D. Uchic, Science **312**, 1188 (2006).

F. F. Csikor, C. Motz, D. Weygand, M. Zaiser és S. Zapperi, Science **318**, 251 (2007).



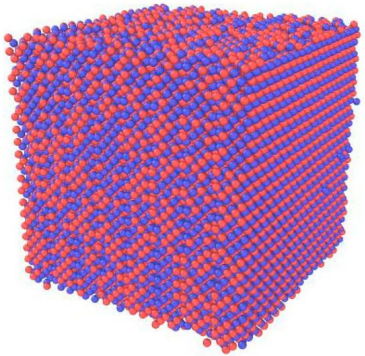
Micropillar compression test



Ispánovity, Péter Dusán, et al., Nature communications 13.1 (2022): 1975.

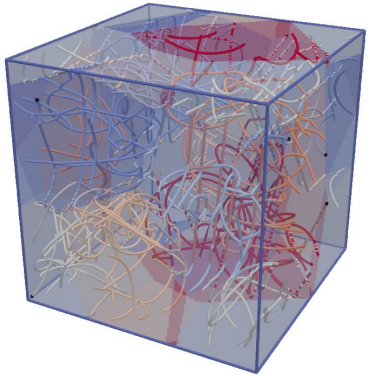
Modeling Plasticity

MD



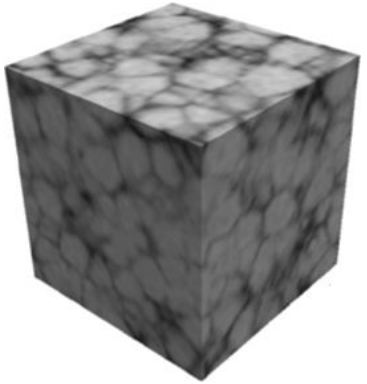
Z. Cui, X. Zhou, Q. Meng
Metals 10.12 (2020): 1660.

DDD



R. LeSar and L. Capolungo
Theory and Modeling (2020): 1079-1110.

CDD



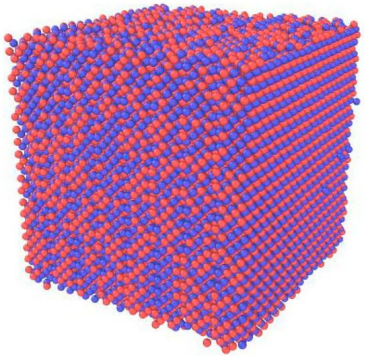
A. El-Azab and G. Po. *Handbook of Materials Modeling: Methods: Theory and Modeling* (2020): 1583-1607.

degrees of freedom, computational cost, realistic description

simulated time and length scale

Frameworks of modeling plasticity

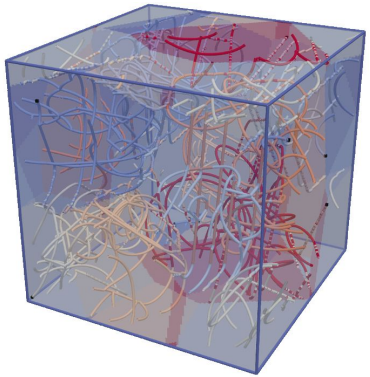
MD



Z. Cui, X. Zhou, Q. Meng
Metals 10.12 (2020): 1660.

- ❑ unit: atom/molecule
- ❑ interaction potentials

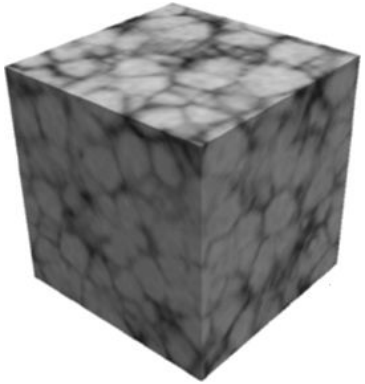
DDD



R. LeSar and L. Capolungo
Theory and Modeling (2020): 1079-1110.

- ❑ unit: dislocation line
- ❑ stress fields + PK force

CDD

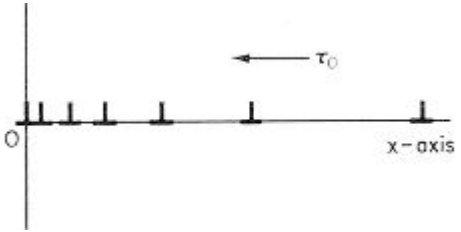


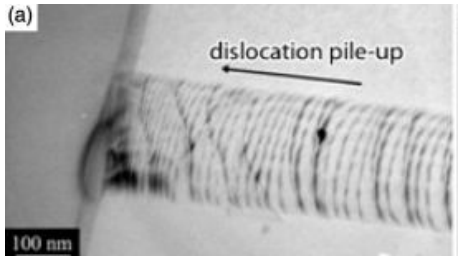
A. El-Azab and G. Po. *Handbook of Materials Modeling: Methods: Theory and Modeling* (2020): 1583-1607.

- ❑ coarse graining
- ❑ PDE for densities

Dimensional complexity

1D DDD

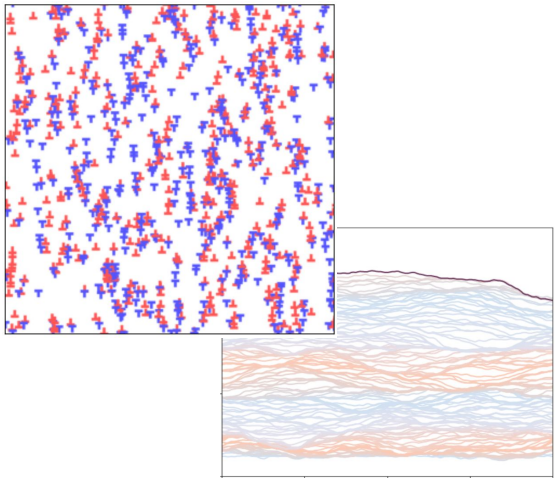




- Dislocation pile-ups

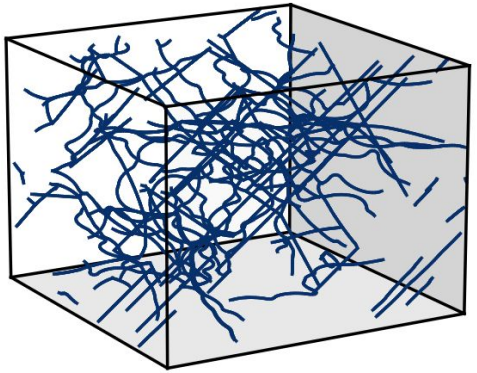
Hull, Derek, and David J. Bacon. *Introduction to dislocations*. Butterworth-Heinemann, 2001.

2D DDD



- Single-slip systems
- Dislocation depinning

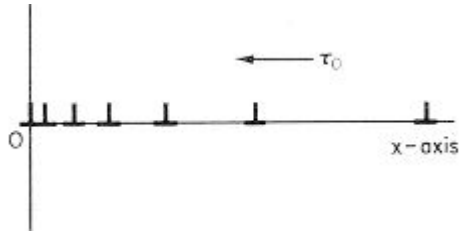
3D DDD

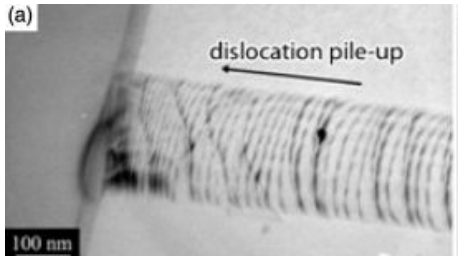


- Multi-slip systems

2D DDD modeling of single-slip dynamics

1D DDD





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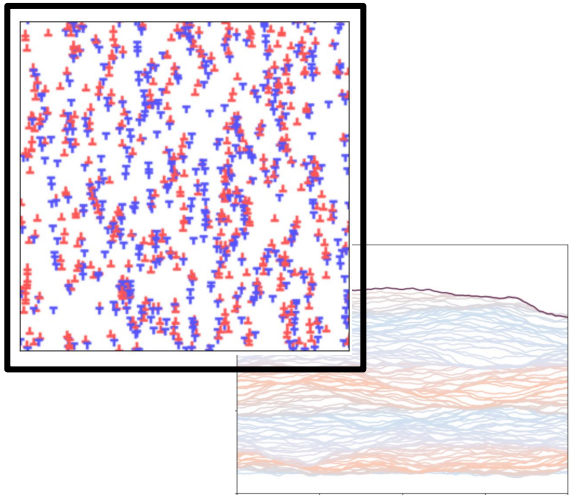
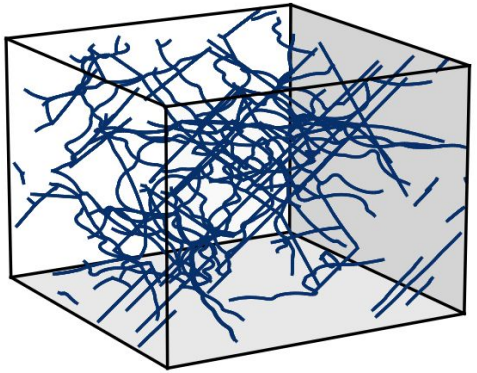
2D DDD



- **Single-slip systems**
- Dislocation depinning

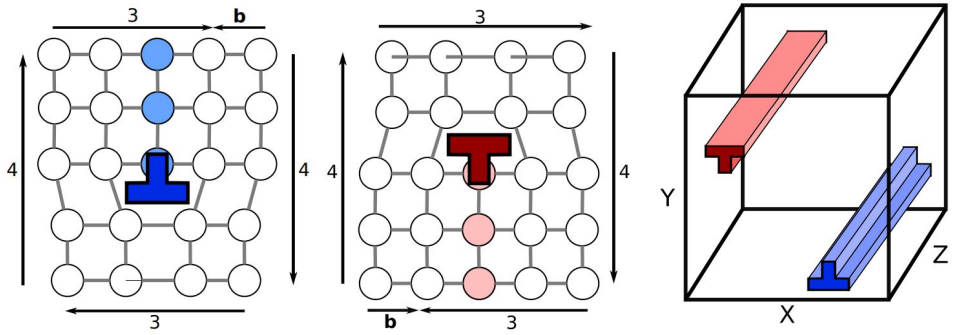
3D DDD



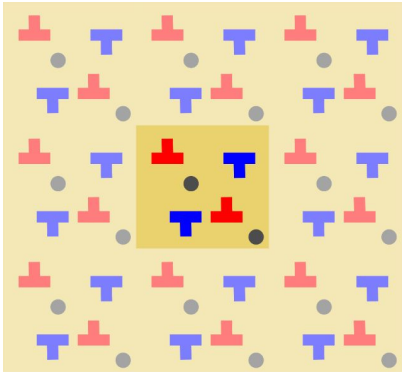
- Multi-slip systems

Model composition

- Edge dislocations
- (Immobile point defects)
- Dynamics: dislocation glides
- PBC

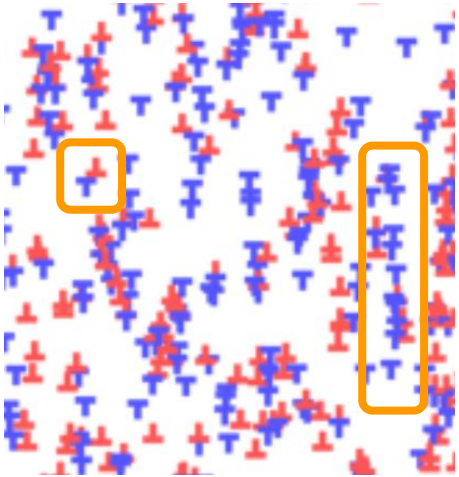


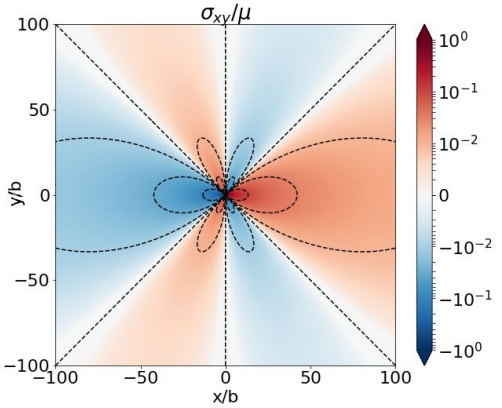
$$B\dot{x}_i = bs_i \left[\underbrace{\sum_{j=1, j\neq i}^{N_{\mathrm{dis}}} s_j \tau_{\mathrm{dis}}(\boldsymbol{r}_i - \boldsymbol{r}_j)}_{\text{disl-disl. int.}} + \underbrace{\sum_{k=1}^{N_{\mathrm{vac}}} \tau_{\mathrm{vac}}(\boldsymbol{r}_i - \tilde{\boldsymbol{r}}_k)}_{\text{disl-p.d. int.}} + \underbrace{\tau_{\mathrm{ext}}}_{\text{external stress}} \right] = b \left[-\frac{\partial}{\partial x_i}(U + s_i \tau_{\mathrm{ext}} x_i) \right]$$



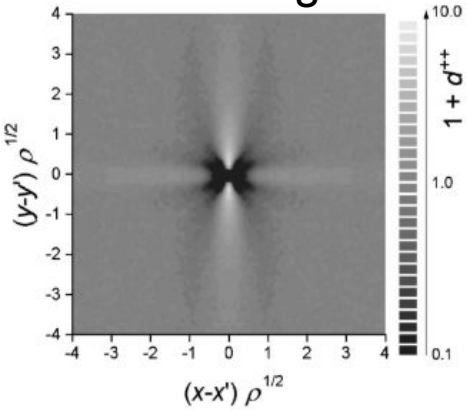
Dislocation correlations

- Anisotropic stress field
- Walls
- Dipoles

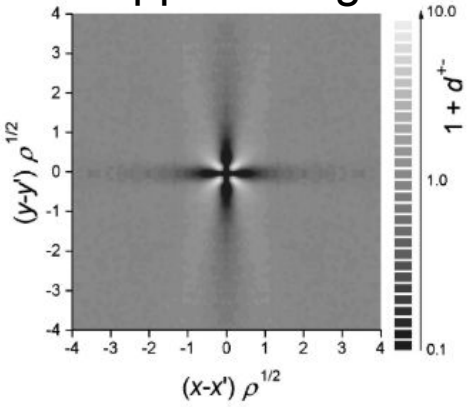




Same sign

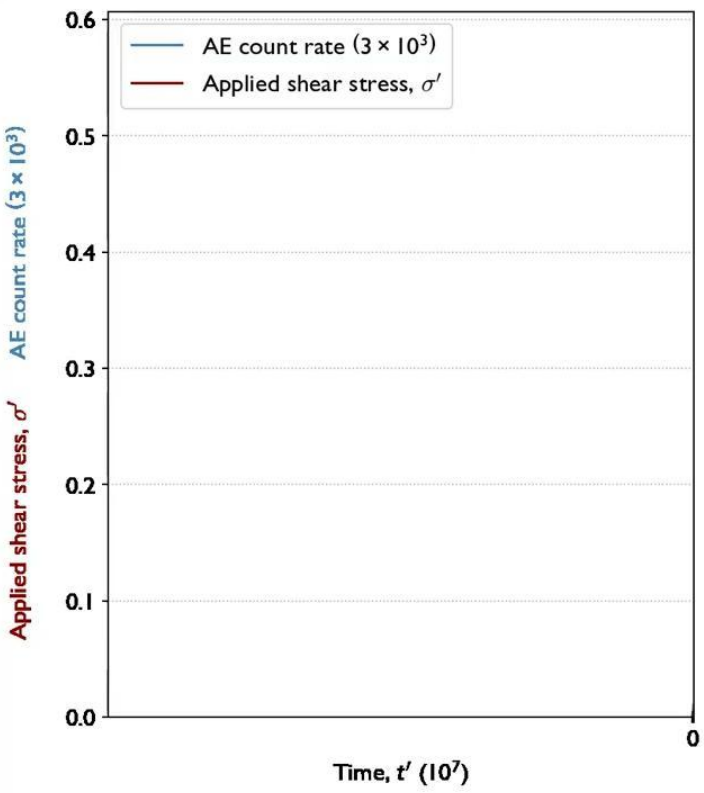


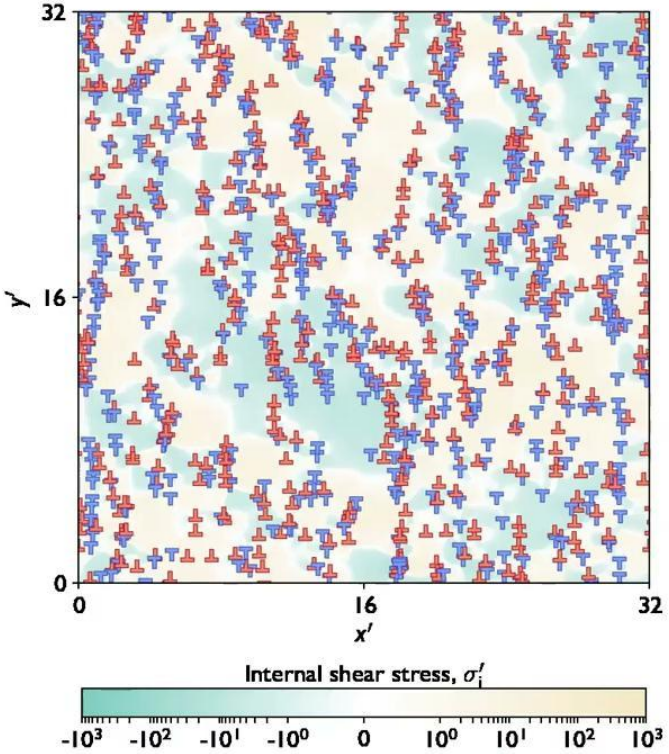
Opposite sign



M. Zaiser, M-C. Miguel, and G. István,*Physical Review B* 64.22 (2001): 224102.

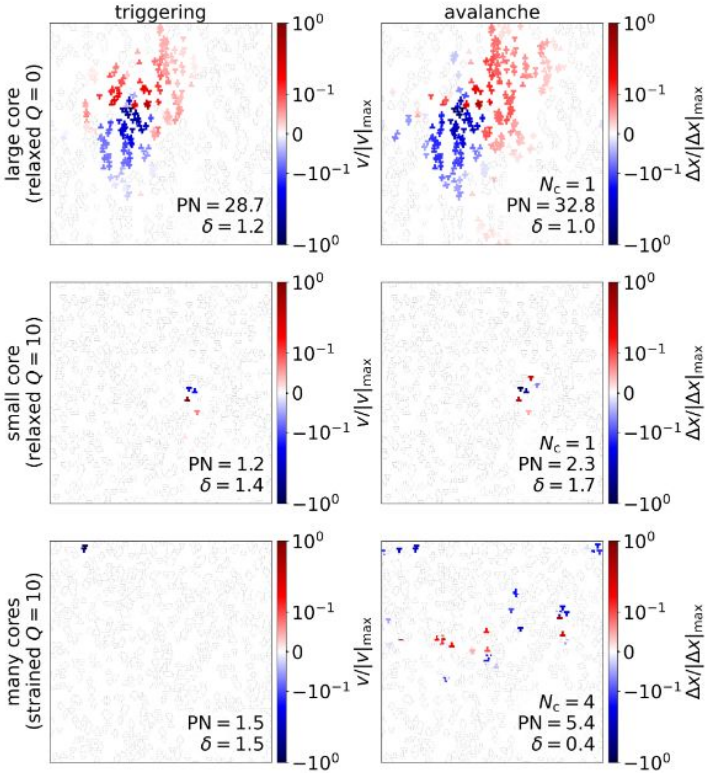
Dislocation avalanches

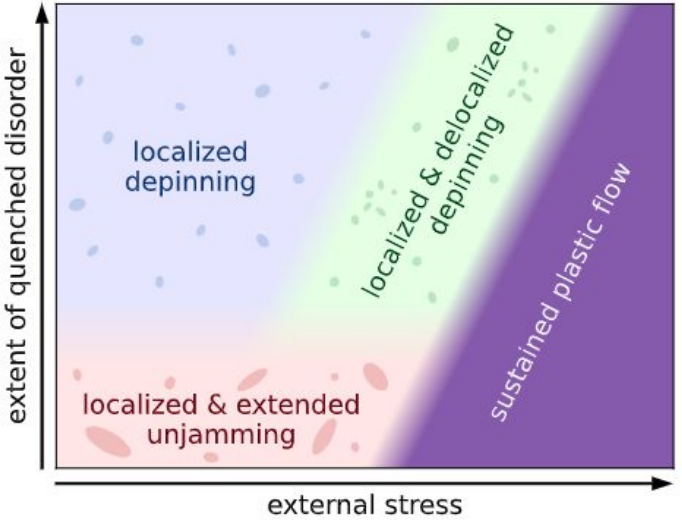




Ispánovity, Péter Dusán, et al., Nature communications 13.1 (2022): 1975.

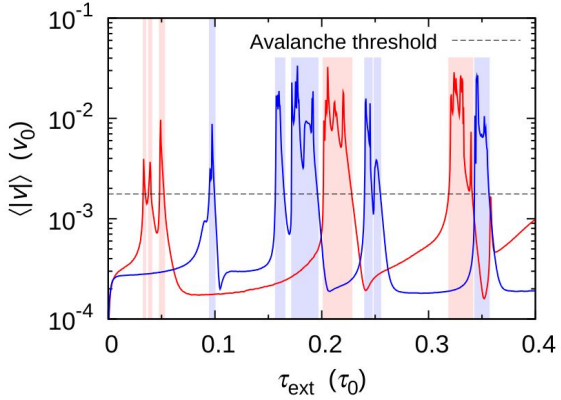
Different regimes of avalanche behaviour

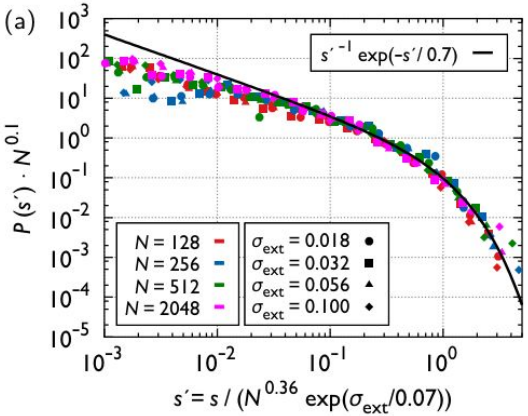


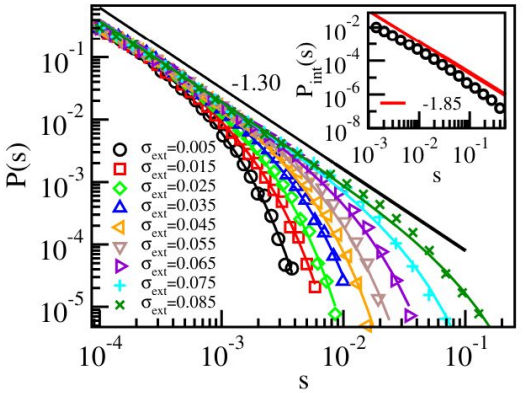


Avalanche statistics

- Scale-free size distribution
- Exponent
  - No point defects: -1
  - Point defects: -1.3







P. D. Ispánovity, et al., *Physical review letters* 112.23 (2014): 235501.

P. D. Ispánovity, et al., P*hysical review letters* 105.8 (2010): 085503.

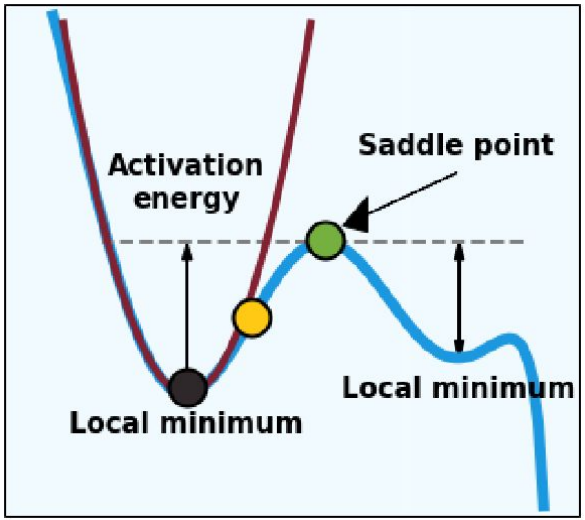
M. Ovaska, L. Laurson, and M. J. Alava, *Scientific reports* 5.1 (2015): 10580.

Linear stability analysis (LSA)

- At stable equilibrium: we are at a local minimum
- Series expansion

$$U(\Delta \boldsymbol{x}) = U_0 + \underbrace{\partial_k U \Delta x_k}_{=0} + \partial_{ij}^2 U \Delta x_i \Delta x_j + \mathcal{O}(\Delta \boldsymbol{x}^3)$$

- Dynamical matrix: $\Lambda_{ij} = \partial_{ij}^2 U$
- Harmonic approximation of the energy landscape

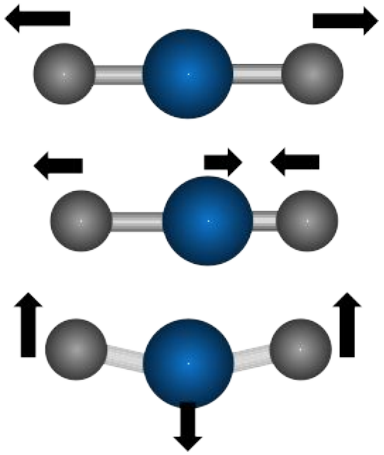


Dynamical modes

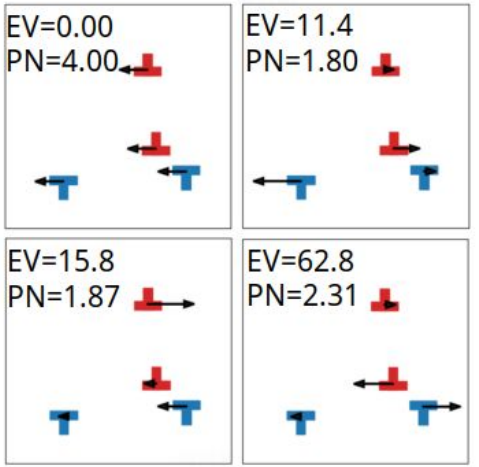
- Eigenvalue problem
  - Eigenvectors: dynamical modes
  - Eigenvalues: steepness of the energy well

EV: eigenvalue
PN: participation number

Molecular vibrational modes

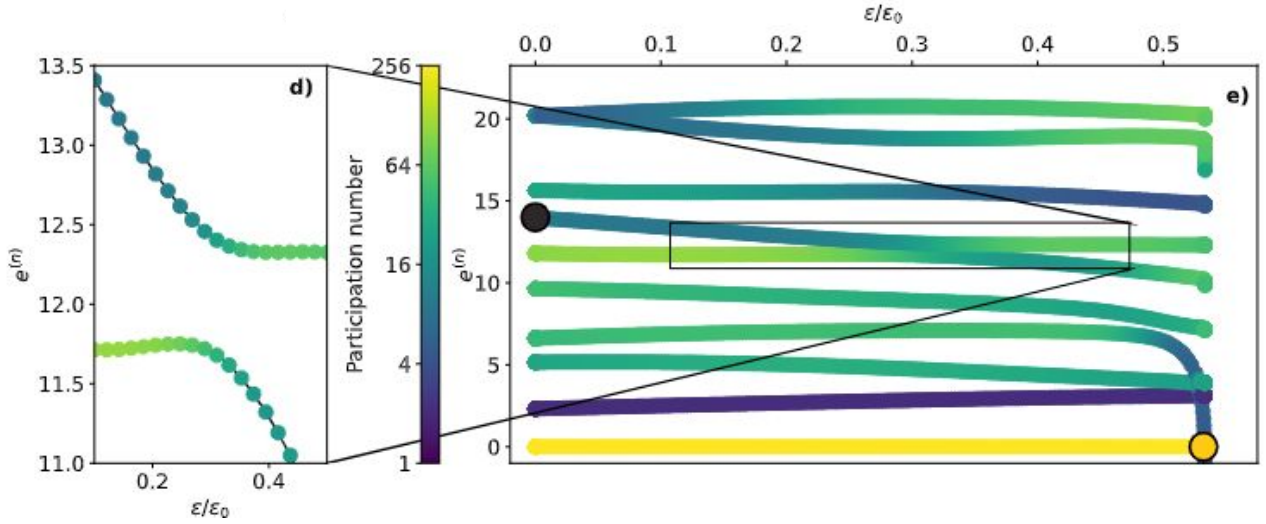


Eigenmodes of DD systems



Connection of modes and plastic events

- Rough energy landscape
- Instability at the saddle point
- Dynamic modes evolve into avalanches



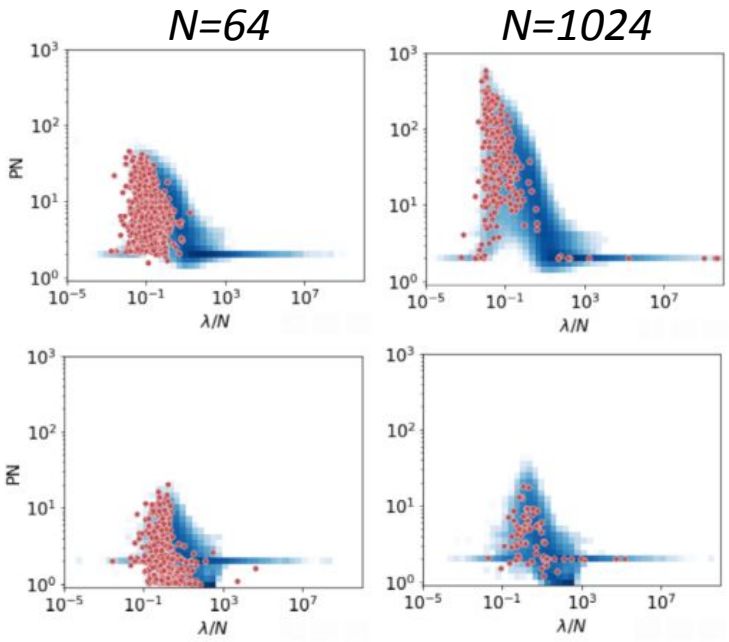
Spectrum of dynamical modes

No quenched disorder

- ❏ Localized modes (dipoles)
- ❏ Large modes (extensive scaling)
- ❏ ‘Wall’ of low eigenvalues (activation)

Great extent of quenched disorder

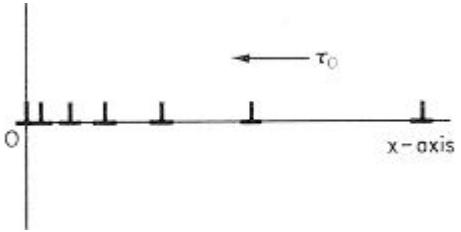
- ❏ Localized modes (dipoles)

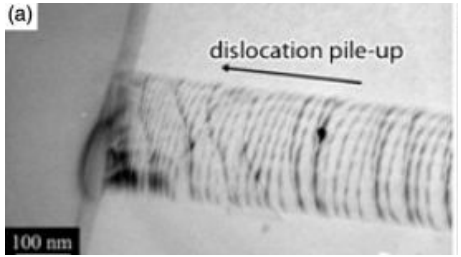


λ: eigenvalue
N: number of dislocations
PN: participation number

2D DDD modeling of dislocation depinning

1D DDD

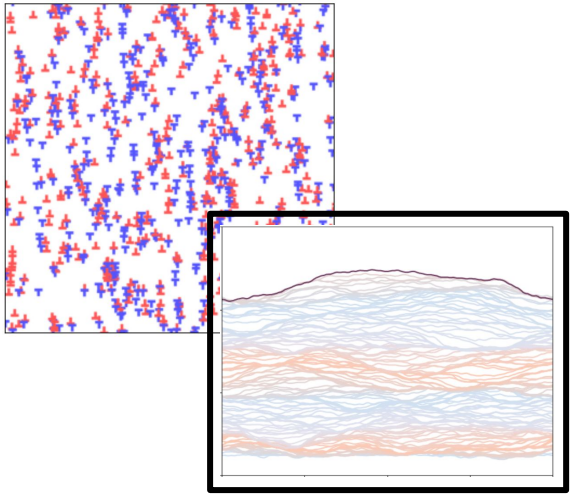




- Dislocation pile-ups

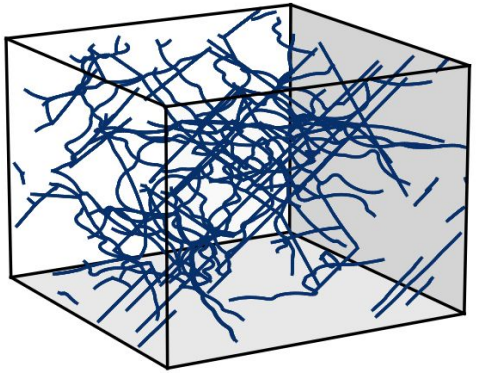
Hull, Derek, and David J. Bacon. *Introduction to dislocations*. Butterworth-Heinemann, 2001.

2D DDD



- Single-slip systems
- **Dislocation depinning**

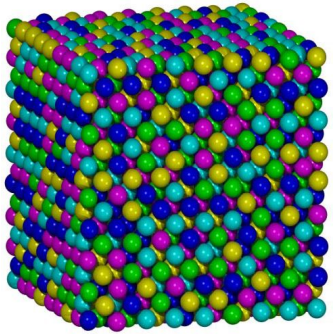
3D DDD

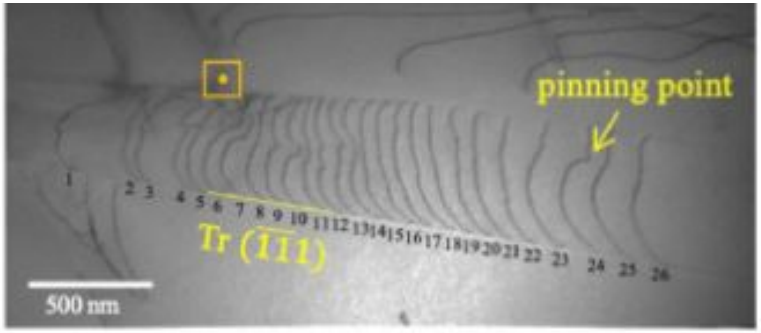


- Multi-slip systems

Dislocation depinning in high entropy alloys

- High entropy alloys (HEA)
  - Multi-principle-element (at least 5)
  - Atomic radius differences
  - Immense lattice distortion
  - Heterogeneous internal stress field
- Impact on dislocations
  - Rough dislocation lines
  - Stick-slip dynamics

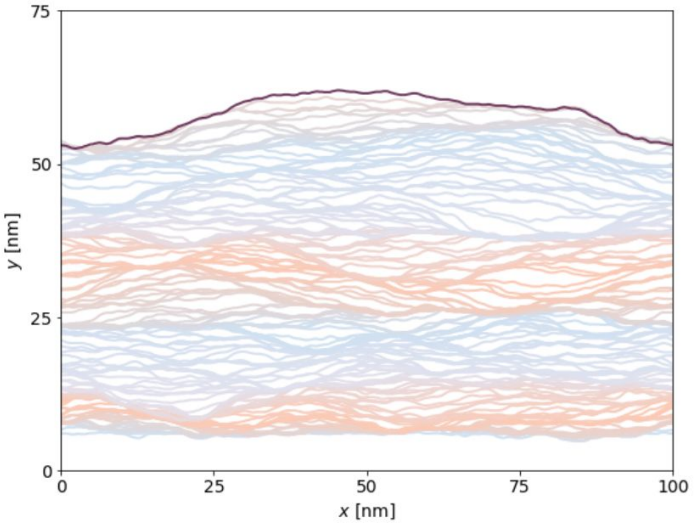




Zhang, Chen, et al., *Acta materialia* 241 (2022): 118394.

Model composition

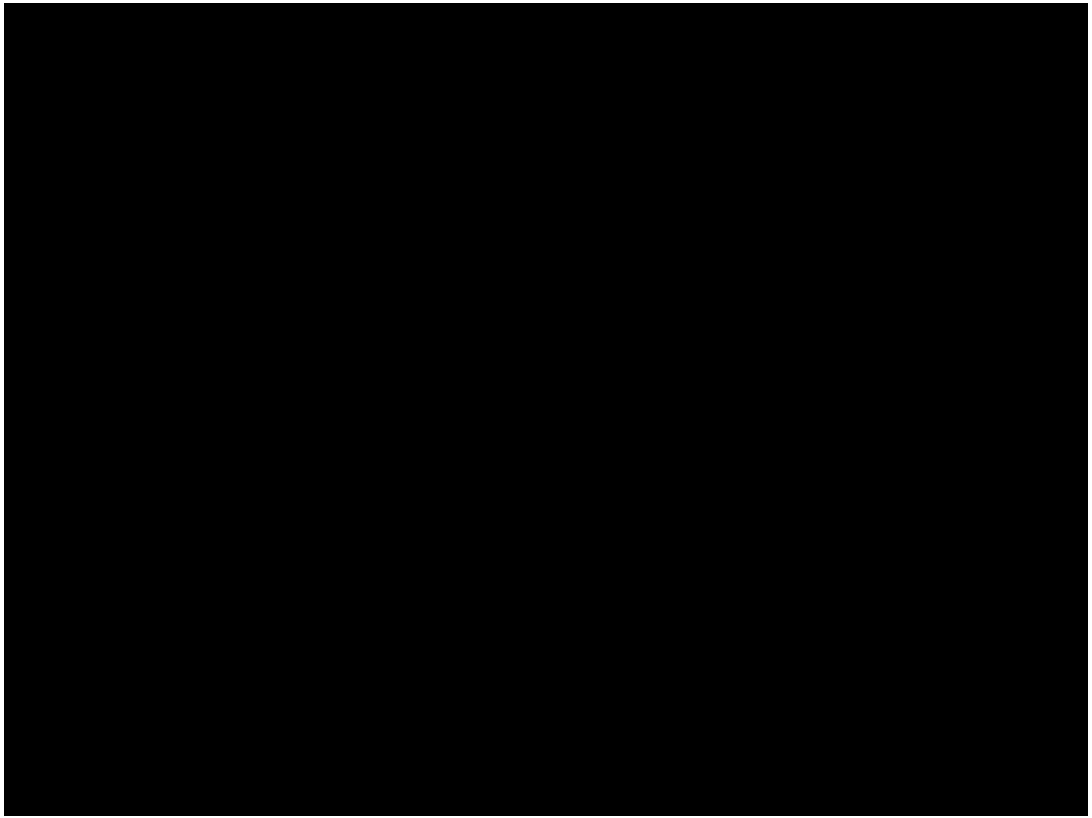
- Vertical and horizontal dislocation segments
- Heterogeneous pinning stress field
  - Gaussian distribution
  - No spatial correlations
- Random dynamics



$$\tau(\boldsymbol{r}) = \tau_{\mathrm{ext}}(\boldsymbol{r}) + \tau_{\mathrm{self}}(\boldsymbol{r}) + \tau_{\mathrm{pin}}(\boldsymbol{r})$$

$$\tau_{\mathrm{self}}(\boldsymbol{r}_i) = \sum_{j}^{\{s\}} \tau_s(\boldsymbol{r}_i - \boldsymbol{r}_j) + \sum_{j}^{\{e\}} \tau_e(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

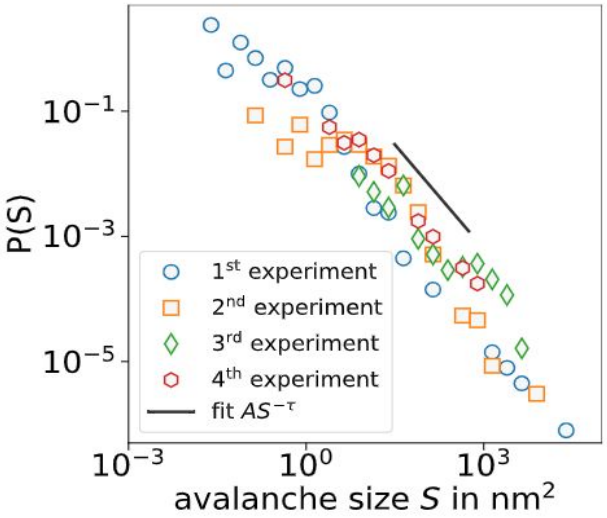
Intermittent dislocation motion



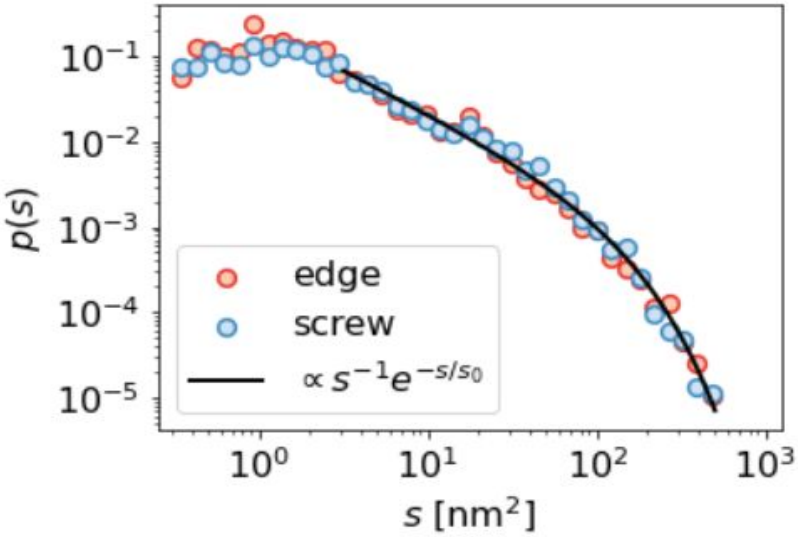
Slip size distribution

- Scale-free distribution
- Exponent: -1

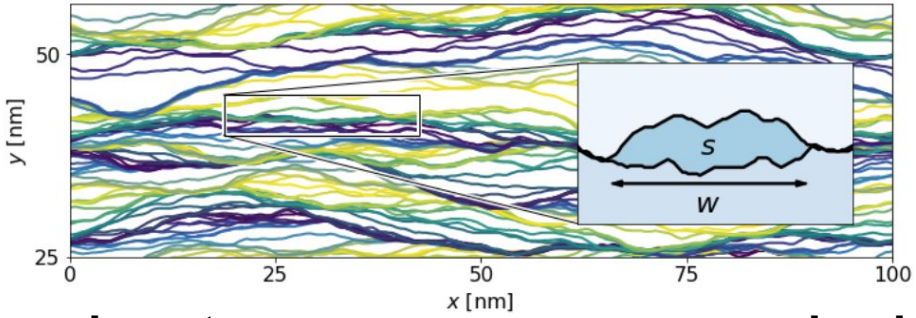
experiment



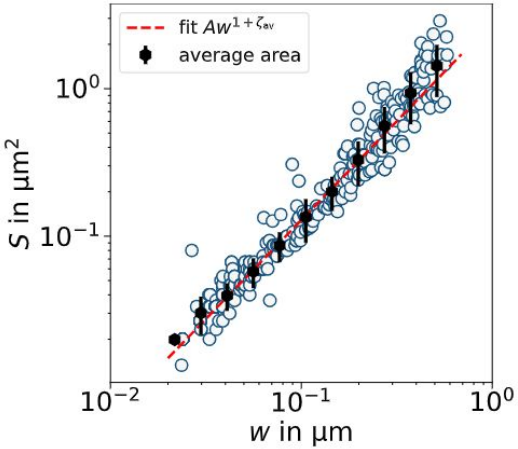
simulation



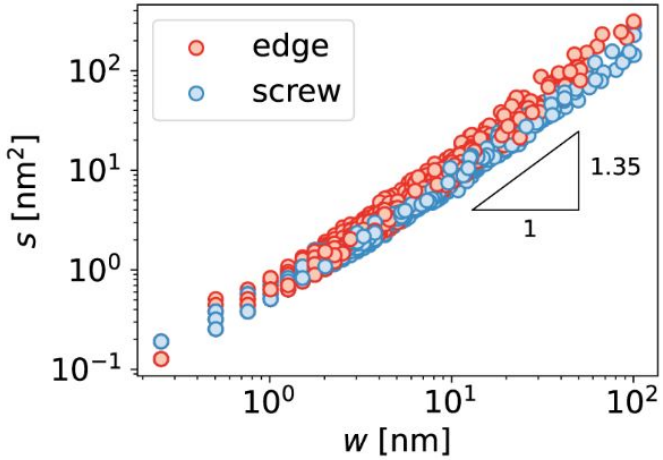
Fractal dimension of slip events



experiment

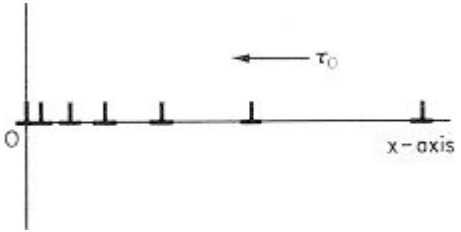


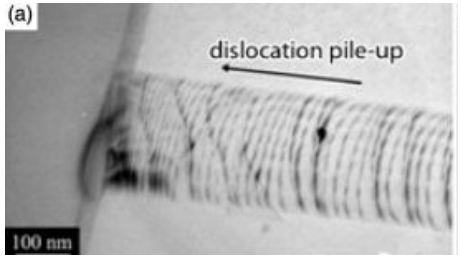
simulation



2D DDD modeling of dislocation depinning

1D DDD

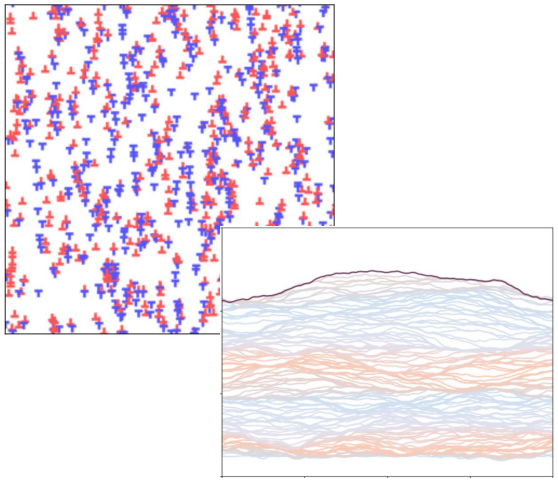




- Dislocation pile-ups

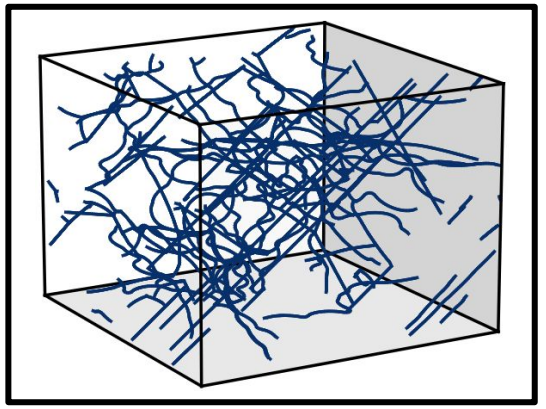
Hull, Derek, and David J. Bacon. *Introduction to dislocations*. Butterworth-Heinemann, 2001.

2D DDD



- Single-slip systems
- Dislocation depinning

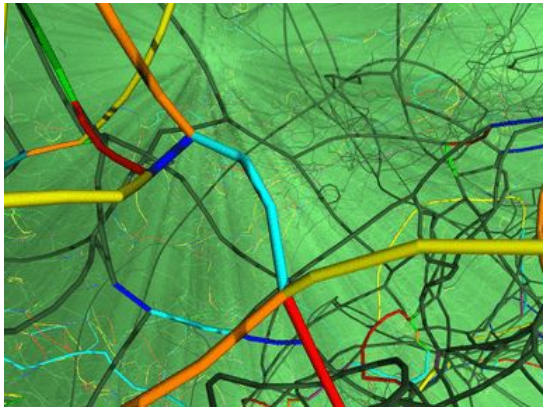
3D DDD



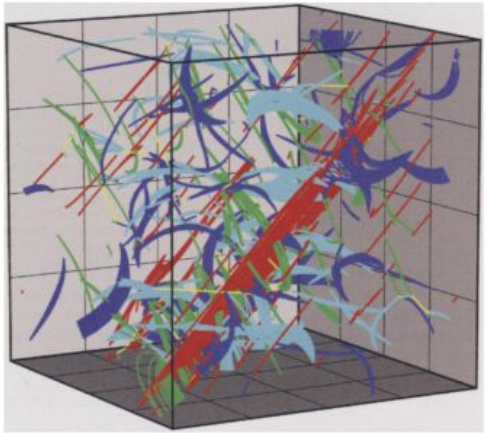
- **Multi-slip systems**

Model composition

- Non-physical dislocation nodes
- Straight dislocation segments
- Dislocation junctions
- Usually multi-slip



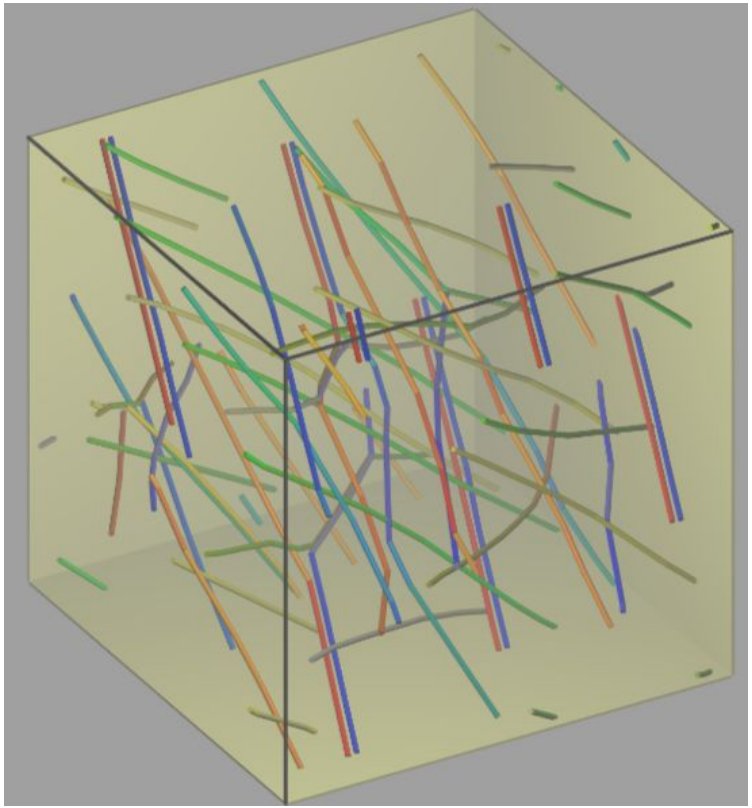
V. V. Bulatov et al., Nature 440.7088 (2006): 1174-1178.



F. F. Csikor et al., *science* 318.5848 (2007): 251-254.

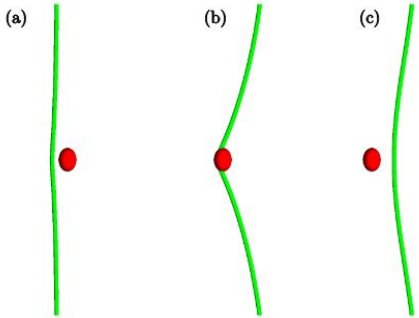
Special case: single-slip

- Less complex structure
- Dipoles
- Similar to 2D

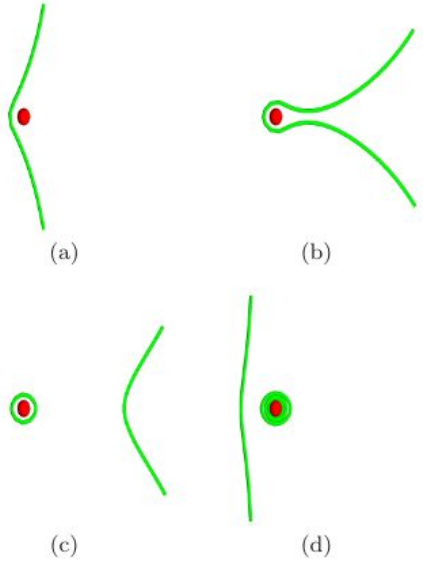


Interaction with precipitates

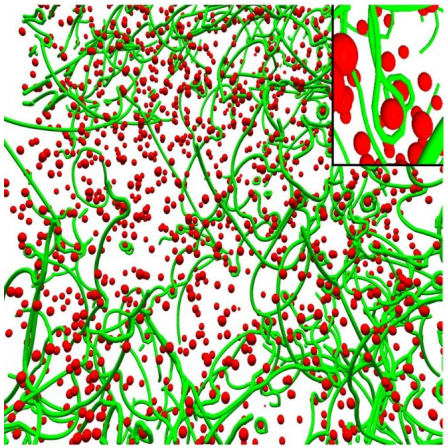
weak precipitates



strong precipitates



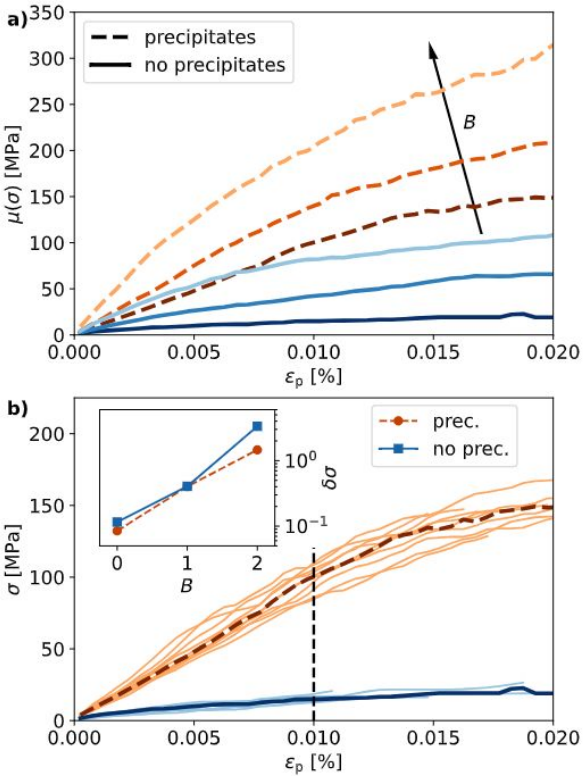
Orowan loop



A. Lehtinen, et al. *Scientific reports* 8.1 (2018): 6914.

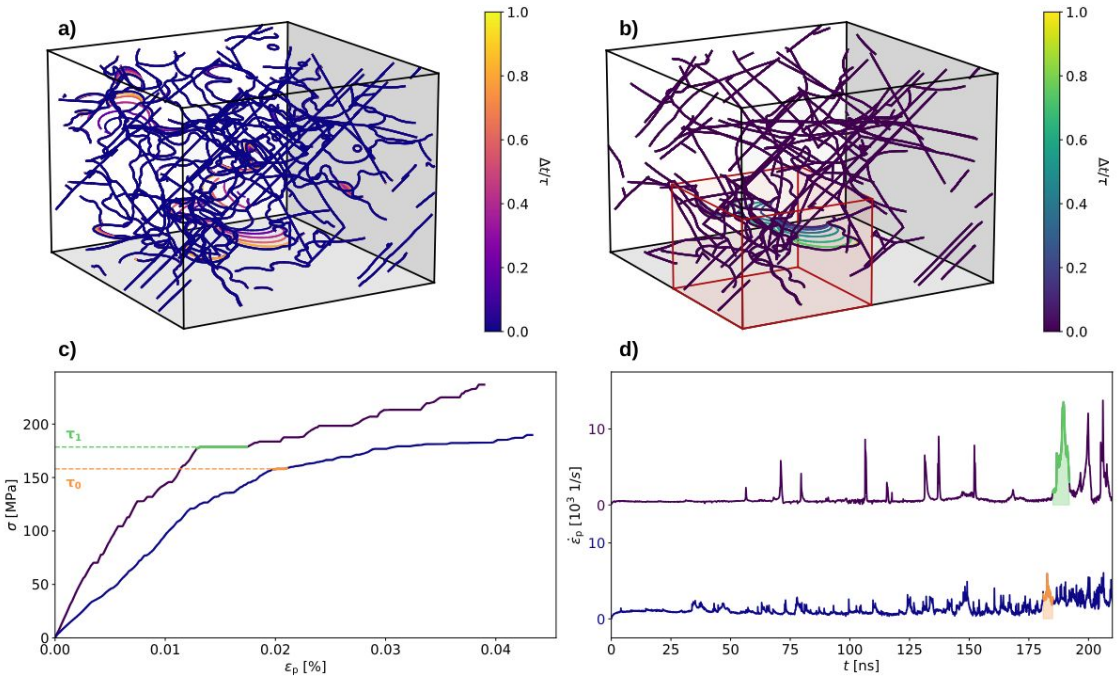
A. Lehtinen, et al., *Physical Review E* 93.1 (2016): 013309.

Size- and precipitate-related hardening



- Fluctuations at this size regime
- Smaller subregions are harder
- Configurations with precipitates are harder

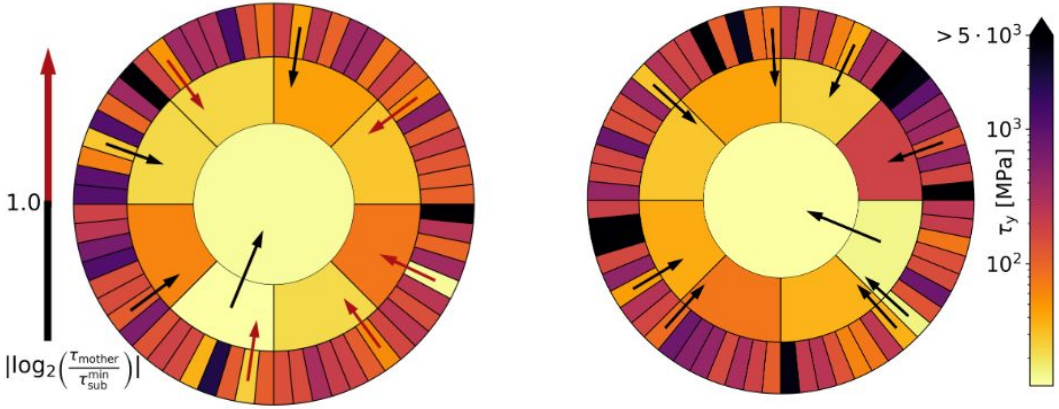
Weakest-link behaviour



- Similar behaviour during global and local quasi-static loading:
  - Similar plastic events
  - At similar stresses

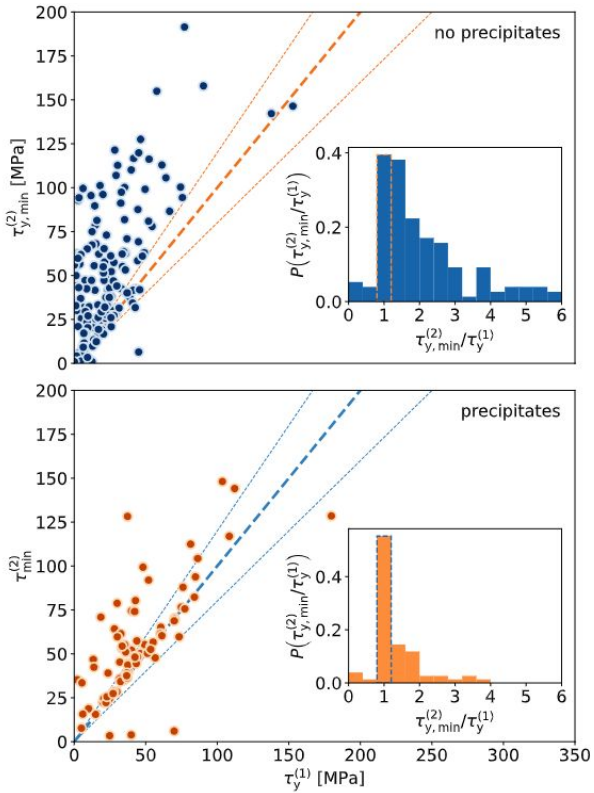
No precipitates vs strong precipitates

no precipitates **strong precipitates**



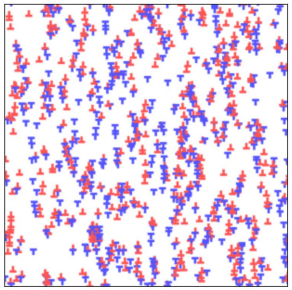
worse inheritance

better inheritance



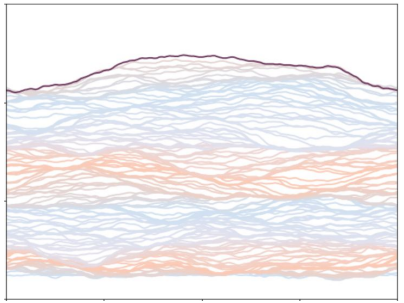
Summary

2D DDD (straight)



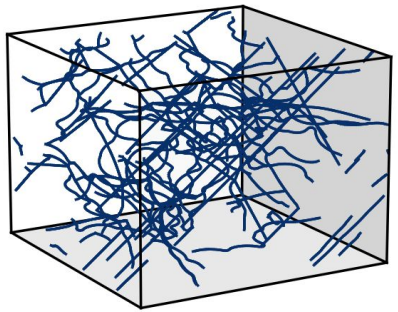
- Scale-free avalanches
- Different behaviour w/ and w/o point defects
- Dynamic modes related to avalanches

2D DDD (curved)



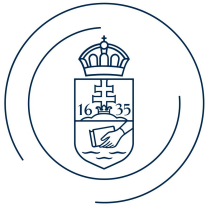
- Depinning dynamics
- Scale-free plastic slips
- Non-trivial dislocation shape

3D DDD



- Weakest-link behaviour
  - Better with precipitates
- Hardening
  - size-related
  - precipitate-related

Thanks to…



ELTE

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- ❑ Stefan Sandfeld
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- ❑ Peter Derlet

- ❑ Marc Legros