Semester Report - Semester II

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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

In the previous semester I investigated the local yield stresses in 2D model crystals using discrete dislocation dynamics (DDD) simulations. Simultaneously, I started to get familiar with the technical details of the 3D DDD code ParaDiS which I will use to investigate single slip plasticity in 3D. Such a situation corresponds to the deformation of HCP materials (such as Zn) oriented for basal slip. Generally, 3D DDD simulations do not predict the formation of dipoles and dipole walls contrary to 2D systems. However, experimental results suggest that one can expect dipoles to arise in a single slip scenario even in a 3D case. My goal is to study the emergence of dipolar structures and the behaviour during relaxation into such a system. Another aim of our research is to study local yield stresses and the eigenmodes of dislocation structures in 2D systems with the presence of *Peierls stress*, that is, in a realization where the crystal exhibits resistance against dislocation motion.

2 Research carried out during this semester

2.1 Single slip in 3D DD systems

In this semester I continued to get familiar with the 3D DDD code, ParaDiS. After several necessary modifications, test configurations were created consisting of dislocation loops on parallel planes. Configurations of fairly large loops were found to collapse and eventually annihilate even for relatively large number of loops. Thus, our focus is now on studying systems containing only a few loops (or even only a single one) with radii some orders of magnitude larger than size of the simulation cell. Such a case is shown in Fig. 1. Note, that the loop due to the periodic boundary conditions appears as a collection of nearly straight random segments.

We started to collaborate with the group of T. Hochrainer on the relaxation of 3D single slip systems. The data obtained by the fellow group are hard to interpret as there are no indisputable signs of relaxation. Therefore, our primary purpose is now to reduce noise by introducing a nodewise low pass filter in the velocity components to exclude the effect of oscillations in practically relaxed configurations. My partial results are promising but further investigation is needed. Another objective that is already completed was to implement a more sophisticated average velocity calculator than the original one of the simulator.

Our final aim is a publication that captures the generic features of 2D and 3D single slip discrete dislocation systems and outlining the essential similarities and differences of the two cases.

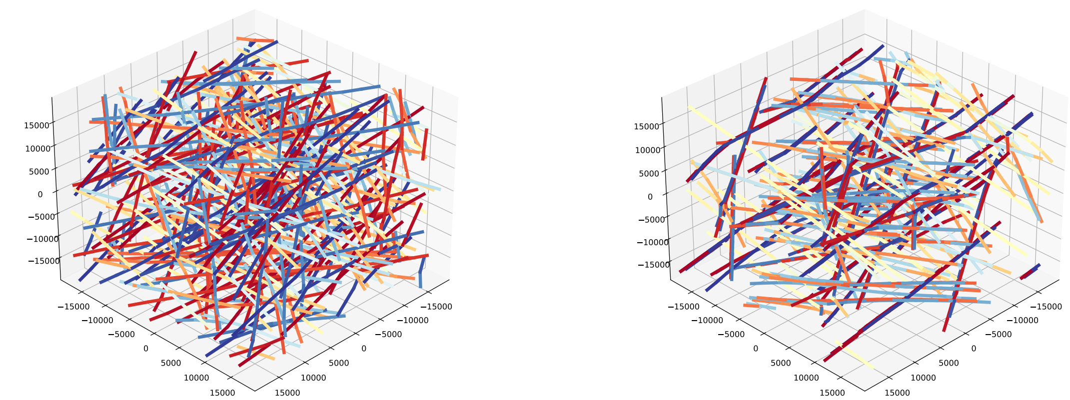

Figure 1: An initial configuration of a single loop and its periodic images (left) and the intermediate state of the same system during relaxation (right). The displayed region is the simulation cell including the dislocation lines. Colours indicate the type of the dislocation: red and blue (according 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.

2.2 2D DD systems

Previously, I computed the statistics of local yield stresses in 2D discrete dislocation systems. This semester I developed a method to characterize the morphology of dislocation avalanches. For this purpose, firstly, the contribution of individual dislocations was calculated. Then, the structure was fit with a ellipse characterizing 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 (see Fig. 2). The result 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. In the future, we aim to to use this method to characterize the morphology of avalanches in more developed phases of the event. This method should also be combined with the result of G. Péterffy utilizing linear stability analysis in order to achieve a deeper understanding of the studied process.

I assisted to G. Péterffy in the implementation of Peierls stress in his 2D DDD simulator. The first tests are promising and we already obtained a reasonable number of relaxed configurations in the presence of Peierls stress. We intend to include the future results of this method in both papers being prepared about the dynamics properties of 2D discrete dislocation systems.

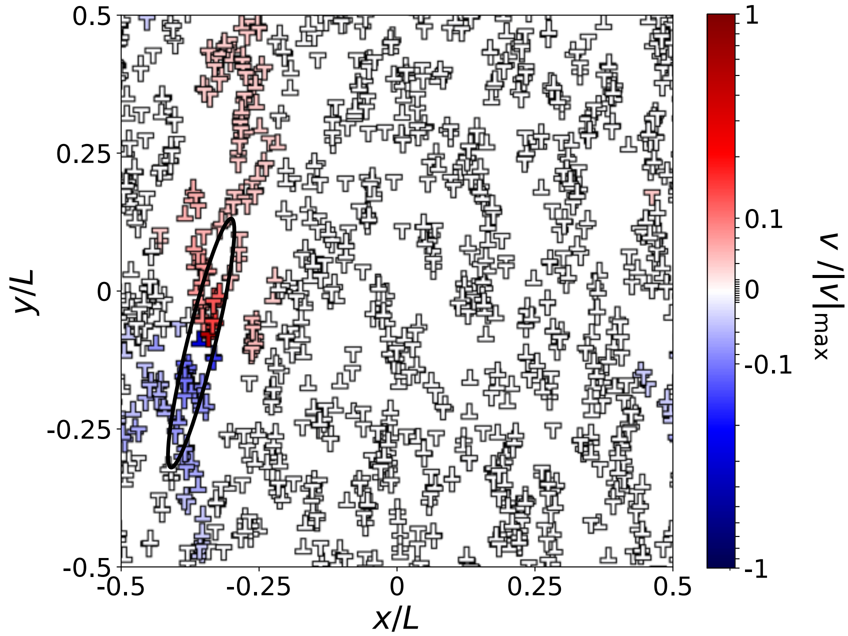

Figure 2: The initial morphology at the beginning of an avalanche during loading of the whole system.

3 Publications

I am involved in the preparation of 3 publications:

- A first-author publication on local yield stresses in 2D discrete dislocation systems is in preparation. The vast majority of the data is available and the preparation of the paper has started recently.
- I cooperate with G. Péterffy et al. in their poject on linear stability analysis of discrete dislocation systems. The majority of the results is available. After obtaining and evaluating the data in the presence of non-zero Peierls stress systems the preparation of a publication can start.
- I cooperate with T. Hochrainer et al. in a poject on the relaxation in 3D single slip systems. We are in the initial stage of our research yet.

4 Studies

I attended 3 courses this semester:

- *Rácshibák II. EA* (FIZ/1/025E)
- *Technology of Materials (intenzív kurzus)* (FIZ/1/031E)
- *Kutatószeminárium 10.*, course at Eötvös József Collegium (BMVD-200.227f/EC)

5 Teaching activity

I held the practice of the course *Hőtan és folytonos közegek mechanikája (emelt szint)* (hotanef19va, 1.5 hours once a week). I held around two third of each occasion the remaining part lectured by P. D. Ispánovity. I was responsible for composition of the four assignments and corrected the half of the overall approx. 180 assignments.

6 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`)