Semester Report - Semester III

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PhD Program: Materials science and solid state physics

Supervisor: Péter Dusán Ispánovity

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

1 Introduction

In the previous semesters I investigated the local yield stresses in 2D model crystals using discrete dislocation dynamics (DDD) simulations. Furthermore, I carried out some research on 3D single-slip systems using the modified code of ParaDiS. 3D single-slip set-up corresponds to the deformation of HCP materials (such as Zn) oriented for basal slip. Additionally, I made attempt together with G. Péterffy to incorporate *Peierls stress* (that is, lattice resistance against dislocation motion) in his 2D DDD simulator (SDDDST).

2 Research carried out during this semester

2.1 Length scales in 2D crystal plasticity

In this semester I continued my investigation on local yield stresses in 2D discrete dislocation systems. It was revealed that while in the presence of quenched disorder (e.g. point defects) systems follow weakest-link principles quite straightforwardly, in pure dislocation systems lacking inherent length scales links often get immensely extended leading to a much more non-trivial weakest-link picture. Recently our thoughts about this subject were condensed into a manuscripct which we hope to submit for publication very soon.

2.2 Implementation of Peierls stress

I assisted to G. Péterffy in the implementation of Peierls stress in his 2D DDD simulator, SDDDST. After some promising results this direction of investigation was halted due to the emerging numerical difficulties.

2.3 3D single-slip

Our previous results clearly indicate the formation of dipolar structures in 3D single-slip dislocation systems. The novelty of this findings come from the fact that beforehand there were no signs of dipoles and dipole walls in 3D numerical works only in 2D models. In this semester further 3D simulations were executed. Besides running relaxation simulations, I also created configurations with numerical creep experiments. Simple quantitative ways of describing the structures (e.g. in terms of dipole content) is already outlined and the implementation of the necessary numerical background is in progress by a BSc member of our research group.

2.4 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. ML methods could possibly enable us to predict plasticity based on merely the initial, relaxed structure. My supervisor outlined several other future projects related to my research interest where ML methods could be useful. Therefore, I intend to broaden further my knowledge on ML in order to employ it in those projects.

3 Publications

I am involved in the preparation of 3 publications:

- A first-author publication on local yield stresses and length scales in 2D discrete dislocation systems is in the very final stage of preparation. Hopefully, the manuscript will be submitted to the Physical Review Letters soon.
- 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.
- I take part in a international collaboration on the relaxation and dipole formation in 3D single slip systems. We are in an intermediate stage of our research with significant result on both experimental and numerical sides.

4 Conferences

I attended the XIII. Országos Anyagtudományi Konferencia, a Hungarian offline conference which took place on the 10-12th October 2021. The title of my presentation was *Lokális folyásfeszültségek vizsgálata 2D modell kristályokban*.

5 Studies

I attended 3 courses this semester:

- *Bulk nanostructured materials* (FIZ/1/040E)
- *Data Mining and Machine Learning* (FIZ/3/084)
- *Research seminar 11.*, course at Eötvös József Collegium (BMVD-200.227i/EC)

I received grade “excellent” for all of these courses.

6 Teaching activity

I held the practice of the course *Mechanics* (mechf19va, 1.5 hours once a week). I was responsible for composition of all classes, the four assignments and four written exams. I corrected all (approx. 100) exams and consulted with the tutors, assigned the students, on demand. My corresponding workload was approx. 1-1.5 workdays a week.

Since this semester I am *de facto* co-supervisor of two BSc students. Their work is related to local yield stresses in 2D and to 3D single-slip systems. I consult with them regularly (approx. once in every two weeks with each).

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`)