Semester Report - Semester I.

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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 the case of crystalline materials similar studies have been in a quite embryonic form so far. In order to fill this gap during my PhD research we study local yield stresses in a bottom up approach starting with low scale 2D discrete dislocation systems.

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 more close to real physical systems. These models, however, are usually hard to interpret due to their complexity. 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 done this semester

2.1 Local yield stresses in 2D dislocation systems

In order to study local yield stresses SDDDST (Simple Dicrete Dislocation Dynamics Simulation Toolkit) was utilized. This framework was developed in the Department by Péterffy & Ispánovity (`https://github.com/pgabor/sdddst`). The local yield stress statistics was the main topic of my MSc thesis as well and this work was continued and deepened during the first semester of my PhD. I made several improvements in the SDDDST code in order to make it more suitable for my purposes. The studied 2D systems are characterized by their dislocation and vacancy numbers: N_{dis} and N_{vac}, respectively. The number of types of systems was increased significantly in comparison with my MSc work. At the moment results with 3 different N_{dis} values (256, 1024 and 4096) are available with 5, 7 and 1 different vacancy concentrations, respectively. Many distinct results of my research (such as the behaviour of box-subbox correlations, see Fig. 1) imply that these 2D systems can be characterised well using weakest link arguments which are commonly used on the mesoscale level. In these models regions are activated when the weakest (most susceptible) subregion (link) is activated. However, the new results of this semester with various vacancy concentrations clearly indicate that these weakest link models match much better the systems rich in vacancies. The probably most important achievement of this investigation was obtaining the *link dimension* D defined by equation

$$N(l) \propto l^D, \tag{1}$$

where $N(l)$ is the number of links that can be activated inside a box of linear size l. From the link dimension and the yield stress distributions the *link-size dimension* was also extracted (see Fig. 2).

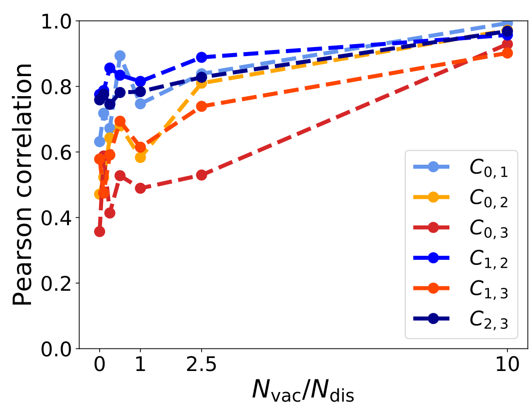

Figure 1: The Pearson correlation $C_{i,j}$ for different $N_{\text{vac}}/N_{\text{dis}}$ ratios. Here $C_{i,j}$ is the correlation between the the yield stress of boxes and the yield stress of their softest subboxes (that is, the one characterized with the lowest local yield stress). There are 4^i and 4^j boxes and subboxes in a single system, respectively. As the number of vacancies is increased the $C_{i,j}$ correlations tend to 1.0 which one would expect in a ideal weakest link model.

A few consultations were arranged with Craig Maloney (Northeastern University, Boston), Sylvain Patinet (Laboratoire PMMH, ESPCI, Paris) and Damien Vandembroucq (Laboratoire PMMH, ESPCI, Paris) who mainly study model amorphous solids. My future plan is to reveal the similarities and differences between the amorphous and crystalline behaviour based on their and my results.

2.2 3D dislocation systems

A new version of the 3D discrete dislocation dynamics (DDD) code called ParaDis was obtained from Ryan Sills (Rutgers University, New Jersey) who will be my consultant in the future should any technical issue arise related to ParaDis. I studied the manual of ParaDis and will start utilizing it in the the very near future.

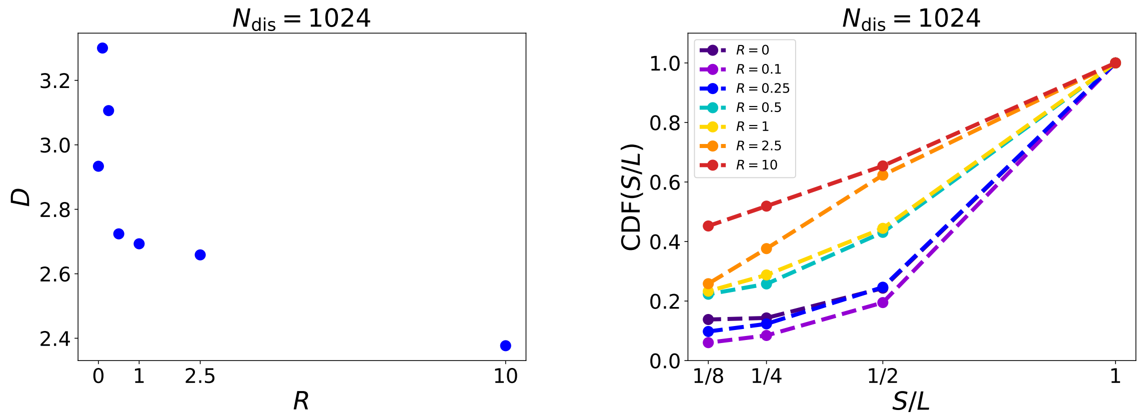

Figure 2: The dependence of link dimension on ratio $R = N_{\rm vac}/N_{\rm dis}$ (left) and the distribution of link size S for different R values (right). Here L is the linear size of the simulation cell. The results clearly show that high vacancy concentration localises the links. It is noted that S is not precisely the linear extent of the link itself rather the linear size of the box in which the link can be triggered.

3 Publications

I am involved in the preparation of 2 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 already and the preparation of the paper itself is likely to start in the near future.
- A joined the project carried out by G. Péterffy et al. on linear stability analysis of discrete dislocation systems. The majority of the results is available.

4 Studies

I attended 3 courses this semester:

- *Rácshibák I. EA* (FIZ/1/024)
- *Diffrakciós módszerek az anyagtudományban I.* (FIZ/1/038E)
- *Kutatószeminárium 9*, course at Eötvös József Collegium (BMVD-200.227e/EC)

5 Conferences

This semester I presented at two online 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*

6 Teaching activity

A contributed in the composition and corrected the 4 assignments of the course *Mechanika* (mechf19va, 2 hours twice a week). My workload was approximately 3-3.5 hours per week on average.

7 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`)