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Strain-rate-dependent predictability of discrete dislocation plasticity

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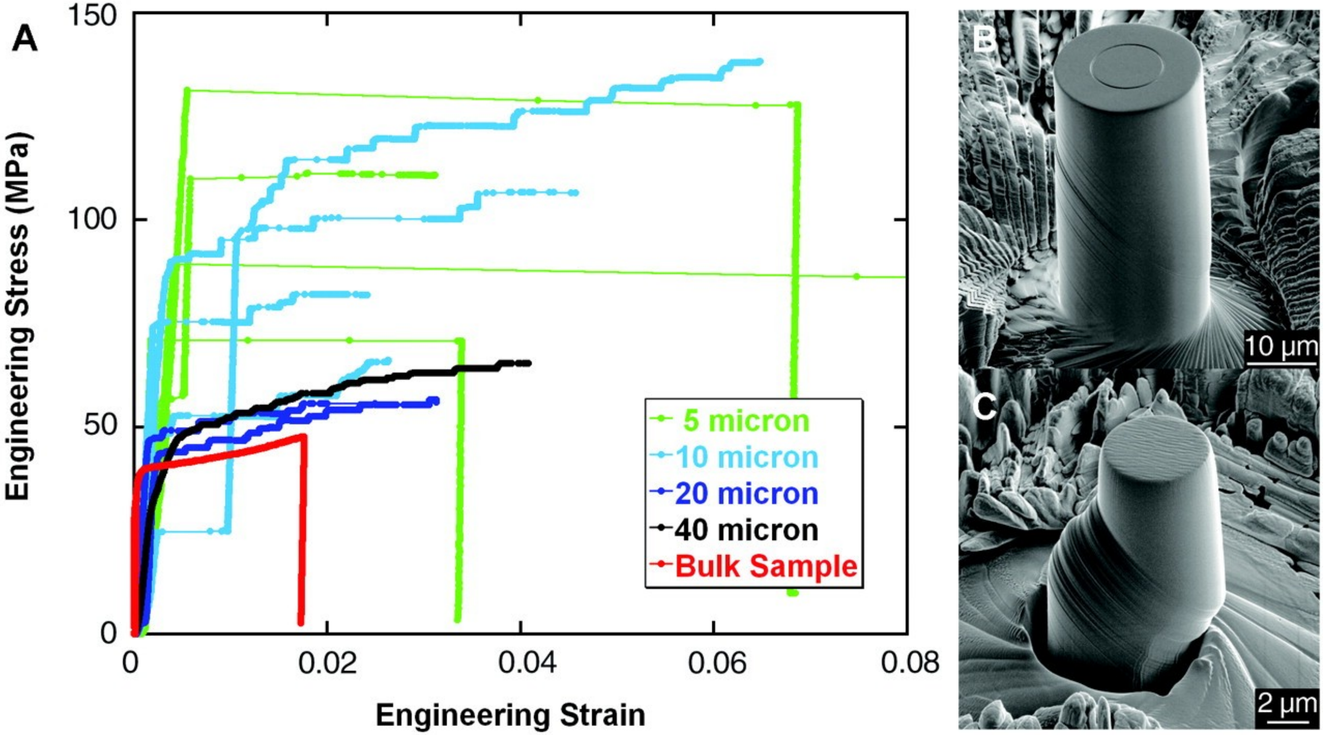
Motivation

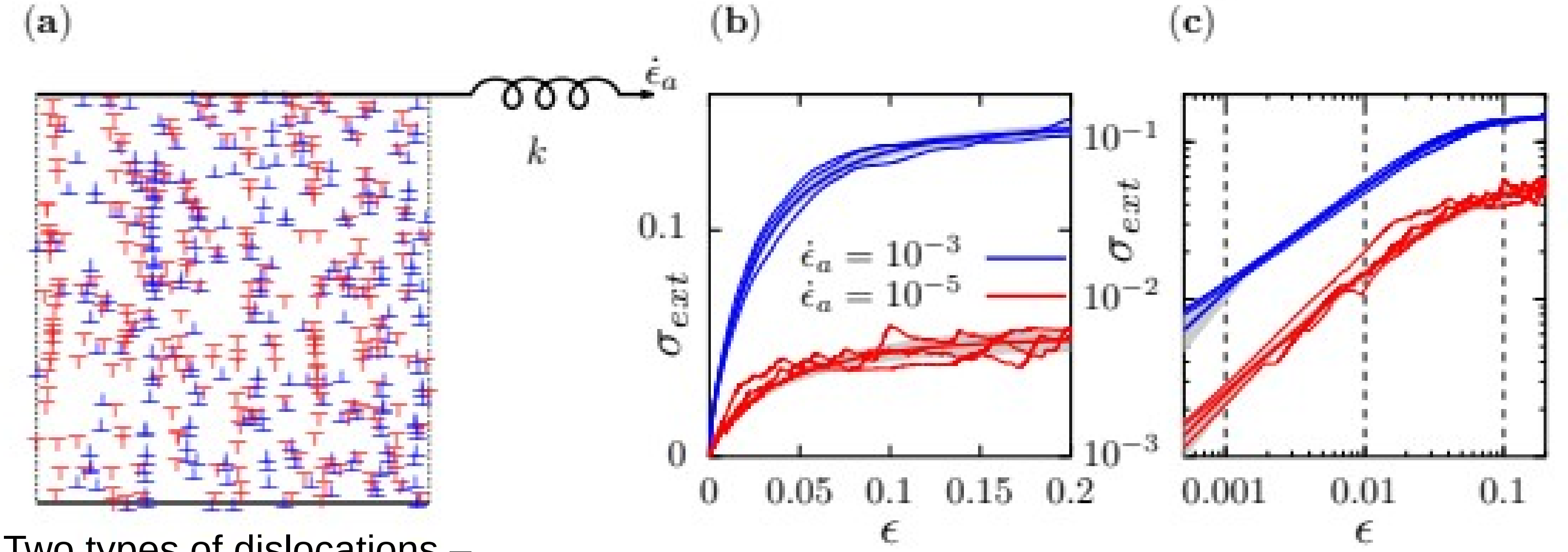


M. D. Uchic et al. Science 13 Aug 2004: Vol. 305, Issue 5686, pp. 986-989
Sample Dimensions Influence Strength and Crystal Plasticity

2D model – shear deformation

Discrete dislocation dynamics (DDD) simulations

Peach-Koehler equation: $$\frac{\dot{x}_i}{Mb} = s_i b \left[\sum_{j \neq i}^{N} s_j \sigma_{disl}(\mathbf{r}_i - \mathbf{r}_j) + \sigma_{ext} \right]$$



Two types of dislocations – opposite Burgers vectors

Strain-rate controlled loading: $$\sigma_{ext} = k[\dot{\epsilon}_a t - \epsilon(t)]$$

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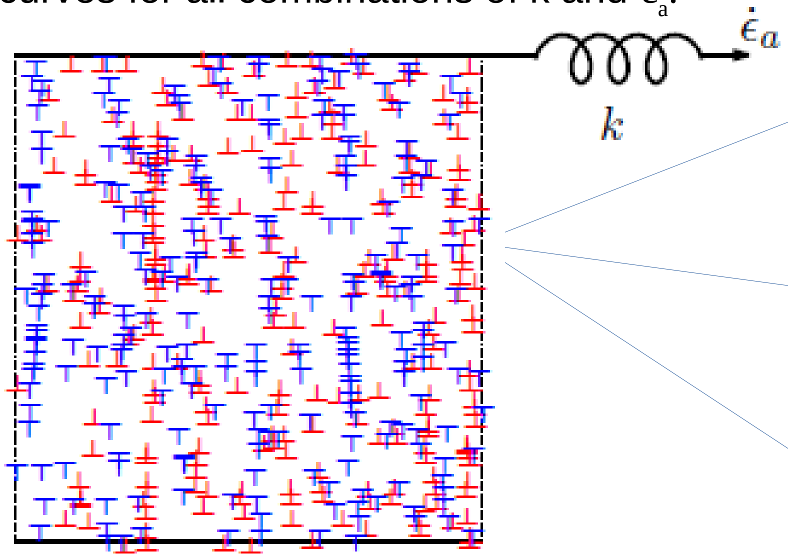
Predictability of stress-strain curves

In total 10000 dislocation configurations were generated and equilibrated. Afterwards the strain-rate controlled loading was performed with DDD to obtain stress-strain curves for all combinations of k and $\dot{\varepsilon}_a$.

k=0.1; 1; 10

$\dot{\varepsilon}_a=10^{-5}; 2*10^{-5}; 5*10^{-5}; 10^{-4}; 10^{-3}; 10^{-2}$



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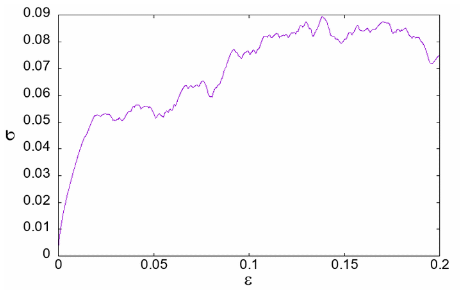

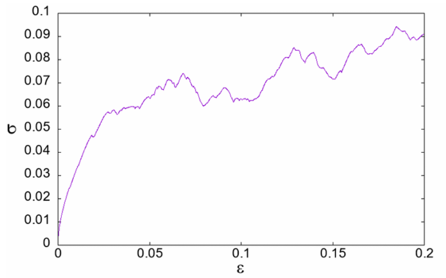

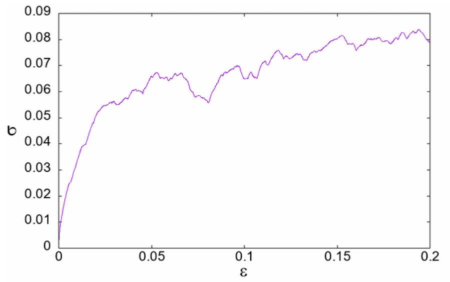

ML models:

- Linear regression
- Fully connected neural network
- Convolutional neural network

$$r^2 = 1 - \frac{\sum_i [\sigma_{ext}(i) - \sigma_{ext}^{fit}(i)]^2}{\sum_i [\sigma_{ext}(i) - \langle \sigma_{ext}(i) \rangle]^2}$$

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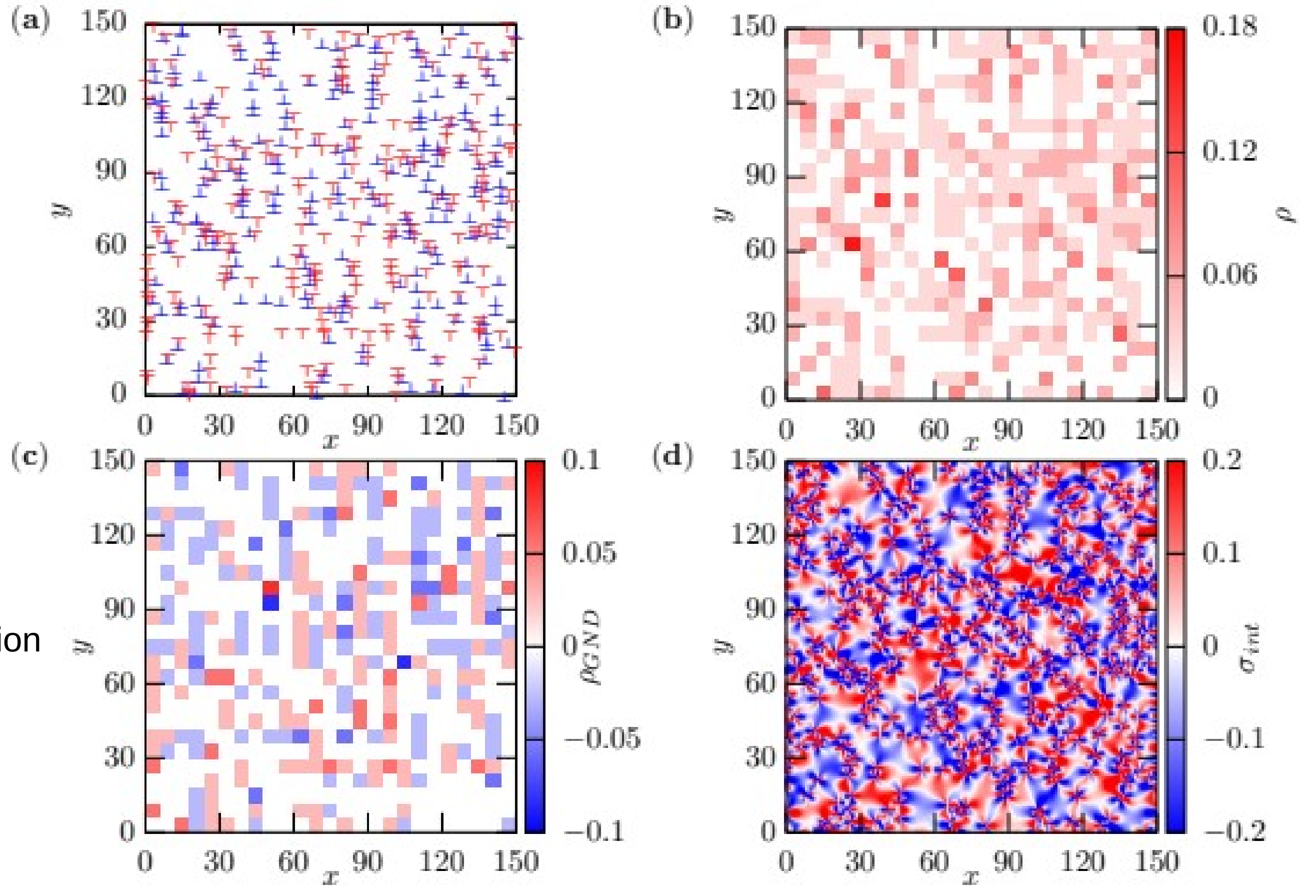
Input fields

Initial configuration

Dislocation density



Geometrically necessary dislocation density

Stress field

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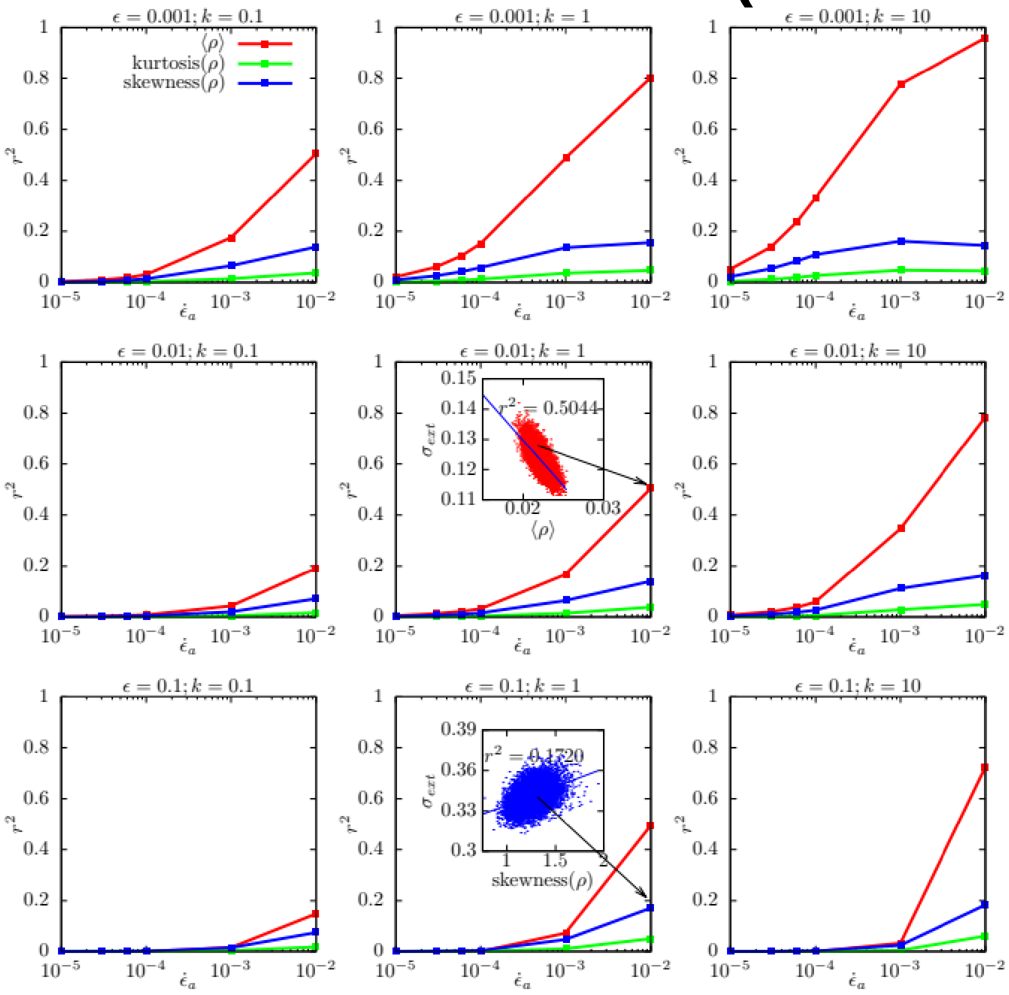
Linear correlations (density)



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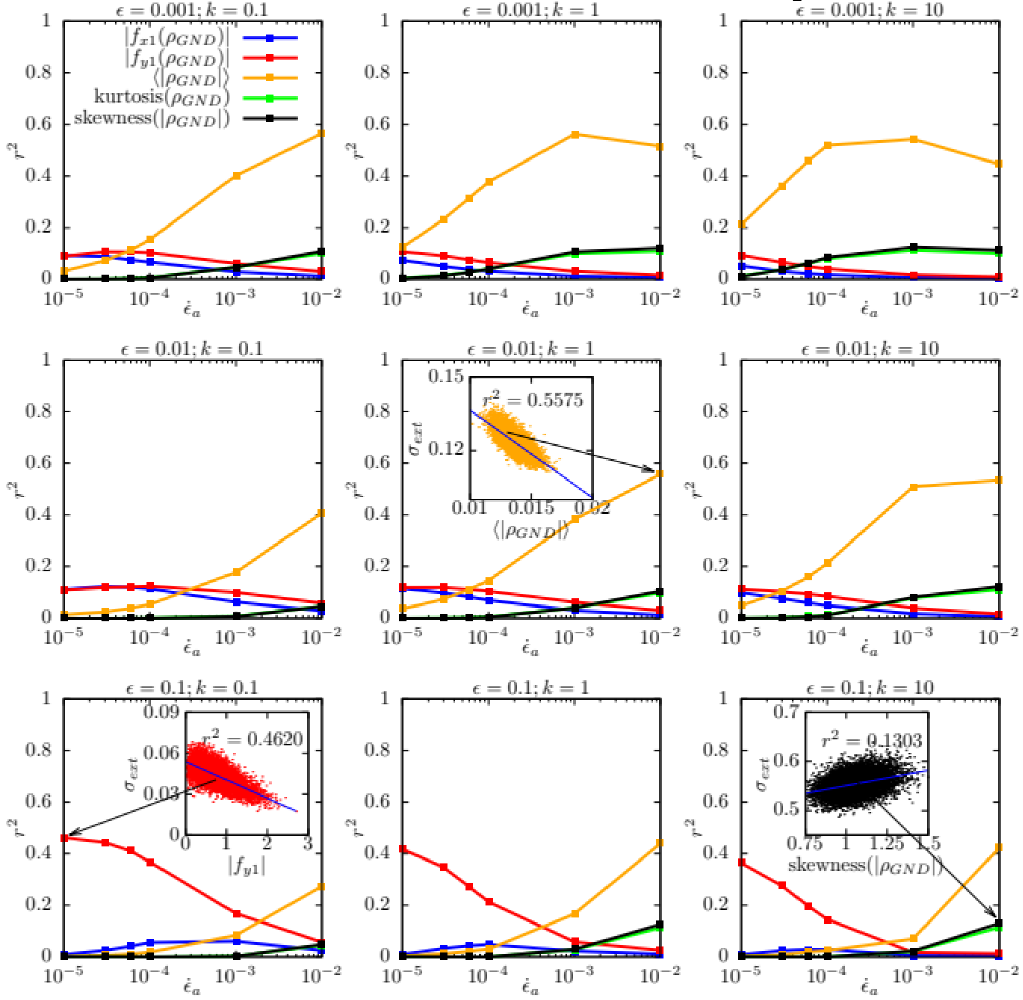
Linear correlations (GND)



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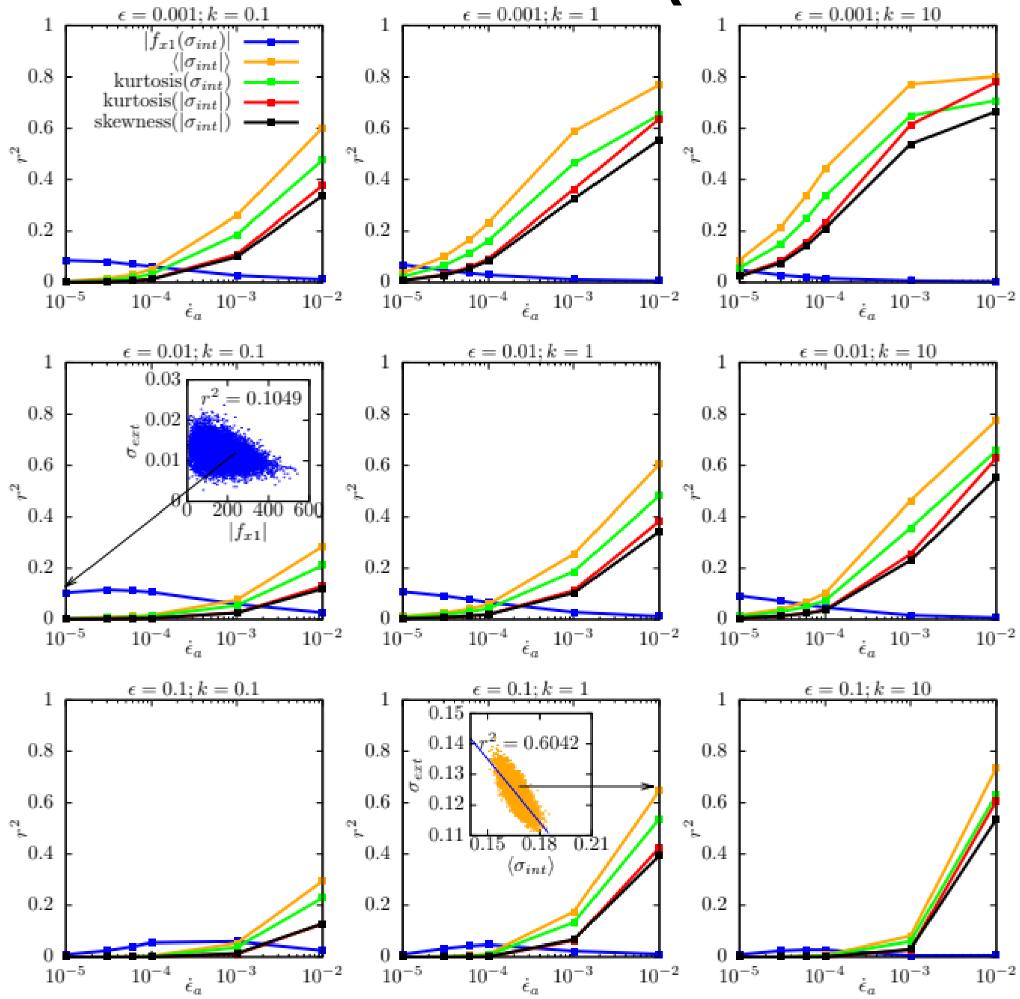
Linear correlations (stress field)



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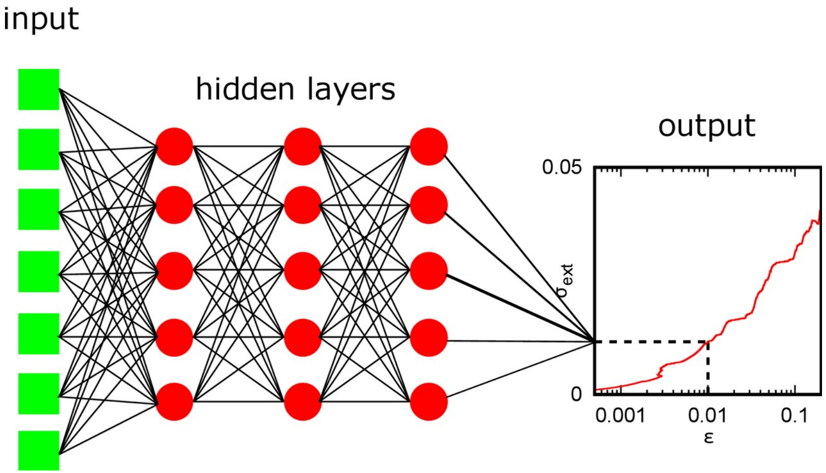
Linear regression and fully connected neural network

Linear regression

$$\sigma_{ext} = a_0 + \sum_{i=1}^{N_{\text{in}}} a_i x_i$$

features extracted from the fields as input

Fully connected neural network



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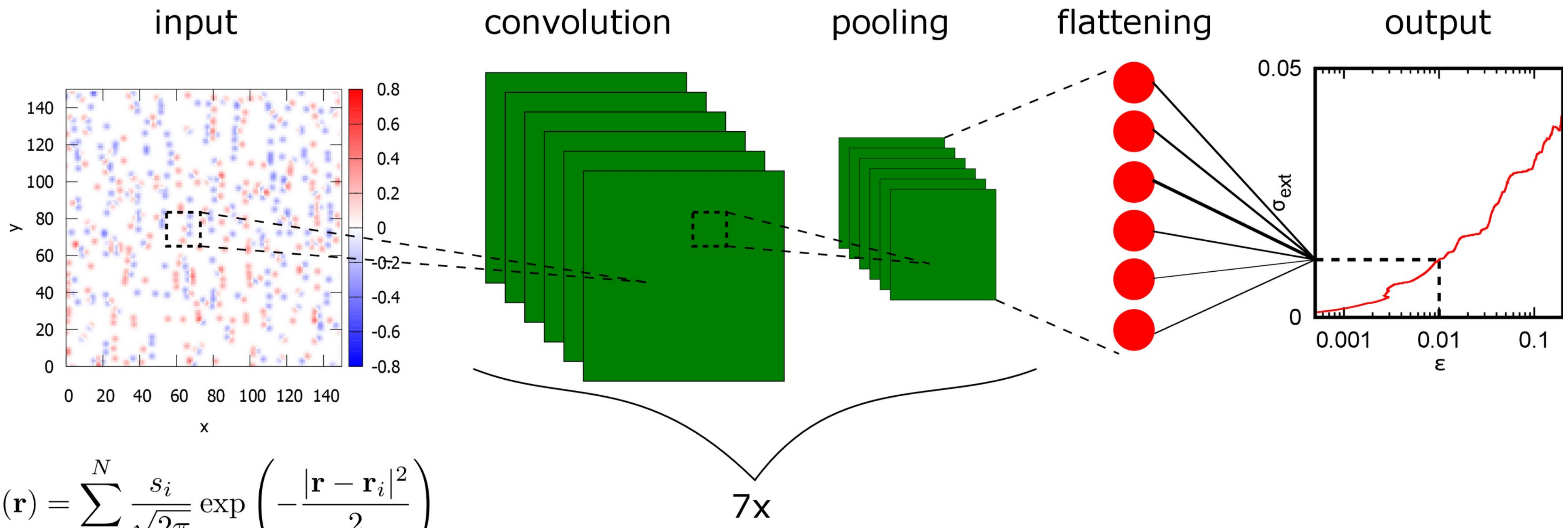
Convolutional neural network



$$J(\mathbf{r}) = \sum_{i=1}^{N} \frac{s_i}{\sqrt{2\pi}} \exp\left(-\frac{|\mathbf{r}-\mathbf{r}_i|^2}{2}\right)$$

image of the initial configuration

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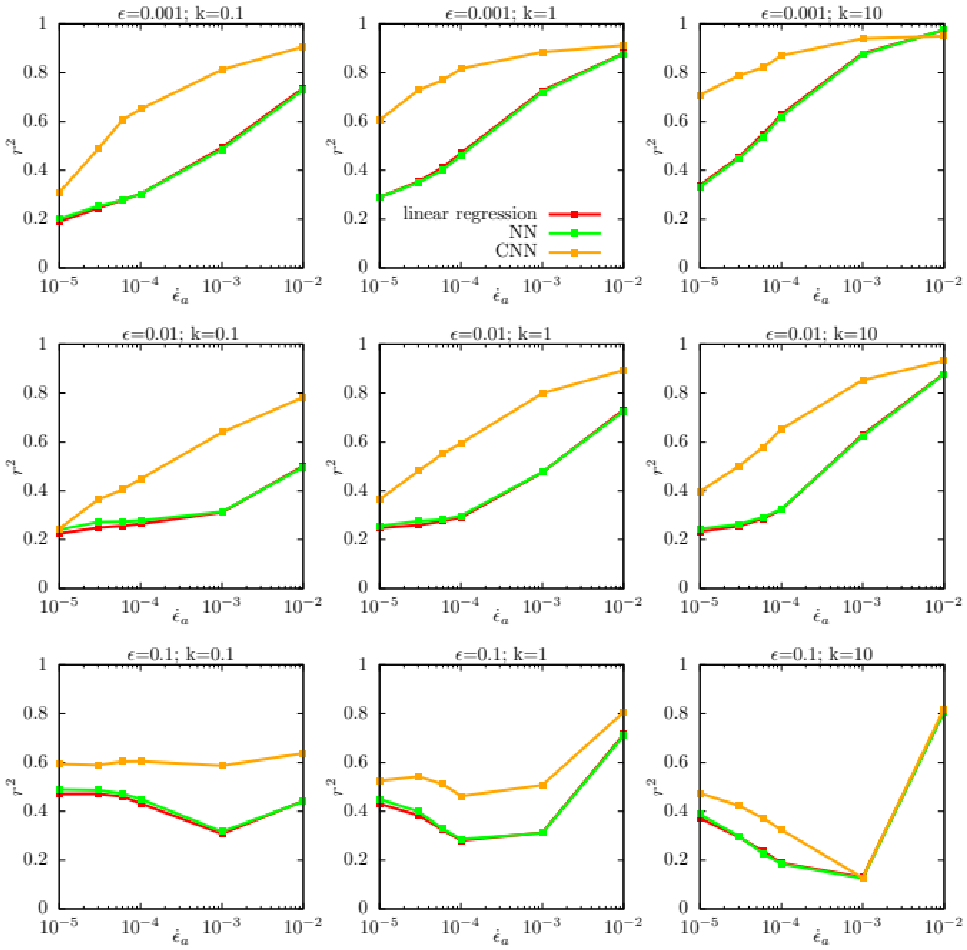
Predictability – test set results

$$r^2 = 1 - \frac{\sum_i [\sigma_{ext}(i) - \sigma_{ext}^{fit}(i)]^2}{\sum_i [\sigma_{ext}(i) - \langle \sigma_{ext}(i) \rangle]^2}$$



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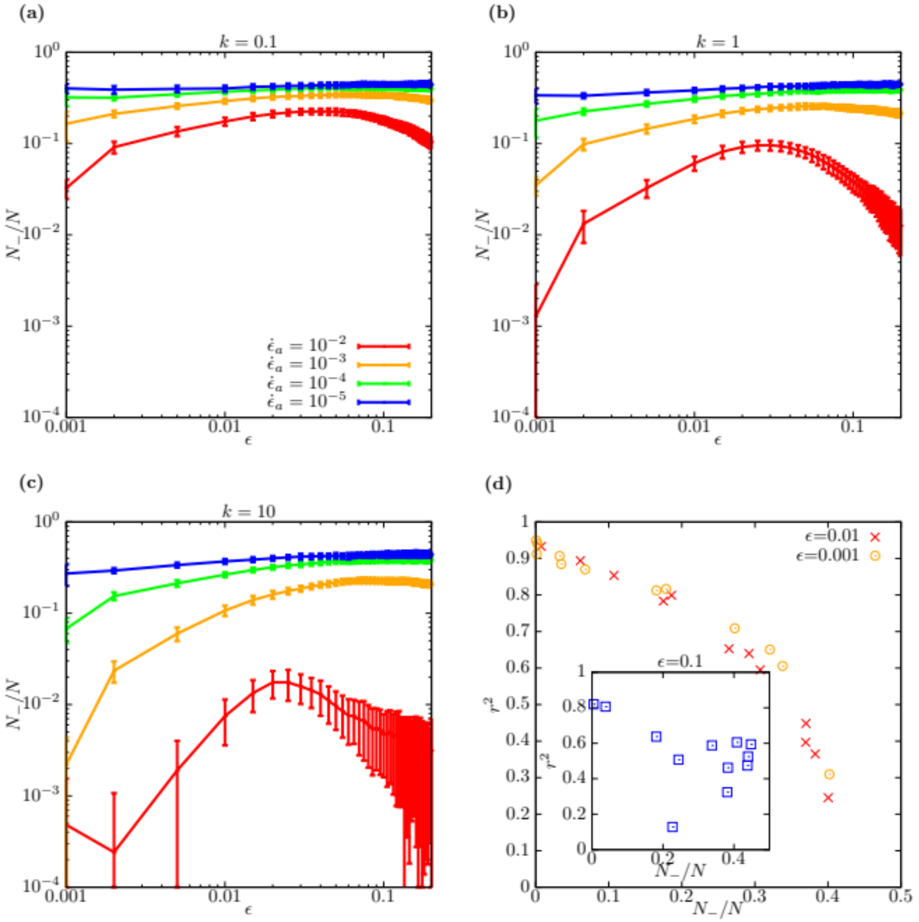
Complexity of dislocation dynamics



The fraction of dislocations moving against the external stress explains the increasing predictability at lower strains but not the non-monotonic behaviour at the highest strain.

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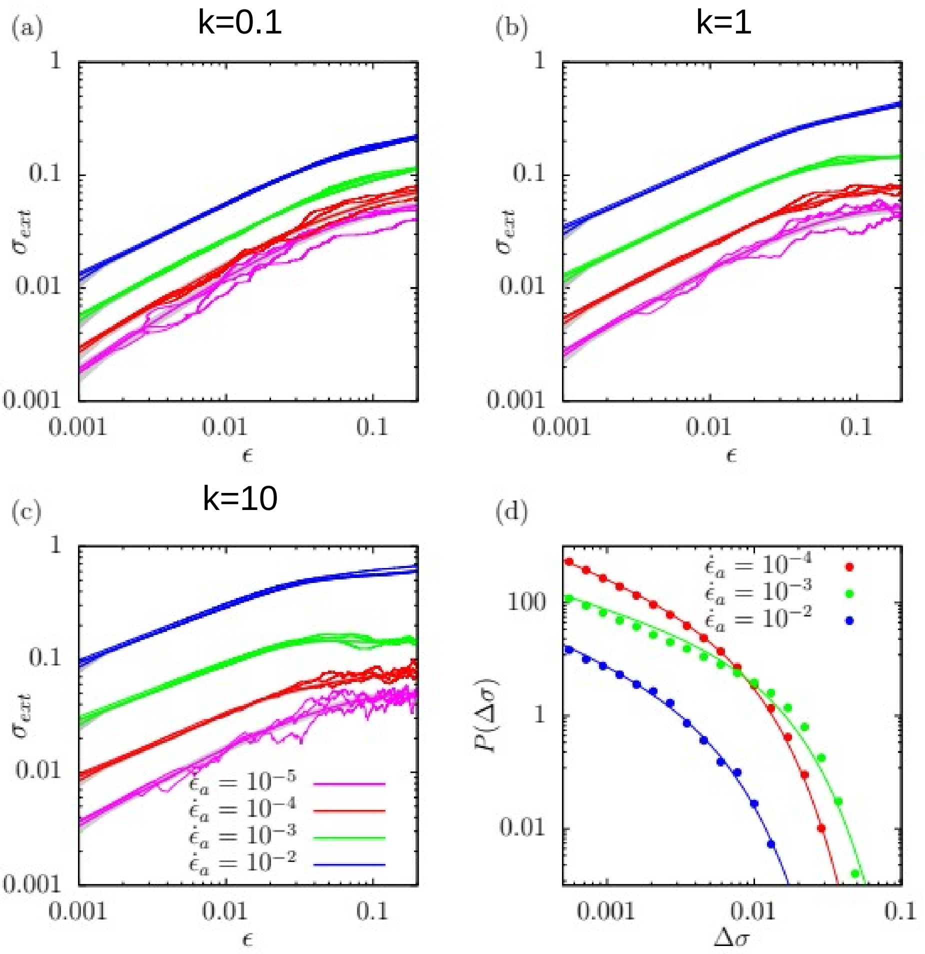
Stress drops distribution



Transition from fluctuating to smooth plastic flow explains the non-monotonic behaviour of the predictability.

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Outlook

- Extension of the model to three dimensions
- More complex dynamics: dislocation junctions, locks, multiplication
- Higher computational cost
- Strain rate effect could still be observed due to decreased dynamics complexity at high strain rates

Conclusions

- At low strain values the predictability increases with strain rate
- At high strain values the predictability exhibits non-monotonic behaviour
- The increasing predictability is related to the complexity of the dislocation dynamics
- The non-monotonic predictability is related to a transition from fluctuating to smooth plastic flow

Thank you for your attention!