**\section\*{Description of the topic}**

In the past few years, thanks to the experimental and numerical investigation in crystal plasticity, it became clear, that the deformation properties of micron scale crystals elementary differ from what one would expect of bulk samples. In this size scale random avalanches characterise the plastic deformation implemented by the collective motion of dislocations \cite{Dimiduk1188}. Therefore, only statistical methods can be used to describe the properties of deformations. The aim of the doctoral thesis is to reveal these almost completely unknown statistical properties by experimental investigation, and to better understand the phenomena by investigating them with computational simulations. Considering the advancement in nanotechnology, more and more materials are used in the industry, the behaviour of which is elementary affected by these phenomena, therefore, the results achieved has a large engineering potential.

**\section\*{Background and aims}**

\markboth{**Background and aims**}{Numerical models}

**\subsection\*{**Numerical models**}**

As the first part of my thesis I would like study the statistical properties of the processes in micron sized samples (e.g. the stress-strain curve, a comparison with a weakest-link model, dislocation-pattern formation) with new models.

Regarding dislocation avalanches, it is known, that they can modelled not only with computational expensive discrete dislocation dynamics (DDD) simulations\cite{PhysRevLett.112.235501}, but also with larger scale mesoscopic models based on the continuum theory of dislocations\cite{1742-5468-2005-08-P08004}. The appearing free parameters in such models have never been calibrated with larger scale models, but with such method one would get an effective model, which shows the similarity with the lower scale model in the properties attributed to those fitted parameters. The benefit of such model lies in its effectiveness, which means, that using the same computational resource and running time larger systems can be also investigated. It is possible only if there exist quantities definable and measurable on the macroscopic state, which properly describe the processes occurring on the microscopic state. Such a model is even more progressive if the similarity of the behaviour is reflected not only on the properties fitted via the parameters but on other respects as well, and if the applicability of the model is wider than the applicability of the original model.

\begin{enumerate}

\setcounter{enumi}{0}

\item My aim is to develop a new mesoscopic model based on the continuum theory of dislocations and to calibrate its parameter such a way, that the behaviour of the model approaches as close as possible the behaviour of the lower scale DDD model in the properties investigated.

\end{enumerate}

Since the first observation of dislocations it is known, that they almost never distributed in the material in a homogeneous way, but they form themselves into patterns. This microstructure has an important consequence when it comes to macroscopic behaviour, because such dislocation systems leads to the appearance of persistent slip bands during cyclic deformation leading to fatigue and finally the failure of the material. But dislocation patterns are also responsible in that phenomenon, that the deformation response of different micron sized rods (called micropillars) strongly differ from sample to sample. Most of the models describing dislocation patterning use a phenomenological approach, and while ones use parameters without explained microscopic origin, others predict behaviours never observed. This is the reason why the model meant a large advancement, which uses DDD as a basis and set up the continuum model of dislocations, where each parameter appearing in the model have been defined through the microstructure and makes it possible to investigate dislocation patterns\cite{PhysRevB.93.214110}. The possibility of pattern formation can be shown by applying linear stability analysis on the model, which also connect the macroscopic parameters to the properties of the patterns, e.g. to the size of the characteristic wavelength \cite{PhysRevB.93.214110}. Even though one can hardly state anything on the developed patterns and its robustness, numerical implementations of the mathematical model make it possible to investigate these properties.

\begin{enumerate}

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\item My aim is to develop a new mesoscopic model based on the continuum theory of dislocations, which is capable to observe and describe dislocation pattern formation beyond the linear stability analysis and makes it possible to investigate the robustness of the patterns evolved.

\end{enumerate}

**\subsection\*{Experiments}**

\markboth{**Background and aims**}{**Experiments**}

Most of the experiments in connection with dislocation avalanches consist of preparing the micron sized samples in a scanning electron microscope and then move them to another device to perform the nanoindentation test. As the fabrication with the focused ion beam and the indentation happened in separate devices, one cannot follow in situ the staircase-like structures appearing on the surface of the sample. With a nanoindenter, which fits into the vacuum chamber of a scanning electron microscope with the samples together, one could perform in situ experiments.

Large amount of data can be obtained originated from the structural changes in the samples by detection of the acoustic signals. However, it is challenging to assign the different parallel competing processes to the signals they emit, because most of the signals -- in case of bulky samples -- come from the inner part of the sample, and the change can be observed only on microscopic scale. With an acoustic emission detector, if one can track the compression in site, one can couple the processes with the signals detected, with special regards to dislocation avalanches. With this technique we could gain a completely new measurement setup making it possible to perform new measurements unknown in the literature.

\begin{enumerate}

\setcounter{enumi}{2}

\item My aim is to develop a nanoindenter, which makes it possible to setup a measurement, where one can in situ follow the deformation of micropillars in a scanning electron microscope, while the acoustic signals emitted by dislocation avalanches are detected with an attached acoustic emission detector.

\end{enumerate}

Regarding that the size scale available for simulations and experiments are in the same order of magnitude, the results obtained from these two methods are directly comparable. This is a unique feature which helps to better understand submicron plasticity.

**\section\*{Methods}**

\markboth{Methods}{Numerical models}

**\subsection\*{**Numerical models**}**

Based on the work of \citet{1742-5468-2005-08-P08004} I developed and programmed a cellular automaton (CA) model. In this model the material is consist of an ensemble of small, separated units, which interact via the emerging stresses due to plastic deformation. The model handles the flow stress on cell-level ($\tau\_w$) and it is considered as a random variable and calibrated via lower scale, discrete dislocation dynamic (DDD) simulations such a way, that the distribution of the external stress at the first avalanche shall be the same that one gets for DDD simulations. The expected value of $\tau\_w$ 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. Since $\tau\_w$ is a probability variable, the plastic response of the system differs from sample to sample, and its time evolution is nondeterministic for one realisation. To compare the desired parameters, numerous simulations must be evaluated therefore.

The CA model is applicable on materials with internal disorder that undergo strain softening, if the fracture is due to strain localisation. To model this behaviour a softening mechanism has been introduced. The disorder in the material is provided by the distribution of $\tau\_w$. The origin of this internal disorder is not necessarily originated from the disorder of dislocations, even more, the material investigated does not even have to be crystalline. The material can be any metallic glass, metallic foam, or any other material that meets the above described criteria, that can be considered homogeneous on a larger scale.

To investigate dislocation patterns, I developed a CA model, that contains additional stress terms in the equation of motions compared to the model used above. These stress terms are originated from the dislocation correlations described by the continuum theory of dislocations in local density approximation. In such a model random processes still play an important role, which reflected at one hand on the initial flow stress-distribution, and on the other hand, on the nondeterministic time evolution of the system. Because of these stochastic processes the details of the evolving dislocation patterns differ from sample to sample but analysing more simulations one can identify the common properties of them. The characteristic wavelength of the pattern can be obtained from the dislocation density of the individual realisations by averaging the patterns in the Fourier space. The robustness of the system can be investigated by varying the strength of the stochastic terms and by applying extremal dynamics. By this latter I mean that I suppose that only those dislocations are moving on which the forces are the largest.

**\subsection\*{Experiment}**

\markboth{Methods}{**Experiment**}

With commercially available devices displacement can be measured up to subnanometer precision with capacitive sensors, and objects can be also moved with similar precision with special linear motors. The stress-strain curve of the sample can be express with the displacement of the tip of the nanoindenter and the force acting on the tip. To obtain these values I designed the body of a nanoindenter consisting three main parts as shown in Fig.~1. The displacement of the frame $d$ relative to the stage can be prescribed with a linear motor. The displacement of the tip $e$ relative to the frame is measured with a capacitive sensor. With these data one can express the change in the shape of the sample as $\epsilon = d - e $, and the elongation of the spring as well, which is also $\epsilon$. From this latter one can calculate the force acting on the tip by knowing the spring constant.

\begin{figure}[htbp!]

\centering

**\includegraphics**[width=1\textwidth]{rugo}

\caption{Schematic structure of the nanoindenter. The unique design of the spring makes it possible, that the tip moves in the deformation axis only. The displacement of the tip relative to the frame is measured by a high precision capacitive displacement sensor. The frame can be moved relative to the stage with nanometer precision.}

**\label{fig:rugo}**

\end{figure}

To this end, the nanoindenter body is machined from a single piece of aluminium, where numerous lamellae form the spring, folding them one after each other. Electric discharge machining provided high enough precision to fabric such a fine and fragile arrangement. With this setup one can measure the force in the direction of the deformation with \si{\micro\newton} precision, while during this measurement the tip does not move in the perpendicular directions, otherwise the measurement of $d$ with the precision required would become impossible.

No air provides the damping in the vacuum chamber in the absence of the air, therefore permanent magnets placed below the holder of the tip provides the damping required.

**\section\*{Results}**

\markboth{Results}{ }

\begin{enumerate}

\item I showed, that crystalline materials can be resolved into a system of smaller units, where the size of the units are larger than the correlation length of the dislocations, and such systems can be effectively investigated with cellular automata. By investigating the regime of small deformations, one can calibrate the parameters of the model such a way, that the model shows similar properties to discrete dislocation dynamics simulations. This similarity manifest in the distribution of the external stress of the first avalanches, in its scatter, in its scaling properties with the system size, and in the stress-strain curve. Such a system can be characterised with independent exponents. One of them is the exponent of the power-law-like distribution of the external stress at the first avalanche. While the other one can be obtained by investigating the scatter of the external stress at a given strain value. \cite{PhysRevB.95.054108}

\item I showed, that such materials with internal disorder, which can be considered homogeneous on a larger scale, and which undergo strain softening, and whose failure is due to strain localisation, can be effectively modelled with cellular automata. I showed that, that with increased disorder, even though the onset of plastic regime appears at smaller stresses already, a large increase in the applicable highest external stress and in the achievable plastic strain until failure can be observed. \cite{Tuzes2017}

\item It is enough to consider the terms of the equations of motion in the continuum theory of dislocations up to the local density approximation to observe dislocation pattern formation. I showed, that the equations of motion can be solved with a cellular automaton in the presence of stochastic terms and the patterns evolved are in a good agreement with the prediction of the linear stability analysis applied on the original equations of motion. \cite{PhysRevB.98.054110}

\item I designed and carried out a nanoindentation tool, which makes it possible to perform in situ deformation experiments in a scanning electron microscope, and to which an acoustic emission detector can be attached to associate the processes observed in the electron microscope to acoustic signals detected. The novel design of the spring in the nanoindenter makes it possible to measure the displacement of the tip relative to the frame with a high accuracy capacitive sensor, and the spring makes it also possible to determine the force acting on the tip. \cite{hegyi}

\end{enumerate}

**\section\*{Further possibilities}**

\begin{itemize}

\item The parameters of the model mentioned in point 2 can be calibrated via lower scale, molecular dynamic models, so that the prediction of the model implemented would have a relevance on concrete materials.

\item The cellular automata mentioned in point 1 and 3 could be merged together. In a hopefully successful case the resulted model would show applicability extended to the regions of the two separate models.

\item The aim of the nanoindentation tool mentioned in point 4 has the purpose to facilitate to obtain large data on deformations of numerous micropillars. Performing these experiments is a current topic in our research group. The part of the setup which causes the largest noise or difficulty can be identified and improved to make the measurements more valuable. There is a possibility to considerable decrease the mass of the part between the springs and the tip making it possible to track the deformation of the micropillars even faster and more precise.

\end{itemize}

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