Semester Report - Semester IV

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PhD Program: Materials science and solid state physics

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PhD Thesis title: The Role of Curvature and Internal Disorder in Dislocation Systems

1 Introduction

Recent experimental and numerical investigations revealed that plastic properties of micron and sub-micron scale crystalline materials profoundly differ from their macroscopic counterparts. In this size regime irreversible deformation is characterised by large fluctuations both in time and space. In particular, deformation proceeds in intermittent localized strain bursts. Consequently, in this size-scale the stress-strain curve of deformed single-crystal specimens is not as smooth as in bulk materials. Thus, the measurable quantities, such as stress or strain, become stochastic as well. The aim of the PhD research is to investigate the theoretical background of this technologically rather important phenomenon.

It was shown in the case of amorphous solids that the positions of the plastic events responsible for the irreversible deformation correlates strongly with the *local yield stress* values. Consequently, this local measure can be utilized to connect the initial microstructure and the plastic activity. In this PhD research we adopt the concept of local yield thresholds and study them in a bottom up approach starting with low scale 2D discrete dislocation systems.

Another step forward could be not only predicting plastic activity from local yield stress values but merely from the miscrostructure itself. Such a method could skip the computationally costly step of determining local yield stresses. A natural choice of the framework for this purpose could be machine and deep learning due to the general high performance in a wide range of applications and its increasingly developing algorithms.

Another interesting related problem is the the impact of dislocation curvature on the fundamental properties of the systems. Discrete dislocation systems are usually investigated in one of two ways. One group is the 2D studies which are generally more efficient computationally and more easy to interpret. However, this approach is usually criticized for its simplicity. The other possibility is to create a 3D model closer to real physical systems. These models, however, are usually hard to interpret due to their complexity and they are also less feasible computationally. An intermediate approach can be the investigation of 3D single slip systems where dislocation curvature is already included but several complicated dislocation mechanisms (such as reactions, cross-slip, climb, etc.) are not present. One purpose of my research is to implement such a model and, subsequently, to obtain local yield stress statistics in these 3D systems as well and utilize them as input parameters in continuum dislocation dynamics (CDD) models.

2 Research carried out during earlier semesters

2.1 Length scales and weakest-link behaviour in 2D crystal plasticity

As the continuation of my MSc research I computed the statistics of local yield stresses in 2D discrete dislocation systems. To this end a modified and employed the 2D discrete dislocation simulator (SDDDST) developed by G. Péterffy. I constructed a method to characterize the morphology of dislocation avalanches. The algorithm is based on the velocity of individual dislocations and it can characterize the properties of the event such as size, eccentricity and orientation. The method was applied to study the initial state of the avalanches to understand their nucleation. The local yield stresses showed surprisingly high correlation between the activated dislocations in subsystems and their own subsystems. Less surprisingly, the triggered avalanche nuclei were found to be much smaller in systems populated with point defects as well. Our results indicate that a *dynamic length-scale* (characterizing the typical size of plastic events) can be introduced based on weakest-link arguments. This dynamic length-scale is intimately connected to the type of interactions in the system. Namely, this scale diverges in scale-free systems dominated by long-range dislocation interactions while as short-range quenched disorder starts to dominate, events get localised. Thus, one can distinguish two different university classes of plasticity. The one corresponding to systems with great extent of short-range interactions obeys the traditional weakest-link picture while the other corresponding to scale-free systems exhibits a non-conventional weakest-link behaviour.

2.2 Single slip in 3D DD systems

In order to study the behaviour of 3D single-slip systems we obtained the 3D DDD code, ParaDiS. After several necessary modifications carried out by myself, test configurations were created consisting of large dislocation loops on parallel planes. Such a configuration is shown in the left panel of Fig. 1. Note, that the loop due to the periodic boundary conditions appears as a collection of nearly straight seemingly random segments. Relaxed configurations (right panel) exhibit a highly-ordered structure consisting a large number of dislocation dipoles. This is a phenomenon which was observed exclusively in 2D discrete dislocation systems so far. However, this results clearly show that this dipolar structure may exist in 3D systems as well if they are oriented for single-slip. This is in accordance with recent unpublished experimental research of our collaborators showing the signs of dipoles and dislocation walls in real life HCP materials. These results imply that the dipolar and wall structures are not simply 2D DDD artifacts as they are often interpreted.

We also intended to utilize ParaDiS to study the relaxation process of dislocation configurations in 3D single-slip systems. However, due to the severe numerical noise, no genuinely decisive result could be obtained yet.

2.3 Prediction of local yield stress with ML

In connection with my PhD course *Data Mining and Machine Learning* a started familiarizing myself with machine learning methods. In the process I made my first attempts of predicting local yield stresses from the structural properties of the relaxed dislocation systems. The predicting power of my models is modest at their recent state and no genuinely novel underlying physics was discovered so far. The reliable prediction of local yield stresses could have immense importance due to the practical limitations of the direct determination of local yield stresses related to the high computational cost of dynamical simulations even in 2D.

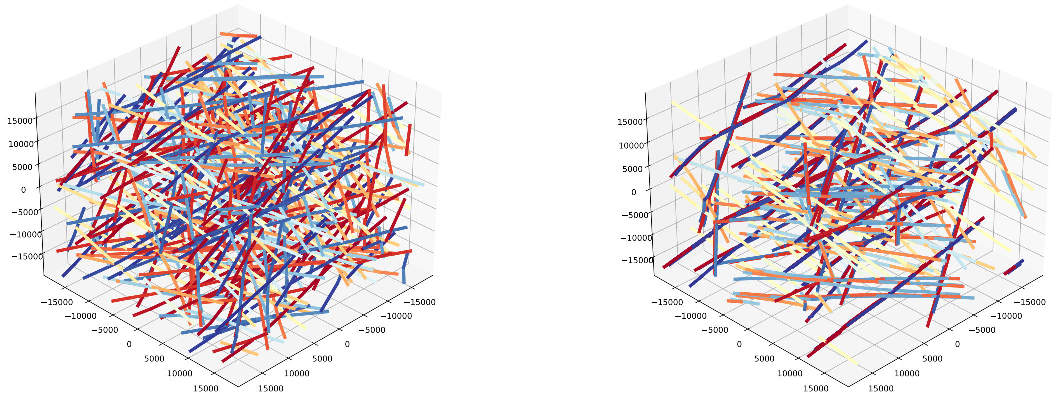

Figure 1: An initial configuration of a single loop and its periodic images (left) and the nearly relaxed systems (right). The displayed region is the simulation cell including the dislocation lines. Colours indicate the type of the dislocation: red and blue (according to the conventional colouring of 2D) are edge dislocation segments and yellow is screw dislocation segment. The right panel confirms the formation of narrow dipoles in this 3D system.

3 Research carried out during this semester

3.1 Length scales and weakest-link behaviour in 2D crystal plasticity

I prepared and submitted a manuscript of our results discussed above about weakest-link behaviour and 2D discrete dislocation systems. I also continued the analysis of the available results and started preparing another publication focusing on the method of morphological characterization of plastic event and on the dislocation-scale interpretation of weakest-link behaviour in our model. Namely, we found that if links (associated with plastic events) are located within the loading region of our specimen, very high correlation of region and subregion yield stresses arise. However, if links are intersected by the boundary of the loaded region (that is, practically always in scale-free systems with diverging link size) these correlation will be much weaker yielding a non-conventional weakest-link behaviour. In order to distinguish intersected and intact links I proposed a overlap function describing the resemblance of plastic events before and after subregion division.

Addiotionally, I (unofficially) co-supervised a BSc student, B. Mendei, and guided him to learn the use of the method utilized for local yield stress calculations. He started to study the local yield stress statistics in pre-strained systems.

3.2 Single slip in 3D DD systems

I (unofficially) co-supervised a BSc student, B. Bonifert. Together with my supervisor I outlined a few strategies to characterize the emergence dipolar dislocation structures in 3D single-slip systems. The characterization are partially done on the available numerical data.

3.3 Applications of ML in materials science

After my initial attempts of employing ML methods for the prediction of local yield stresses we started to collaborate with mathematicians from the Mathematics Institute of ELTE. After some initial discussion and studying the literature, a large amount of raw data was generated by me in this semester in order to obtain a large enough training data for deep learning based approaches. We intend to predict local yield stresses with artificial neural networks fed with images representing the equilibrium dislocation microstructure.

We also outlined another possible application of machine learning algorithms on our available results. This method would predict stress-strain curves along with their stress-drop structure based on acoustic emission (AE) signals. The training data will be the AE time-series available from micropillar compression tests in the Department. I studied the literature searching for the appropriate method to employ. Based on that knowledge, firstly, we will try to develop a deep learning based method. As input data, we intend to use spectrograms of the acoustic time-series obtained via wavelet-transformation. I already started the testing of the input data generation.

4 Publications

I am involved in the preparation of 3 publications:

- A first-author publication on local yield stresses, length scales and weakest-link behaviour in 2D discrete dislocation systems is has been recently submitted.
- I started preparing a first-author follow-up article on the weakest-link behaviour in 2D DD systems.
- I cooperate with G. Péterffy et al. in a project on linear stability analysis of discrete dislocation systems. The majority of the results is already available.

5 Conferences

I presented my research at 3 Hungarian conferences.

- XXI. Eötvös Konferencia, 25-26 September 2020, presentation title: *Lokális folyásfeszültség vizsgálata DDD szimulációkkal*
- IX. Eötvözet Konferencia, 18-19 December 2020, presentation title: *Lokális folyásfeszültségek vizsgálata 2D modell kristályokban DDD szimulációk segítségével*
- XIII. Országos Anyagtudományi Konferencia, 10-12th October 2021, presentation title: *Lokális folyásfeszültségek vizsgálata 2D modell kristályokban*.

I intend to participate in the *10th International Conference on Multiscale Materials Modeling* with a presentation. My abstract has not yet been accepted.

6 Teaching activity and supervising

- 2020/21 fall semester: *Mechanika* (mechf19va, practice, 2 hours twice a week). I helped during the composition of the 4 assignments and corrected them.
- 2020/21 spring semester: *Hőtan és folytonos közegek mechanikája (emelt szint)* (hotanef19va, practice, 1.5 hours once a week). I held approx. 2/3 of the practices. I was responsible for composition of the four assignments and corrected the half of the overall approx. 180 assignments.
- 2021/22 fall semester: *Mechanics* (mechf19va, practice, 1.5 hours once a week). I was responsible for composition of all classes, the four assignments and two written exams. I corrected all (approx. 100) exams and consulted with the tutors, assigned to the students, on demand.
- 2021/22 spring semester: *Hőtan és folytonos közegek mechanikája (emelt szint)* (hotanef19va, practice, 1.5 hours once a week). I was responsible for composition of all classes, the four assignments and two written exams. I corrected about one third of the (approx. 100) assignments and all the exams.
- In the last two semester I de facto co-supervised two BSc student in our research group. I consulted with them regularly (approx. once in every two weeks with each).

7 Other scientific activity

I chaired the Physics and Informatics section of the *XXIII. Eötvös Konferencia*, 22-23 April 2022.

8 Previous publications

I am first author of a published paper:

- Berta, D., Groma, I., & Ispánovity, P. D. (2020). Efficient numerical method to handle boundary conditions in 2D elastic media. *Modelling and Simulation in Materials Science and Engineering*, **28**(3), 035014. (`https://dx.doi.org/10.1088/1361-651X/ab76b1`)