Stochastic Properties of Micron-scale Plasticity

Final report, PD grant of Péter Dusán Ispánovity

Introduction

The plastic response of most crystalline and amorphous metals exhibit 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 several intriguing issues related to the stochastic features of plasticity, grouped in five distinct objectives in the proposal. In this report the summary of the research is given in the same structure below.

Summary of the Research Performed

1. *Experimental and numerical investigation of stochastic properties of micron-scale plasticity*

   (1.1) Plastic response of a large number of identical micropillars.

   Micropillars are cylindrical samples with diameters in the micrometer range. These specimens have been known to exhibit strong fluctuations upon compression. Consequently, the stress-strain curves, and thus the yield stress, of identically prepared pillars differ from each other. The previous studies on the plastic properties of micropillars mostly focused on the properties of individual samples differing in material, shape and fabrication method. Within this objective, therefore, we aimed at giving an in-depth statistical characterization of the fluctuations. To this end, 42 identical pillars were fabricated on the surface of a pre-deformed copper single crystal oriented for single slip (see Fig. 1 for a subset). The stress-strain curves were obtained using a nanoindenter equipped with a flat punch diamond tip. The subsequent analysis showed that (i) based on the average stress-strain curves a yield stress can be defined that is characteristic of the whole ensemble, (ii) the stresses of individual realizations measured at a given strain follow a weakest link distribution (Weibull) and (iii) complementary 2D and 3D discrete dislocation dynamics (DDD) simulations yield identical results, showing that these properties do not depend on fine details of the actual set-up, rather, they represent general features of micron-scale plasticity.

   [1] P. D. Ispánovity, Á. Hegyi, I. Groma, G. Györgyi, K. Ratter and D. Weygand, *Average yielding and weakest link statistics in micron-scale plasticity*, Acta Mater. **61**, 6234 (2013).

   (1.2) Weakest-link hypothesis.

   Although the results summarized in point (1.1) above indicate a weakest-link phenomenon accompanying micron-scale plasticity, we aimed at identifying its origin as well. Two different types of 2D DDD simulations were employed as well as a higher scale stochastic continuum plasticity model (SCPM). The latter considers the yield stress to be a local random variable which represents internal disorder originating from the inhomogeneities of the underlying dislocation microstructure. In all models stress-controlled loading procedure was applied. It was found that in every case the stresses corresponding to individual

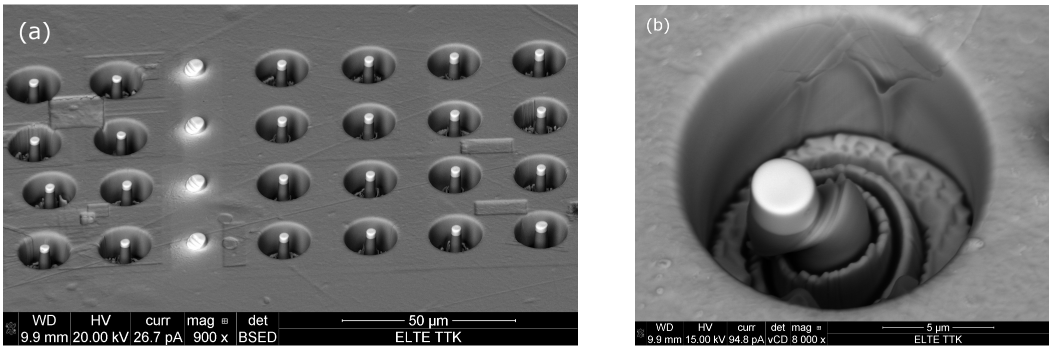

FIG. 1: (a) A group of 24 Cu single crystalline micropillars with a diameter of 3 μm and (b) a compressed micropillar. The specimen fabrications and the compression tests were performed at the Eötvös Loránd University [1].

strain burst events follow weakest link order statistics in the microplastic regime. This finding shows that plastic events can be envisaged as independent random processes that take place at the weakest sites of the specimen. Based on this observation a plasticity theory has been suggested that describes the average and the fluctuations of the individual stress-strain curves using simple scaling relations. In addition, a detailed methodology was proposed for setting the parameters of the SCPM (including the local yield stress distribution) unambiguously in order to precisely model the lower-scale 2D DDD results. As such, a complete multi-scale modelling framework emerges, with a higher scale model correctly capturing the plastic fluctuations, but with a significantly reduced computational speed.

[2] P. D. Ispánovity, D. Tüzes, P. Szabó, M. Zaiser and I. Groma, *The role of weakest links and system size scaling in multiscale modeling of stochastic plasticity*, submitted to Phys. Rev. B (2016) [http://arxiv.org/abs/1604.01645].

2. *The origin of different length scales*

Micropillars with diameters below $\sim$40 μm show fluctuating response and typically a strong size effect, that is, the yield stress of individual pillars increases with decreasing diameter. It was not clear, however, at which size the transition from bulk (size independent) to size-effected flow takes place. We argued in the proposal that the transition diameter must be related to the average dislocation spacing, and thus to the dislocation density, in the pillar. To test this hypothesis a large number of identical micropillars with diameters 3, 6 and 12 μm were fabricated from a strongly pre-deformed sample with an average dislocation distance of about $\sim$0.1 μm. The members of the 3 different sets were compressed as in the previous section. Figure 2 shows the stress-strain curves obtained for each measurement. Surprisingly, one observes a different kind of size effect: instead of hardening usually observed at such pillar diameters the average stress-strain curves are hardly affected by pillar size, but one still finds huge fluctuations in individual curves with magnitudes decreasing with diameter. So size effects manifest in the fluctuations instead of yield strength in this case. This change is attributed to the high dislocation content in the pillars, which are 30-120 times larger in diameter than the average dislocation spacing, confirming our main assumption regarding the role of the dislocation density in the size effect.

[3] Á. Hegyi, P. D. Ispánovity, Z. Dankházi and I. Groma, manuscript under preparation (2016).

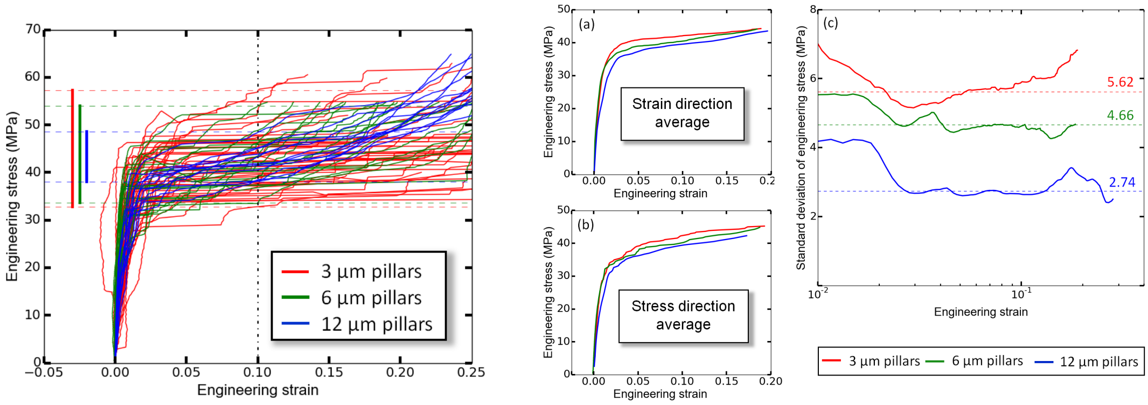

FIG. 2: Stress-strain curves of the compressed micropillars of different diameters (left panel), and their statistics (right panels). The average stress-strain curves show only weak size effects irrespective of the averaging direction [panels (a) and (b)], whereas the fluctuations decrease considerably with increasing pillar size [panel (c)]. The specimen fabrications and the compression tests were performed at the host institution [3].

3. *Role of spatial and dynamical correlations in the fluctuating response*

It is long known that due to the long-range mutual interactions of dislocations strong spatial and temporal correlations develop in dislocation structures, and they play an important role in the physics of these systems. Correlations, for instance, are crucial in the continuum theory described in point 5 below. This objective aimed at studying different aspects of this phenomenon in order to obtain a deeper understanding of correlations and their role in plasticity.

X-ray line profile analysis is not only capable of determining the net dislocation content in the sample but also to extract some parameters of the internal correlations. Within this project the effect of an elastic external load was investigated experimentally that induces a certain 'polarization' of the dislocation structure [4]. In the theoretical considerations, we described this polarization in terms of the dislocation-dislocation spatial pair correlation functions and calculated analytically the form of the broadened Bragg peaks. It was found that the cubic decay of the peak (corresponding to zero applied stress) is complemented by a $x^{-1}|x|^{-3}$ type asymmetric additive component proportional to the applied stress. Indeed, the analysis of the diffraction peaks obtained on *in situ* elastically compressed copper single crystals revealed quantitative equivalence with the theory. The strength of the method lies in its applicability: it is not only useful for determining externally applied stresses, but also for monitoring internal stresses within the sample [4].

The main motivation of the proposal was to study stochastic properties in crystalline samples. Such fluctuations, however, are not restricted to this class of materials but are also observed in metallic glasses and many other types of materials (granular packings, rigid foams, colloid systems, etc.), hinting at generic features of stochasticity. So, in parallel with the trends in the community, we broadened the scope of the research to include amorphous materials in order to obtain a more solid understanding of the phenomena. In an experimental study time correlations of plastic events were investigated observed during torsional deformation of a Vitreloy bulk metallic glass [5]. The events were identified as torque drops and also by detecting acoustic emission signals. The analysis of waiting times between subsequent events revealed long-range temporal correlations in the plastic activity reflecting the self-organized build-up of shear bands. To explain the measured event sequences a simple model was proposed based on the stress concentrations at the shear band tips [5]. In a numerical work, on the other hand, the focus was on identifying the role of the microstructural disorder in the formation of the shear bands, that is, system spanning correlations in the local plastic strain field [6]. It was found that increasing disorder in the local yield stress distribution (that is, increasing standard deviation with keeping the average fixed) leads to (i) larger amount of plasticity in the microplastic regime and (ii) more importantly, it significantly delays shear band formation, making the material ductile. A quantitative method was also suggested how to predict shear band nucleation. The results are expected to be applied in the design of bulk metallic glasses or other disordered systems, like metallic foams or crystalline samples with significant dislocation content [5].

[4] I. Groma, D. Tüzes and P. D. Ispánovity, *Asymmetric X-ray line broadening caused by dislocation polarization induced by external load*, Scr. Mater. **68**, 755 (2013).

[5] Zs. Kovács, M. Ezzeldien, K. Máthis, P. D. Ispánovity, F. Chmelík and J. Lendvai, *Statistical analysis of acoustic emission events in torsional deformation of a Vitreloy bulk metallic glass*, Acta Mater. **70**, 113 (2014).

[6] D. Tüzes, M. Zaiser and P. D. Ispánovity, *Disorder is good for you: The influence of local disorder on strain localization and ductility of strain softening materials*, submitted to Int. Journ. Plast. (2016) [http://arxiv.org/abs/1604.01821].

4. *Statistical properties of dislocation avalanches*

(4.1) Acoustic emission measurements. Experimental measurements of the stochastic properties of plasticity are mostly based on detecting AE signals for bulk samples, and measuring the stress drops in micromechanical testing for micron-scale samples. The latter method is not applicable for large samples, because of the huge number of events and because the corresponding stress drops are undetectable with the traditional set-ups. On the other hand, AE signals originating from small volumes are typically weak, so performing AE measurements on micro-pillars did not seem feasible.

In the proposal we aimed at performing a coupled AE and micromechanical testing measurement in-situ in an SEM chamber. To this end, in co-operation with experts from Charles University, Prague, a device capable of performing this simultaneous measurement was built. The long development phase led to a successful measurement on a micropillar fabricated from an Al-5% Mg alloy exhibiting the Portevin-Le Chatelier effect. Exceptionally good correlation was found between the events and the stress drops corresponding to the collective depinning of dislocations from the solute Mg atoms. A new pillar fabrication method was also proposed that leads to high-quality, non-tapered, rectangular geometries with a significantly reduced fabrication time.

[7] Á. Hegyi, P. D. Ispánovity, M. Knapek, D. Tüzes, K. Máthis F. Chmelík, Z. Dankházi, G. Varga and I. Groma, *Micron-scale deformation: a coupled in-situ study of strain bursts and acoustic emission*, submitted to Microsc. Microanal. (2016) [http://arxiv.org/abs/1604.01815].

(4.2) High-precision statistics from numerical modelling. Strain bursts associated with the sudden collective motion of dislocations dominate micron-scale plasticity, but they are present during the deformation of large specimens, too. To understand the nature of dislocation avalanches in full detail is, therefore, central to our understanding of plastic flow. In an international collaboration with scientists from four European countries we aimed at giving an in-depth description of avalanche statistics based on different 2D DDD models [8]. The results obtained shed new light on the critical properties of plasticity, as it turned out that they contradict the mean-field depinning model suggested earlier to

describe yielding. Namely, from the stress and system size dependence of the avalanche distributions (Fig. 3) it was found that criticality is not only observed at a single applied stress value which could be identified as the yield stress (as speculated before), but is present all along the stress strain curve, even at zero stress [8].

In a complementary study, the inter-avalanche regions were investigated, and based on 2D and 3D DDD simulations it was found, that these segments exhibit reversible plasticity attributed to reversible dipole stretching in 2D and dislocation bow-out in 3D [9]. This phenomenon leads to a measurable change in the elastic moduli of the system, typically in the range of ∼10% regardless of the dislocation density. The system size dependence of the plastic responses reveals size effects in this model system and decreasing stress fluctuations with increasing size obeying simple scaling forms [9].

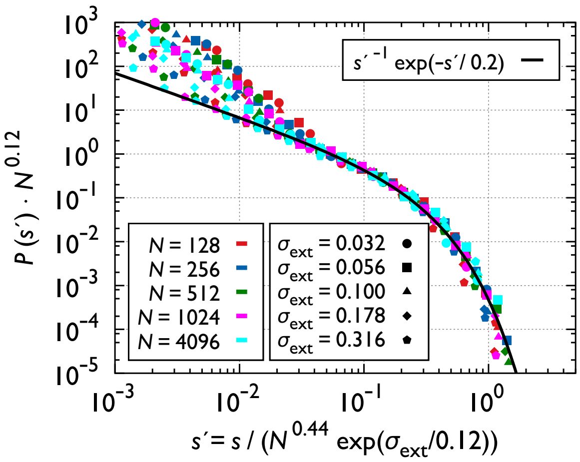

FIG. 3: Scaled avalanche distributions obtained from a 2D discrete dislocation simulation of stress-controlled loading for different system sizes N and applied stresses σ_{ext}. The scaling collapse in the cut-off region signals the presence of extended criticality described in the text [8].

[8] P. D. Ispánovity, L. Laurson, M. Zaiser, I. Groma, S. Zapperi and M. J. Alava, *Avalanches in 2D Dislocation Systems: Plastic Yielding is not Depinning*, Phys. Rev. Lett. **112**, 235501 (2014).

[9] P. Szabó, P. D. Ispánovity and I. Groma, *Plastic strain is a mixture of avalanches and quasi-reversible deformations: Study of various sizes*, Phys. Rev. B **91**, 054106 (2015).

5. *Derivation of a stochastic continuum plasticity model*

Discrete dislocation dynamics is a powerful tool to investigate plasticity on the level of individual dislocations, but due to its weak scaling properties, it cannot be applied for volumes larger than a few μm^3. For technical applications, therefore, it is essential to develop higher-scale continuum plasticity models based on the output of DDD modelling. The aim of this project objective was twofold: (i) to further develop the existing continuum models in order to account for dislocation pattern formation and (ii) to incorporate stochastic effects to account for dislocation avalanches.

Firstly, the existing continuum model of Groma that is based on a phase-field formalism was extended to tackle high geometrically necessary dislocation concentrations, often observed close to grain boundaries when the material is subject to external load [10]. To this end, the phase field functional of the model was extended based on dimensionality considerations that stem from the scale-freeness of the dislocation-dislocation mutual interactions (being proportional with $1/r$). It was shown that the so derived evolution equation correctly describes the evolution of continuum dislocation densities in a channel geometry (see Fig. 4).

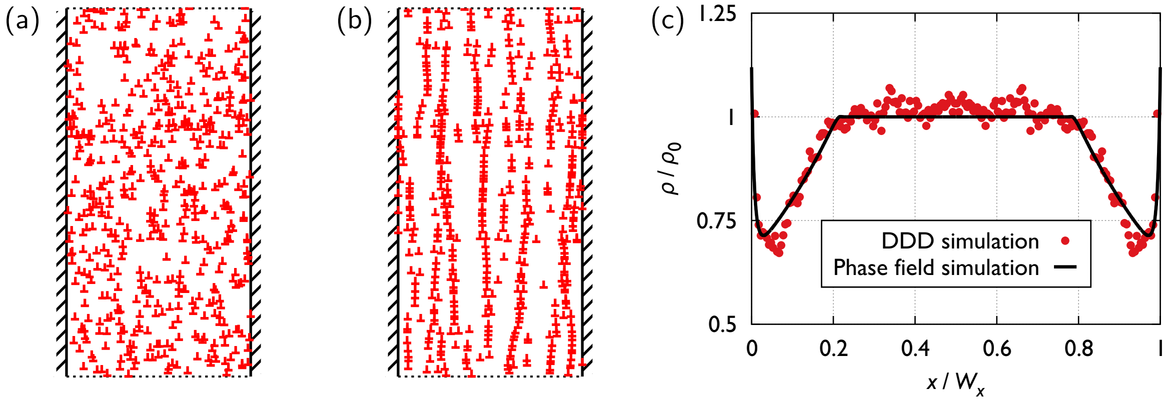

FIG. 4: Geometrically necessary dislocations in a finite channel of width W_x periodic in the y direction. Panel (a) depicts a random initial configuration and panel (b) shows the corresponding equilibrated dislocation distribution. In panel (c) the dislocation density (ρ) profile of the relaxed state is seen obtained by averaging over a large, statistically equivalent ensemble of simulations, while the solid line is the prediction of the continuum theory [10].

In a subsequent study dislocation pattern formation was investigated in the continuum model using linear stability analysis of the trivial solution [11]. It was shown that the model developed for plane strain single slip problems is indeed able to produce patterns similar to those obtained by DDD and experiments. Although many phenomenological models have been proposed so far on dislocation patterning, this is the first one derived directly from the equations of motion of dislocations. So, contrary to the phenomenological models, it is able to explain the physical meaning and the origin of the parameters appearing in the equations, thus providing a deeper understanding of the phenomenon [11].

The continuum models described above are deterministic, so they can account for patterning, but stochastic features are absolutely absent in them. The stochastic plasticity model used in [2] and [6], on the other hand, gives a quantitative description of strain bursts, but does not include patterning. Our aim was to unify the two models, to account for the two phenomena in a single stochastic continuum plasticity model. To this end, the evolution equations of [11] were discretised in space, and the deterministic yield stress of the model was replaced by a stochastic local yield threshold, as in [2] and [6]. The resulting model turned out to match DDD simulations not only in terms of the observed patterns (see Fig. 5) but also in the avalanche dynamics, described in point 4.2 and [8]. So this unified model exhibits great potential for applications because it establishes a missing connection between pattern formation and strain bursts, that is mechanical properties and stochasticity [12].

[10] I. Groma, Z. Vandrus and P. D. Ispánovity, *Scale-free phase field theory of dislocations*, Phys. Rev. Lett. **114**, 015503 (2015).

[11] I. Groma, M. Zaiser and P. D. Ispánovity, *Dislocation patterning in a 2D continuum theory of dislocations*, submitted to Phys. Rev. B (2016) [http://arxiv.org/abs/1601.07831].

[12] P. D. Ispánovity, S. Papanikolaou and I. Groma, manuscript under preparation (2016).

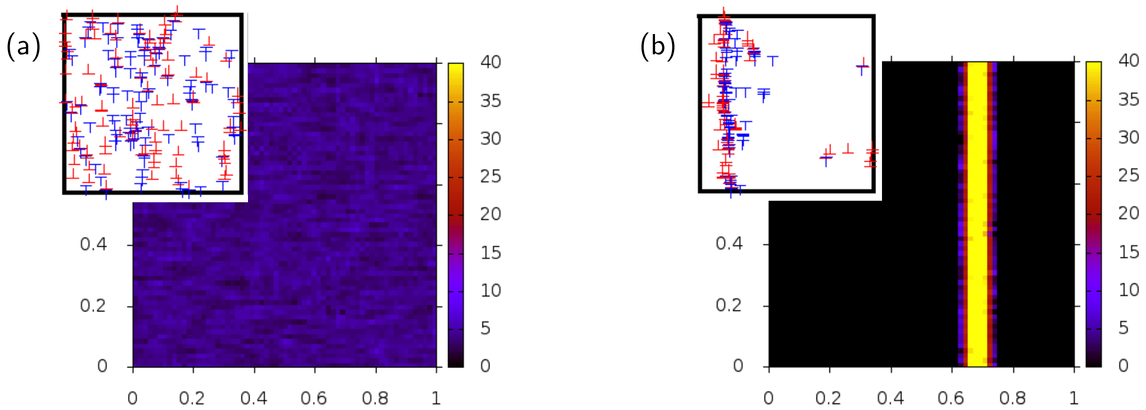

FIG. 5: Dislocation patterns derived from the stochastic continuum model (color map) and from DDD simulations (insets) without external stress (a) and at the onset of yielding (b). It is noted, that not only the observed patterns are statistically similar, but the strain burst size distributions are also equivalent [12].

Summary

The research performed within the frames of this grant are 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 12 publications related to this project 6 have been published, 4 are submitted (but already accessible at an open manuscript database), and 2 are under preparation. All the published papers appeared in high-impact journals with D1 classification (that is, they belong to the top 10% of the given field), two of them in Physical Review Letters.