# Experimental and Theoretical Investigations of Dislocation Avalanches

*Final report, KH-125380*

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## Introduction

The plastic response of most crystalline and amorphous metals exhibit random spatio-temporal fluctuations. For micron-scale samples this stochasticity appears in the form of unpredictable sudden localized strain bursts with magnitudes varying on a wide range, posing a significant challenge for material design at this scale. Stochasticity, however, is not constrained to small specimens, it is also present in bulk samples as indicated by acoustic emission measurements. Its importance is not lesser in this case, since dislocation avalanches are expected to have a strong impact on the dislocation pattern evolution, thereby affecting several macroscopic mechanical properties. The aim of the project was to investigate intriguing issues related to the stochastic features of plasticity. In this report the summary of the performed research is given grouped in three distinct but related sub-topics.

## Summary of the performed research

1. *Characterization of dislocation avalanches in metals*

   *(1.1) Deformation of Zn micropillars.*

   Dislocation avalanches that are responsible for the accumulation of plastic strain in crystalline specimens are challenging to investigate experimentally. Two state-of-the art techniques available are (i) micropillar compression and (ii) the detection of acoustic signals emitted during plastic strain. The first method is only suitable for quite small samples (max. ~20 $\mu$m) whereas acoustic emission (AE) measurements have been only performed on bulk samples so far.

   One of the main aims of the project was to couple these two type of experiments, that is, to perform AE measurements on micropillars while being compressed *in situ* in a scanning electron microscope (SEM). Such an experiment could answer the long standing issue: how should one interpret AE data in terms of strain and/or stress evolution within the material.

   Micropillars with various diameters were fabricated using a focused ion beam (FIB) in the SEM lab of the Research and Instrument Core Facility at the Eötvös University. As a base material a Zn single crystal was used and the pillars were oriented for nearly perfect basal slip. The sample preparation proved a difficult task, as pure Zn is extremely soft and a sophisticated polishing procedure had to be developed in order to prevent twin formation and recrystallization close to the sample surface. Unfortunately, this unexpected difficulty slowed down the experimental work considerably. The final procedure involved a final polishing step with Ar ions in collaboration with Szilvia Kalácska, EMPA Thun, Switzerland. A SEM picture of an 8 $\mu$m micropillar is shown in Fig. 1(a).

   Subsequent *in situ* compression of the pillars was performed by a custom made nanoindenter stage equiped with a diamond flat punch tip. The resolution of the device in terms of force is around 1 $\mu$N and in terms of displacement around 0.1 nm. A compressed micropillar is seen in Fig. 1(b) and representative stress-strain curves of pillars of various sizes are plotted in Fig. 1(c). It was tested using electron backscatter diffraction (EBSD) that all pillars were single crystals both before and after compression proving that nor sample preparation nor compression did not introduce twins, that is, only basal dislocation glide took place during deformation.

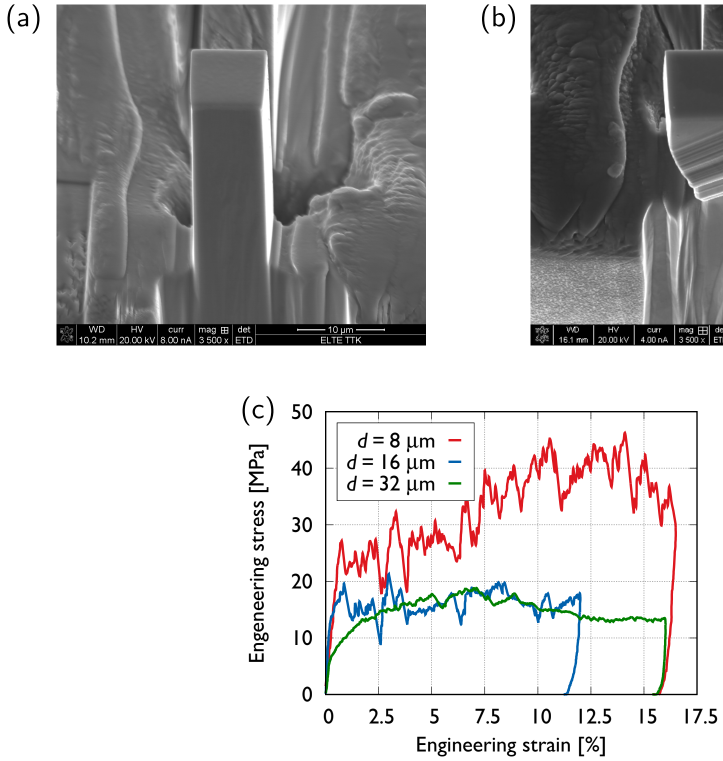


FIG. 1: SEM picture of a FIB milled micropillar before [panel (a)] and after [panel (b)] *in situ* compression. Panel (c): representative stress-strain curves of pillars with various diameters. Size-effects are clearly observed as well as the decrease of the stochasticity as the sample size increases.

*(1.2) Acoustic emission (AE) measurements.*

Within the framework of this project an extremely sensitive AE device has been purchased and installed at the Department of Materials Physics, Eötvös University. The *in situ* AE detection during micropillar compression and subsequent noise reduction of the AE signals were performed with the assistance of expert colleagues from Prague involved in this project.

The nanoindenter was equipped with a piezoelectric acoustic sensor which was connected to the amplifier through the wall of the vacuum chamber of the SEM. The results obtained during micropillar compressions were beyond our previous expectations. First of all, the AE data were found to be in perfect correlation with the observed stress drops (that mark dislocation avalanches), which confirms that the main source of AE in this sample is indeed dislocation activity. As seen in Fig. 2 all AE events correspond to an anelastic event. In addition, at large stress drops several acoustic events can be detected, as also seen from the event rate in Fig. 2(a) and from the zoomed figure of Fig. 2(b).

In addition, the analysis of the waiting times between subsequent acoustic events reveal very complex avalanche dynamics: a typical stressdrop on the stress-strain curve is eventually the result of several (typically 2-10) subsequent plastic events as we concluded from the AE measurements. According to Fig. 3(a) approx. 80% of the events follow each other within 10 ms, whereas the rest have a lag of more than 1 s in between. When a smaller deformation rate is applied, only the large waiting time portion of the distribution is affected,

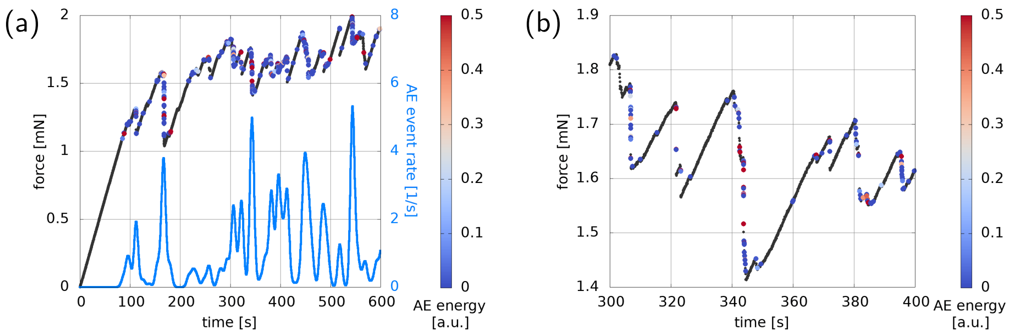


FIG. 2: Compression of an 8 $\mu$m Zn micropillar coupled with AE measurement. (a) Force vs. time plot, the force drops correspond to individual slip events. The colour dots mark to the detected AE signals whereas the light blue curve is the AE event rate that exhibits pronounced peaks around large force drops. (b) Zoomed figure: AE events can only be detected where plastic deformation takes place.

therefore, the intermittent dynamics within a single avalanche is unaffected by the rate. To elaborate further on this finding we investigated the rate of events after each mainshock (defined as an event with released energy between two predefined and varied bounds) and it was found to decay as $1/t$ (for more than 3 orders of magnitude) in agreement with the empirical Omori law that corresponds to earthquakes. In addition, according to Fig. 3(b) larger rates correspond to larger mainshocks, again a well-known fact for earthquakes usually referred to as productivity law. Our finding thus means that the dynamics of plastic events that take place in micron sized samples with durations on the ms scale are analogous to those of earthquakes that may span several km-s and months. These results are not only the first successful combination of micromechanical and AE measurements but yield insight to the very nature of dislocation avalanches by linking their properties to those of earthquakes. We will, therefore, submit our results to a high impact journal soon.


[1] Péter Dusán Ispánovity, Dávid Ugi, Gábor Péterffy, Dániel Tüzes, Szilvia Kalácska, Zoltán Dankházi, Michal Knapek, Kristián Mathis, František Chmelík and István Groma
*Dislocation Avalanches: Earthquakes on the Micron Scale*
manuscript under preparation (2020).


2. *Pattern formation of dislocations*

*(2.1) Stochastic continuum dislocation dynamics (SCDD).*

During plastic deformation dislocations organise into distinctive patterns. Since the amount of dislocations is the key factor affecting the yield strength of a single crystalline material, these patterns lead to the inhomogeneity of the local strength of the material. It was shown earlier, that an inhomogeneous local yield stress distribution leads to an avalanche-like deformation process that is identical to the one observed experimentally.

Therefore, to obtain an in-depth theoretical description of dislocation avalanches it is essential to understand the patterning phenomenon in full detail. To this end, a SCDD model was established based on the variational framework of continuous dislocation dynamics [2]. It was shown, that if the local yield stress distribution is narrow, than dipolar walls perpendicular to the dislocation slip direction form with a well-defined distance between them. This result is in-line with previous linear stability analysis of the deterministic evolution equations.

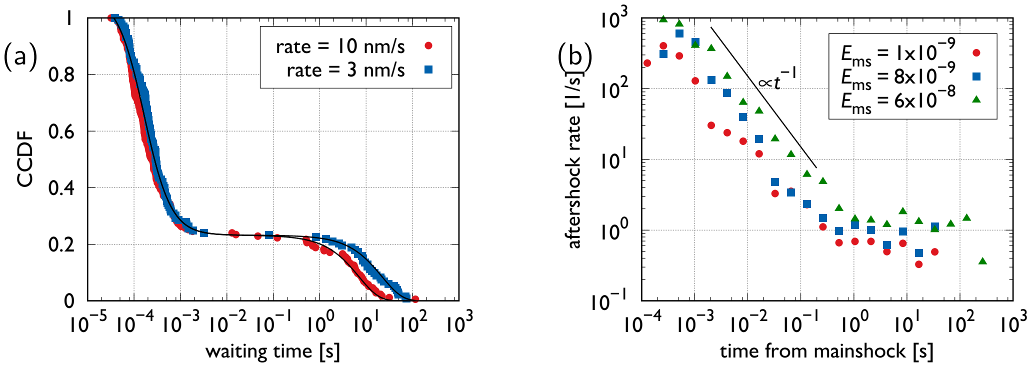


FIG. 3: (a) Complementary cumulative distribution function of waiting times between subsequent AE events. Notice that almost 80% of the data fall below 10 ms, and the rest is typically above 1 s. When the deformation rate is altered only the tail of the distribution is affected. (b) Average AE event rate after mainshocks with various energies $E_{\mathrm{ms}}$. The rate in every case decays as $1/t$ and the rate increases with mainshock energy.

According to discrete dislocation dynamics (DDD) simulations periodic patterns predicted by the linear stability analysis do not form, but a slightly different pattern emerges instead. In particular, dipolar walls do form but they are not equidistant. To account for this phenomenon in the SCDD model the local yield threshold distribution was chosen to be a wide Weibull distribution, in line with previous studies on DDD systems. Precise agreement in the patterning characteristics was found in terms of spatial two-point correlation functions: upon increasing stress dislocations organise into dipolar walls perpendicular to the slip plane (see Fig. 4 for an example pattern in DDD and SCDD simulations). These anisotropic structures give rise to hysteresis upon stain reversal, that is, the Bauschinger effect. This study, therefore, provides a theoretical link between microscopic features of dislocations and macroscopic continuum descriptions based on the concept of backstress. As such, this study is the first example of a successful multi-scale modelling of the pattern formation of two-dimensional discrete dislocation systems [3].

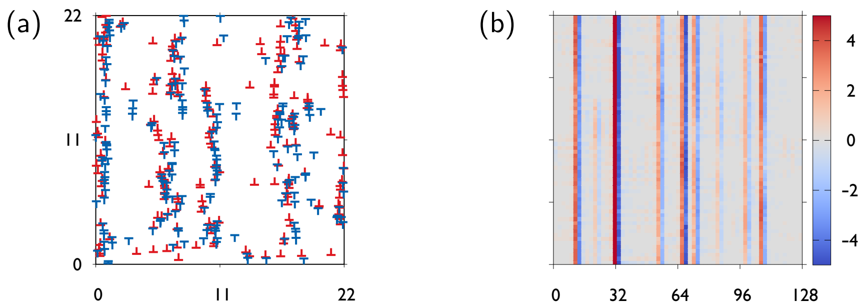


FIG. 4: Dislocation patterns obtained from DDD simulations [panel (a)] and SCDD simulations [panel (b)]. The equivalence of the patterns can be shown using spatial correlation functions [3].

[2] Ronghai Wu, Daniel Tüzes, Péter Dusán Ispánovity, István Groma, Thomas Hochrainer and Michael Zaiser

*Instability of dislocation fluxes in a single slip: Deterministic and stochastic models*

*of dislocation patterning*
Phys. Rev. B **98**, 054110 (2018).
[https://doi.org/10.1103/PhysRevB.98.054110].

[3] Péter Dusán Ispánovity, Stefanos Papanikolaou and István Groma
*Emergence and role of dipolar dislocation patterns in discrete and continuum formulations of plasticity*
Phys. Rev. B **101**, 024105 (2020).
[https://doi.org/10.1103/PhysRevB.101.024105].

*(2.2) Local yield thresholds in discrete dislocation systems.*

In the stochastic continuum formulation described above in point (2.1) a fundamental role is played by the local yield stress distribution that represents the microstructural inhomogeneities leading to the avalanche-like response. Although there are theoretical considerations that may be applied to predict the form of this distribution, we also plan to *'measure'* it directly in DDD simulations. To this end, one needs to test local regions of a large configuration individually after extracting them from the whole system. For such a testing, the initial boundary conditions must be kept fixed. Since so far only periodic boundary conditions were implemented in our DDD simulations, we decided to develop a new method to handle the boundary conditions which is faster than the finite element method (FEM). We, therefore, developed a spectral method that is capable of handling any type of elastic boundary conditions on a rectangular domain [4]. This method indeed exhibits superior computational complexity than FEM and its precision was tested both on analytically solvable test cases and also in systems containing edge dislocations. The application of the method for the problem of local yield thresholds outlined above has been started.

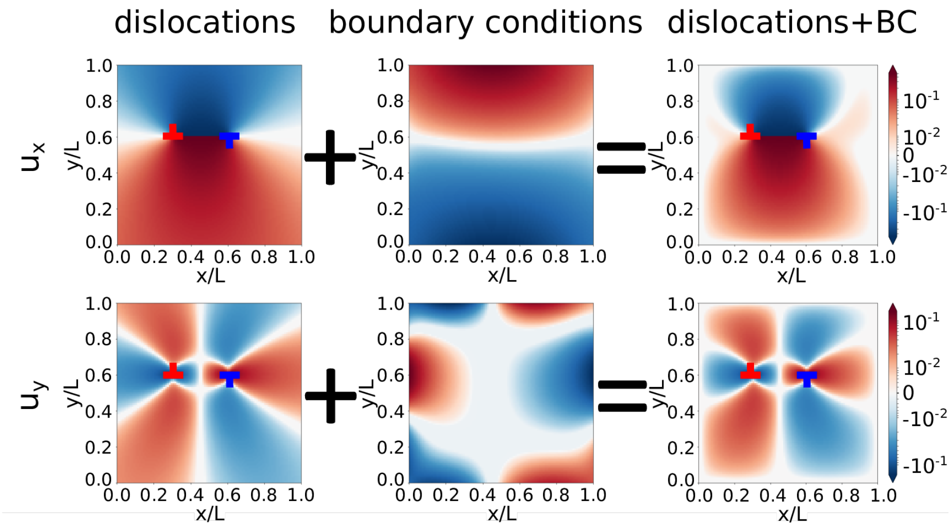


FIG. 5: Displacement field $\boldsymbol{u}$ of a dislocation dipole with zero displacement boundary conditions. The final solution is plotted in the right column. For details see [4].

[4] Dénes Berta, István Groma and Péter Dusán Ispánovity
*Efficient numerical method to handle boundary conditions in 2D elastic media*
Model. Simul. Mater. Sci. Eng. **28**, 035014 (2020).
[https://doi.org/10.1088/1361-651X/ab76b1].

*(2.3) Experimental investigation of dislocation structures formed in micropillars.*

Dislocation patterns that develop during plastic deformation of crystalline matter in most cases exhibit a characteristic length-scale in the order of 1 $\mu$m. Since the stochastic behaviour also appears when the specimen size is in this range or below, it is natural to assume that dislocation patterns may play a central role in the statistics of strain bursts. The dislocation structures in bulk samples are quite different from the ones in nanocrystals both in terms of morphology and dislocation density. The aim of the research was to investigate the emerging dislocation structures at an intermediate scale. The reason is that currently there are no state-of-the-art methods available that could reconstruct a full 3D dislocation microstructure which would be inevitable to validate theoretical results presented in section (2.1) above. In this work, micropillars with 6 $\mu$m diameter were prepared from Cu single crystals, and then deformed *in situ* up to different strain levels. Afterwards, serial slicing was performed on the pillars with FIB and HR-EBSD was performed at every step in order to obtain the full 3D microstructure and the internal stresses within the samples. Scanning transmission electronmicroscopy (STEM) and transmission electronmicroscopy (TEM) images were also captured to validate the HR-EBSD measurements. It was found that a complex network of geometrically necessary dislocations (GNDs) form which resembles cellular structures of bulk specimens that are responsible for the strain hardening observed during compression [5]. However, the GND density levels are an order of magnitude lower than in bulk, so, a large number of dislocations can still escape through the boundary at this size and this gives rise to a size-effect, that is, the yield stress is significantly higher than in bulk. This study thus represents the first thorough 3D mapping of the evolving microstructure at this scale and is expected to serve as a valuable input for discrete dislocation dynamics and crystal plasticity modelling of collective dislocation transport [5].

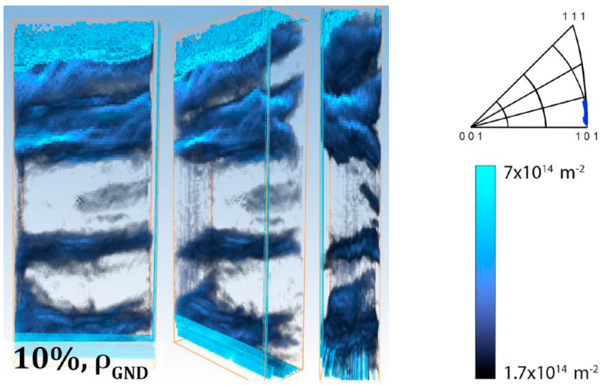


FIG. 6: Distribution of geometrically necessary dislocation density in a Cu micropillar compressed to 10% strain. High dislocation content in the slip bands is clearly visible [5].

[5] Szilvia Kalácska, Zoltán Dankházi, Gyula Zilahi, Xavier Maeder, Johann Michler, Péter Dusán Ispánovity and István Groma
*Investigation of geometrically necessary dislocation structures in compressed Cu micropillars by 3-dimensional HR-EBSD*
Mater. Sci. Eng. A **770**, 138499 (2020).
[https://doi.org/10.1016/j.msea.2019.138499].

*(2.4) Distribution of internal elastic stresses in polycrystals.*

We developed a new theoretical method to determine the internal stresses in grains of different orientation in polycrystalline samples. The theory was tested on neutron diffraction measurements performed on strained steel samples, and the shifts of the Bragg peaks (representing grains with identical orientation) showed perfect agreement with the predictions [6]. This method will help in deepening our understanding of the dislocation patterns developing in different grains with various orientation in a polycrystalline material.

[6] Ádám Takács, Géza Tichy and Péter Dusán Ispánovity
*Strain distribution in polycrystals: Theory and Application for Diffraction Experiments*
Submitted to Journal of Elasticity (2019)
[https://arxiv.org/abs/1812.02247].

3. *Dynamical correlations in discrete dislocation systems*

*(3.1) Implicit time integration scheme for DDD simulations.*

In understanding crystalline plasticity DDD simulations play a fundamental role. In these simulations the motion of individual dislocations are tracked by solving their equations of motion. These tools are numerically exceptionally demanding since dislocation interact via their long-range elastic stress fields, so all the pair interactions have to be summed at every timestep. In addition, the stress field diverges at the dislocation core. Due to these properties the governing equations form a stiff set of ordinary differential equations which needs a tailor-made algorithm for an efficient solution. During the project a specific implicit scheme was developed which introduces a cut-off function for the calculation of the Jacobian [7]. Using this method the simulation runtime could be decreased with up to four orders of magnitude compared to the previous widely used implementation based on 4th order Runge-Kutta explicit schemes. The method was developed and tested for 2D DDD simulations but can be generalized to 3D simulations as well which will have a significant impact on the applicability of these simulations [7].

[7] Gábor Péterffy and Péter Dusán Ispánovity
*An efficient implicit time integration method for discrete dislocation dynamics*
Model. Simul. Mater. Sci. Eng. **28**, 035013 (2020).
[https://doi.org/10.1088/1361-651X/ab76b2].

*(3.2) Linear stability analysis of discrete dislocation systems.*

The linear stability analysis of the equations of motion of discrete dislocations shows the existence of a large number of extended soft modes in equilibrated dislocation configurations at zero applied stress. According to Fig. 7 there exist a large number of modes with low eigenvalue and a large participation number. The latter quantity characterises, roughly speaking, the non-zero elements in the given eigenvector. As seen, there are a number of soft modes and the participation number almost reaches the total number of dislocations. In addition, the larger the system is, the more extended these soft modes get as it is evident from the comparison of Figs. 7(a) and 7(b). These eigenmodes of the dynamical matrix are of utmost importance in understanding dislocation avalanches, since an avalanche occurs when one of the eigenvalues associated with these modes becomes negative. In such a case the corresponding eigenvector defines the velocities of the dislocations at the onset of the event. The existence of extended modes thus explains the previous finding that dislocation avalanches may span the entire system even at zero stress regardless of the system size. This means, that these modes are responsible for the extended critical behaviour of these systems.

We also performed simulations with added point-like impurities (e.g., vacancies or solute atoms). It was shown before that in this case at small applied stresses the system becomes sub-critical with avalanche sizes independent of the system size. Our results shed light on the microscopic origin of this finding since the eigenmodes become localised in this case. This means that avalanches are triggered locally and they exhibit a maximum spatial range, determined by the number and strength of the impurities in the system. These results clarify the physical background of the critical behaviour observed in dislocated crystals and we, therefore, plan to publish them in a high impact journal soon.

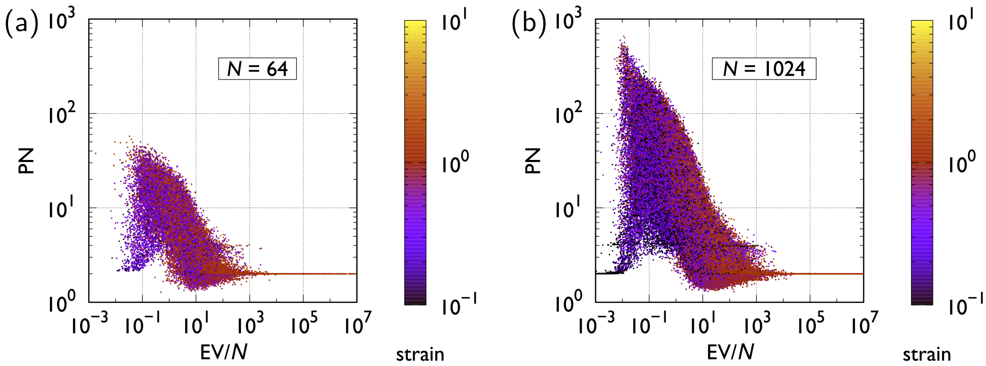


FIG. 7: Eigenmodes of the dynamical matrix for relaxed discrete dislocation configurations. Normalized eigenvectors (EV) are plotted vs. the participation number (PN) for systems that contain different number of dislocations $N$ [panel (a): $N = 64$, panel (b): $N = 1024$].


[8] Gábor Péterffy, Peter Derlet and Péter Dusán Ispánovity
*Universality classes of dislocation systems*
manuscript under preparation (2020).


*(3.3) Depinning transition of a single dislocation in a random solid solution.*

So far, dislocation avalanches of collective dislocation motion and their consequences were considered. However, dislocation themselves are line-like objects with an associated line tension that make them behave like elastic strings. When these lines move through a random field a classical depinning transition may take place.

From the practical point of view, the mobility of a dislocation, that is the multiplier in the velocity-force relation of dislocations, plays a crucial role. These mobilities are commonly upscaled from molecular dynamics simulations for usage in higher scale plasticity models, such as discrete dislocation dynamics and crystal plasticity. Usually it is assumed that dislocation mobilities are independent of the length of the dislocation line.

Through a molecular dynamics study of edge dislocation mobility in random, austenitic Fe0.7Ni0.11Cr0.19 alloy we showed, however, that dislocation mobilities in solid solutions are intrinsically scale-dependent. To help rationalize this observation, we analyze the dislocation line configurations obtained over a range of stresses and temperatures. An analysis of the line roughness reveals the hallmarks of a classic depinning transition: (i) at low temperatures the average dislocation velocity vs. external stress curve shows a second order phase transition at $\sigma_c \approx 95$ MPa where the dislocation line depins [see Fig. 8(a)]. (ii) The roughness analysis of the dislocation profile reveals a scaling behaviour analogous for domain wall depinning in ferromagnets: three distinct scaling regimes exist with fractal dimensions $D \approx 1.2$, 1.5 and 1.8. The regimes with different $D$ are separated by correlation lengths that diverge at the depinning point as seen in Fig. 8(b). At higher temperatures creep sets in, but no new scaling regime is introduced compared to those at low temperatures. We conclude that it is this depinning transition which gives rise to the length-dependence of the mobilities. The implication of these findings is that care must be taken when upscaling mobility information to ensure that the scale-dependence is properly accounted for. As an example, we developed a new dislocation mobility law suitable for discrete dislocation dynamics simulations of random solid solutions which accurately captures the scale-dependence.

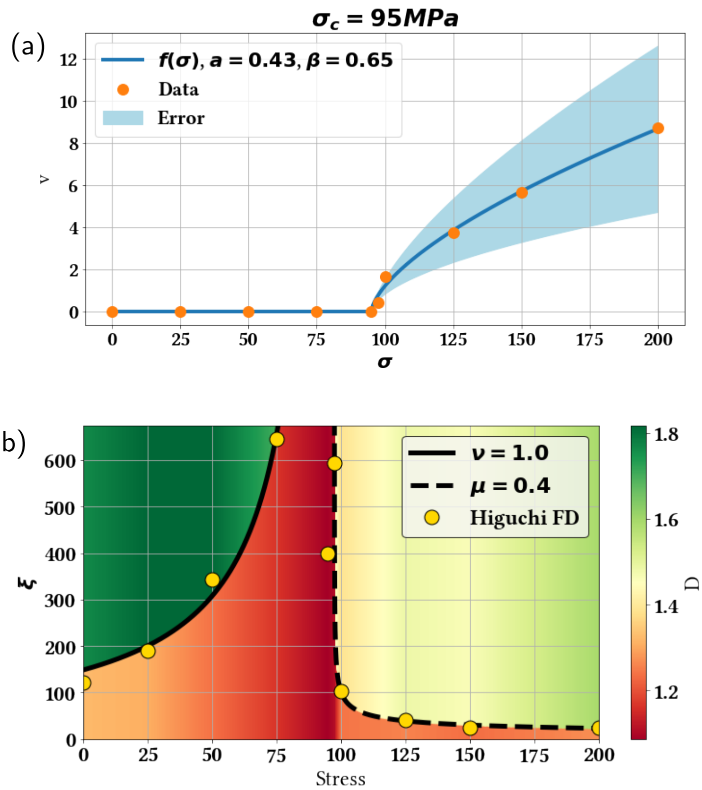


FIG. 8: Depinning transition of a dislocation line in a Fe-Ni-Cr solid solution. Normalized eigenvectors (EV) are plotted vs. the participation number (PN) for systems that contain different number of dislocations $N$ [panel (a): $N = 64$, panel (b): $N = 1024$].


[9] Ryan B. Sills, Gábor Péterffy, Michael E. Foster, Xiaowang Zhou and Péter Dusán Ispánovity

*Length scales and scale-free dynamics of dislocations in dense solid solutions*

manuscript under preparation (2020).


## Summary

The research performed within the frame of this project is absolutely in line with the proposed directions. Significant scientific achievements were made for every objective of the project proposal, as described above. The research activities addressed various different but related issues of stochastic properties of plasticity, and included experimental, theoretical and numerical activities, as well. From the 9 publications related to this project 5 have been published, 1 is submitted (but already accessible at an open manuscript database), and 3 are under preparation.