Stochastic properties of dislocation motion and rearrangement

A PhD thesis by Dániel Tüzes

The topic of my doctoral thesis was inspired by the diversity of the collective and stochastic properties of dislocations. Nowadays the size scales accessible for computational simulations and experiments overlap for crystalline materials. They can be modelled with computers and can be investigated by, for example, scanning electron microscopes, even in an in-situ deformation setup too.

As the first step of my thesis I approached the issue from a theoretical point of view. I developed a cellular automaton model based on the continuum theory of dislocations and investigated the role of the relevant parameters in the region of small deformations. The model handles the flow stress on cell-level () and it is considered as a probability variable and calibrated via lower scale, discrete dislocation dynamic (DDD) simulations. The expected value of and the size of the applied discrete plastic strain on the cells are calibrated via the comparison of the stress-strain curve of the CA model and two other DDD models. The efficiency of the mutliscale modelling is reflected on that that beyond the fitted properties of the model it shows the same type of universality classes with the DDD simulations in several regards. Based on the findings a plasticity model has been also introduced.

The CA model is applicable on materials with internal disorder that undergo strain softening, if the fracture is due to strain localisation. In order to model this behaviour a softening mechanism has been introduced. The disorder in the material is provided by the distribution. The results of the simulations show, that in materials with higher disorder the applicable highest stress is significantly larger and failure occurs at considerably larger plastic strain.

The CA models used above has strong assumptions on dislocation correlations, and in this case such systems may reflect non-physical properties. To this end the equation of motions of the CA model is extended with further stress terms attributable to these correlations. Linear stability analysis (LSA) shows the possibility of dislocation pattern formation and link the free parameters of the model to the characteristic wavelength of the pattern. My simulation results obtained from this CA model follows well the prediction of the LSA, so does a non-discrete model, where in contrary to the extremal dynamics of the CA, hydrodynamic-like transport equations are used. Despite the elemental differences between the models they both built upon the appearing new stress terms attributed to the more precise continuum theory approximation, and therefore they indeed show qualitatively same results, showing the robustness of the theory.

In the last part of my thesis I approached the topic from an experimental point of view. In the micron scale the plastic deformation of crystalline materials show avalanche-like behaviour. The key of the research work is the recognition, that the deformation response of each micron-sized sample is different from sample to sample in this size scale, therefore characterisation of materials must rely on a statistical approach. This requires a large amount of data measured on the samples, and the origin of the data measured must be well interpreted and evaluated. To this and, at one hand, a micropillar-fabrication method is proposed facilitating the mass production of the samples with the required shape. On the other hand a unique experimental setup has been implemented making it possible to track the in-situ compression procedure faster than ever before in an electron microscope, and due to an attached acoustic emission detector coupling the avalanches observed with the acoustic signals detected became possible.