Collective phenomena in dislocation plasticity: jamming, avalanches and yielding

Henri Salmenjoki
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Aalto University
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**Abstract**

When crystalline materials are externally loaded, the irreversible changes in the shape, i.e. plastic deformation, results from the motion of dislocations that are line-like defects in the crystal lattice. Thus, the mechanical properties of crystalline materials, including most metals, are dependent on both the interactions between dislocations with other dislocations and dislocations with other types of crystal defects. Observing crystal plasticity on micron-scale reveals that it proceeds in discrete intermittent events that are avalanches of collective dislocation motion. The size and duration of these avalanches follow power-law distributions which is typical for critical phenomena. As the avalanches are dependent on the features of the unique, initial dislocation structure, micron-scale samples exhibit fluctuations in the stress-strain response and mechanical properties.

This dissertation consists of two parts where we study crystal plasticity with 2D and 3D discrete dislocation dynamics simulations. In the first part, we focus on the seemingly stochastic, avalanche-dominated stress-strain curves of dislocation systems. In Publication I, we use supervised machine learning methods to predict 2D single system stress-response from the initial state of the system. And in Publication II, we find correlations between the subsequent avalanches of the stress-strain curve in both 2D and 3D systems.

The second part considers 3D dislocation simulations with disorder in the form of precipitates. As precipitates block dislocation motion, they are commonly added to increase yield strength of the crystal. In Publication III, we study the effect of precipitate density and strength on the avalanche distributions and yield stress. We find a phase transition between low precipitate density systems, where dislocation-dislocation interaction dominates and the systems exhibit extended criticality, and high precipitate density systems, where dislocations pin to the defects and the systems possess a distinct critical point. Finally in Publication IV, we use unsupervised machine learning to locate the phase transition by using solely the dislocation structures extracted from systems with varying precipitate density.

**Keywords** plastic deformation, dislocations, machine learning

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“Tässä oli tietyistä upottavan ansan mahdollisuus, tienviitta kohti pakkomiellettä ja epätoivoa, yksinäisyyttä, loputonta paneutumista: tämä oli henkinen tila, joka johti ylitosan myrskyihin ja pitkanteeseen apatiaan, joka toi muassa välipitsä tärkeimmän ja mahdollisuuden kytkeytyä muunlaiseen elämään, arkeen, arkiin toimiin, mutta hänellä oli silti palava tarve hakeutua tuohon tilaan aina uudestaan, koska lopulta, kaikesta kuluttavudeesta huolimatta tämä yliväsymystila, tämä ohimoita pakottava, silmään korventava tila oli hänen intohimonsa ja ahkeruuden kantava motivaattori, tämä tarve palata karkotetun alkuidean äärellä, ja totta kai vakavien pyrkimysten lopussa, tietyjen kuumoisen harmonisten ja ylityöläiden päivien jälkeen, mikäli hän oli saattanut jonkin pitkään pohdituttaneen ongelman onnistuneesti jos ettei päättäkseni niin eteenpäin, odotti aina lyynen riemastus.”
— Miki Liukkonen, Elämä: esipuhe


Koirakorttipelin ja työpaikkahuumorin täyteinen aikani CSM:n jäsenenä alkoivat paljon väitöskirja-aiakaa aiemmin, vuoden 2014 kesäällä. Niinpä suuri kiitos avustaa vuosista kuuluu myös kaikille nykyisille ja entisille kollegoilleni. Olen nauttinut lounashetkistä ja kipakoista keskusteluista Leevi Viitasen, Tero
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Ja kuten esipuheille tyyppillinen draamankaari etenee, viimeisenä haluan kiittää perhettäni mittaamattomasta tuesta. Akateemiset taipumukseni olen epäilemättä perinyt vanhemmiltani, Pirjolta ja Kimmolta. Mutta mikä tärkeämpää, heiltä olen saanut aina rakkautta ja kannustusta, joista olen ikuisesti kiitollinen. Lisäksi ylisuuri kiitos kuuluu rakkaalle vaimolle Tuulialle – hän jos kuka on joutunut kestämään minua ja minun "mahdottomuutta kytkeytyä muunlaiseen elämään, arkeen, arkisiin toimiin". Tämä ei olisi onnistunut ilman häntä.

Same in English: I’m grateful to everyone who has helped me during my doctoral studies, especially my colleagues, friends and family.

Helsinki, May 9, 2022,

Henri Salmenjoki
Preface

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Author’s Contribution

Publication I: “Machine learning plastic deformation of crystals”

LL and MJA designed the study. Doctoral Candidate (DC) performed the simulations, designed and implemented the machine learning algorithm, and did the data analysis. LL wrote the first draft of the manuscript and all authors contributed to the final version of the publication.

Publication II: “Avalanche correlations and stress-strain curves in discrete dislocation plasticity”

DC, LL and MJA designed the study. DC performed the simulations and data analysis. All authors contributed in writing the manuscript.

Publication III: “Plastic yielding and deformation bursts in the presence of disorder from coherent precipitates”

LL and MJA designed the study. DC and AL performed the simulations. DC did the data analysis and wrote the first draft of the manuscript. DC, LL and MJA contributed to the final version of the manuscript.

Publication IV: “Probing the transition from dislocation jamming to pinning by machine learning”

DC designed the study with help from LL and MJA. DC performed the simulations and data analysis, implemented the machine learning algorithm and wrote the first draft of the manuscript. All authors contributed to the final version of the publication.
Other publications the author has contributed to


Abbreviations

**DDD** Discrete Dislocation Dynamics

**SC** Simple-Cubic

**FCC** Face-Centered-Cubic

**BCC** Body-Centered-Cubic

**2D** two-dimensional

**3D** three-dimensional

**PBC** Periodic Boundary Conditions

**ParaDiS** Parallel Dislocation Simulator (software)

**ML** Machine Learning

**NN** Neural Network

**ID** Initial Deformation

**GND** Geometrically Necessary Dislocation
1. Introduction

For thousands of years, humankind has used great effort to study metallurgy to be able to produce more durable and processable tools. Originally it started with the aim to manufacture the strongest weapons and finest ornaments but nowadays, especially the desire for micron-scale components in electronics industry has further steered the research towards smaller and smaller samples. Whether the question is about strength of a sword or shaping a metal rod with diameter less than few micrometers, the decisive factor is how the metal behaves under external forces and resists plastic deformation, i.e. irreversible changes in its shape. As most metals have crystalline structure, studying their strength and durability requires fundamental information of crystal plasticity. And on micron-scale, crystal plasticity exhibits interesting, complex phenomena.

Already in 1932 experiments on crystalline zinc showed that plastic deformation occurs in discrete events instead of a smooth transition [1]. Later the origin of these events and crystal plasticity in general was established with the theory of topological line defects called dislocations, formulated simultaneously by Orowan [2, 3, 4], Taylor [5] and Polányi [6]. Since then, the theory of dislocations has succeeded explaining properties of crystals from macro-scale yielding to micron-scale oddities such as the intermittent events that arise from collective dislocation motion, i.e. avalanches. This dissertation focuses on the latter, that is the avalanches and other collective phenomena of dislocations on micron-scale.

During recent decades, new computational tools to study dislocation systems have evolved, especially Discrete Dislocation Dynamics (DDD) software. With DDD software, the physical size of simulated systems can reach multiple micrometers which is unreachable with computational molecular dynamics. Additionally, skyrocketing popularity of applying machine learning methods in materials science has opened new opportunities. In this dissertation, DDD simulations are used in collaboration with machine learning to analyse dislocation systems and the plastic deformation process.

This Chapter builds a foundation for the dissertation and is structured as follows: First, Sections 1.1 and 1.2 introduce the concepts of dislocations and
collective dislocation phenomena, respectively. Then Section 1.3 presents the
used DDD simulation methods. And finally Section 1.4 discusses machine
learning methods from the perspective of this study. The results are presented
in the following Chapters 2 and 3. Chapter 4 concludes the findings.

1.1 Crystal dislocations

The notion of crystal dislocation arises from discontinuities of the lattice struc-
ture. Ideally, crystal lattice is a collection of atoms forming a regular pattern.
These patterns are classified by the cell structure that is repeated to form the
eventual crystal. For example, crystals with Simple-Cubic (SC) structure are
formed by stacking cubic cells with atoms at every corner, or Face-Centered-
Cubic (FCC) by cubic cells with atoms at every corner and center of every face.
But in real materials, these patterns are broken by irregularities, topological
defects called dislocations [7].

In practice, the fundamental dislocations are usually caused by uneven amount
of layers of atoms or displacements of crystal parts with respect to each other,
the former leading to a formation of edge dislocation and the latter to a screw
dislocation. Fig. 1.1 shows a schematic illustration of edge and screw dislocations
in SC crystal. Dislocation can be also a mix of the two types but, in any of these
cases, the irregularity is a line. Additionally crystals can have differently shaped
defects too, such as stacking faults in FCC crystals, where the subsequent atom
layers are stacked in irregular order causing misalignment in the form of plane
defects. Alternatively, some single atoms in the crystal can be replaced by
impurity atoms of different type or even be missing entirely, i.e. vacant, leading
to point defects.

From the different crystal defects, dislocations have the main role in the
plastic deformation of crystals. As a crystal is externally deformed, existing and
nucleating dislocations inside the crystal move and produce plastic strain. This
is illustrated in Fig. 1.2, where an edge dislocation moves in SC crystal due to
Figure 1.2. When driven by an external shearing force acting on the top layer of the crystal, the edge dislocation moves until it exits the crystal from the right-hand side leading to accumulated plastic strain.

an imposed stress. There once the dislocation reaches the right-hand edge of the crystal, it exits and leaves behind a crystal where the top part has shifted by one atomic spacing with respect to the bottom part.

In order to quantify the amount of irregularity caused by the dislocations, they are assigned a ‘topological charge’ [8]. This is done with a Burgers vector $b$ which is the vector measure of discrepancy between the distorted lattice with the dislocation and a reference lattice without any dislocations. Burgers vector is defined as

$$b = \oint_C \partial u \partial l \, dl,$$  \hspace{1cm} (1.1)

where $u$ is the elastic displacement near the dislocation and the integral is taken on a closed circuit $C$ around the dislocation.

The actual force moving the dislocations is given by the Peach-Koehler formula, which states that the force per unit length $f$ is

$$f = (\sigma \cdot b) \times \xi,$$  \hspace{1cm} (1.2)

where $\sigma$ is the local stress field felt by the dislocation and $\xi$ is the dislocation line direction vector. But due to to anisotropy of the crystal lattice, the direction of motion for dislocations is not decided solely on force: in general, dislocations prefer to move in their glide or slip planes (like in Fig. 1.2) which is a plane containing both $b$ and $\xi$. Opposed to gliding, dislocations rarely move perpendicular to their glide plane (i.e. climb).
As is evident from the observations made thus far, dislocations cause displacement fields around them and, thus, generate internal stress fields. And this has two major consequences: Firstly, dislocations interact via the internal stress fields. The magnitude of the stress field at a distance from the generating dislocation can be evaluated with linear elasticity (despite the anisotropy of the lattice). For instance for an infinitely long edge dislocation aligned with $z$-axis, the stress field at point $(x,y,z)$ is [7]

\[
\sigma_{xx} = -Dy \frac{3x^2 + y^2}{(x^2 + y^2)^2} \tag{1.3}
\]

\[
\sigma_{yy} = Dy \frac{x^2 - y^2}{(x^2 + y^2)^2} \tag{1.4}
\]

\[
\sigma_{xy} = \sigma_{yx} = D \frac{x^2 - y^2}{(x^2 + y^2)^2} \tag{1.5}
\]

\[
\sigma_{zz} = \nu (\sigma_{xx} + \sigma_{yy}) \tag{1.6}
\]

\[
\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0, \tag{1.7}
\]

where $D = \frac{Gb}{2\pi(1-\nu)}$ with $\nu$ the Poisson ratio, $G$ shear modulus and $b$ the magnitude of Burgers vector. Thus the long-range (decays $\propto 1/r$ with $r$ as distance) interaction field affecting one dislocation is the superposition of stress fields generated by all other dislocations $\sigma_{\text{interaction}}$.

Secondly, distorted lattice with a dislocation is not in its energy minimum so there is an elastic strain energy associated to the dislocation, comprising of the elastic part and the dislocation core part which is included to avoid the diverging elastic energy at the dislocation line ($r = 0$). As the elastic energy is proportional to the dislocation length, the dislocation tries to minimise it by assuming as short and straight form as possible. This produces self-caused line tension on the dislocation $\sigma_{\text{self}}$. In addition to stress fields from other dislocations and line tension, the local stress field around a dislocation can also contain terms arising from other lattice obstacles for dislocation motion $\sigma_{\text{obstacle}}$, such as grain boundaries in polycrystals, solutes or precipitates in the case of metal alloys. Thus, to conclude, the stress field driving dislocations in Eq. (1.2) is highly complex as it is a sum of contributions of all the internal terms, and the external contribution from loading $\sigma_{\text{external}}$, [9]

\[
\sigma = \sigma_{\text{interaction}} + \sigma_{\text{self}} + \sigma_{\text{obstacle}} + \sigma_{\text{external}}. \tag{1.8}
\]

1.2 Collective dislocation phenomena

Typically metals and other crystalline materials possess a high amount of dislocations, with common dislocation line densities $\rho$ ranging up to $1 \times 10^{15} \text{ m}^{-2}$. 
During plastic deformation, the dislocation structures evolve and nucleate even more dislocations. Due to the complex, long-range interaction between them, dislocations tend to move in a collective fashion.

### 1.2.1 Dislocation avalanches

Collective motion of dislocations leads to avalanches of plastic deformation [10, 11, 12, 13, 14]. These dislocation avalanches are a form of crackling noise which is familiar in many physical systems ranging from earthquakes to magnetic domain wall motion [15, 16, 17]. Fig. 1.3 shows a signal with crackling noise. In the case of dislocations, this sort of signal arises for instance from the measured sum of dislocation velocities $V$ during loading. When one sets a threshold $V_{\text{thres}}$, the signal is separated into parts of low and high activity. As the figure shows, the size of the avalanches $s$ can be characterised for instance by the area below the velocity signal during the active phase.

What systems exhibiting crackling noise have in common is that the events — e.g. dislocation avalanches, earthquakes — occur on wide scale of sizes and durations. For avalanche sizes, this results in a power-law-type probability distribution

$$P(s) \propto s^{-\tau_s} f\left(\frac{s}{s_0}\right),$$

where $\tau_s$ is the critical exponent describing the power-law part and $f(\cdot)$ is a cutoff function typically of exponential family, $f(x) = e^{-x}$, with cutoff avalanche size $s_0$.

In macroscopic samples with large dislocation ensembles the bursty plastic...
events diminish to a seemingly smooth process but observing avalanches is possible by careful procedures. One typical experimental setting is micropillar compression, where a sample with size $\sim 1\mu m$ is compressed to measure its mechanical response, stress $\sigma$ versus strain $\varepsilon$, as shown in schematic of Fig. 1.4. There the dislocation avalanches dominate the plastic response regardless of the fine details of the experiment or material [10, 18, 19, 20].

Evidently crystal plasticity is regulated by size-dependent effects: Famously, ‘smaller is stronger’ as the interplay between the internal (dislocations, other defects) and external (sample size) size-scales leads to smaller micropillars having higher yield strength [10, 21]. Conversely, increasing sample size leads to ‘tamer’ fluctuations and avalanches accumulating smaller part of the plastic strain [22]. On the other hand on macro-scale, compression of single crystal ice has produced crackling acoustic emission signal with power-law distributed amplitudes [23]. And as a bridge between the observations on macro- and micron-scales, a recent study by Ispánovity et al. showed that the bursts of acoustic emission are correlated with the observed dislocation avalanches during micropillar compression [24].

Obviously, the individual, initial dislocation structures vary from one micropillar to another. As the dislocations in these structures cause the avalanche-dominated response (where single avalanche sizes span multiple size-scales), the resulting stress-strain curves have a stochastic-like appearance [25]. Therefore, eventual yielding of the material fluctuates in small samples even if they were made of the same material. This stochastic aspect of crystal plasticity is the question of interest in Chapter 2 covering Publication I and Publication II.

1.2.2 Dislocation jamming, depinning and yielding

The emergence of crackling noise in physical systems with no evident similarity has lead to the notion of universality classes. Systems among a class share the macroscopic properties – the critical exponents of distributions of observables including the event size – despite the differences in the microscopic details of the systems.

Initially dislocation ensembles have been associated with systems that undergo a depinning transition [26, 27]. In depinning, an elastic interface is driven in a field of random disorder that pins the motion. The line exhibits avalanches as it jumps from one pined state to another before undergoing a non-equilibrium phase transition at a critical stress $\sigma = \sigma_c$ where the average avalanche size diverges,

$$\langle s \rangle \propto (\sigma_c - \sigma)^{-\gamma'},$$  

(1.10)

where $\gamma'$ is a critical exponent, and the line enters continuous flow. Systems exhibiting depinning transition include cracks propagating during fracture of heterogeneous medium [28, 29], magnetic domain walls [30, 31] and, even to some extent, shear bands of Portevin–Le Chetaliere effect [32]. Mean-field
Figure 1.4. (a) A schematic of stress-controlled micropillar compression. The tip is lowered to produce a stress on the dislocations that get activated and start to glide in their slip planes. Once the dislocations reach the edge of the pillar, they exit and leave an increment between crystal parts above and below the glide plane. In real world crystals, the number of dislocations does not only decrease as there exist also sources that generate dislocations when they are activated by external forces. (b) The compression results in a staircase-like stress-strain response where the dislocation avalanches produce most of the plastic strain.

approximation of depinning transition has been used to predict dislocation ensemble behaviour and, indeed, a single dislocation in a static random field undergoes a depinning transition [33, 34].

Although experimental observations have yielded power-law statistics from dislocation avalanches agreeing with the mean-field depinning theory [35], it has been recently demonstrated that the critical exponents vary with loading properties including direction and rate, partly due to the anisotropy of the crystal lattice [20]. And after all, pure dislocation systems differ from the assumptions of the depinning theory as the disorder field, that the dislocations explore, is anisotropic and time-dependent, evolving with the dislocation structure (i.e. \( \sigma_{\text{interaction}} \) changes in time). So instead of depinning transition with a distinct critical point, DDD simulations have shown that dislocation ensembles exhibit a state referred to as dislocation jamming [8] with a continuous proximity to a critical point but never reaching it (i.e. ‘extended criticality’) [36, 37, 38].
In dislocation jamming, avalanches are power-law-distributed but the average avalanche size increases exponentially, \( \langle s \rangle \propto e^{\sigma_0/\sigma} \) with some parameter \( \sigma_0 \), instead of Eq. (1.10) as in depinning.

The dislocation ensemble dynamics become more complex when the crystal lattice contains disorder such as precipitates leading to additional static random pinning field \( \sigma_{\text{obstacle}} \neq 0 \) and evolving \( \sigma_{\text{interaction}} \). In case of metals this type of alloying is a fundamental way to improve material strength as the precipitates block dislocation motion and increase yield stress [39]. Additionally disorder can diminish the fluctuations caused by the stochastic-like avalanches [22]. Previously a 2D DDD study showed that, by adding solutes to the dislocation system, dislocations change their dynamics to depinning-like with distinct critical stress which is a trait of transition from dislocation jamming to a different universality class [40]. More importantly, both the amount and strength of the added quenched disorder alters the dynamics. This transition from jamming to depinning is the main topic in Chapter 3 covering Publication III and Publication IV.

As a final note, the distinct types of dislocation dynamics produce an ambiguity in the definition of yield stress \( \sigma_y \) of a crystal: for systems with obstacles, \( \sigma_y = \sigma_c \) can be a natural choice as there the dislocations depin and enter continuous flow. But for pure systems, one needs to resort to an ‘engineering’ definition of \( \sigma_y = \sigma(\varepsilon_y) \) where \( \varepsilon_y \) is a pre-defined yield strain, such as the commonly used 0.2%.

1.3 Simulations of discrete dislocation dynamics

This Section provides introduction to the simulation methods used in this dissertation, namely the two-dimensional (2D) DDD model in Section 1.3.1 and three-dimensional (3D) DDD model in Section 1.3.2. What these models have in common is that the atoms in the lattice structure of the crystal are neglected and the dislocations are modelled as elastic objects interacting via their shear stress fields inside a single crystal.

1.3.1 Discrete dislocation dynamics in 2D

The 2D DDD model is a simplified tool to simulate plastic deformation of crystals. The model simulates a \( L \times L \) region that is a cross-section of a single crystal with infinitely long, parallel edge dislocations that are perpendicular to the simulated box. Dislocations are randomly assigned a Burgers vector pointing in either the positive or negative direction along the \( x \)-axis which, correspondingly, restricts their glide planes to be parallel to the \( xz \)-plane. This is depicted in Fig. 1.5 which shows an example of a 2D DDD initial dislocation structure.

Assuming that the dislocation motion is restricted to the glide plane (i.e.
Figure 1.5. An example of initial dislocation structure from a 2D DDD simulation. The edge dislocations are marked with red $\perp$ or blue $\top$ according to their Burgers vector (positive or negative, respectively).

$x$-direction) and given the symmetries in the system setup, the shear stress field produced by one dislocation reduces to the single relevant component, $\sigma_{xy}$, according to Eq. 1.2. The simulation box is implemented with periodic boundary condition (PBC) meaning dislocations leaving the system at one edge enter the system at the opposite edge. To avoid PBC leading to any discontinuities in the stress field, an infinite number of periodic images in the $x$-direction are taken into account, yielding for single dislocation stress field at point $(x, y)$

$$\sigma_{PBC}'_{xy}(x, y) = \sum_{n=-\infty}^{\infty} \sigma_{xy}(x + nL, y),$$  \hspace{1cm} (1.11)

where $\sigma_{xy}$ is given by Eq. (1.5). This can be evaluated [41], giving

$$\sigma_{PBC}'_{xy}(x, y) = D \pi \sin(2\pi x/L)[\cosh(2\pi y/L) - \cos(2\pi x/L) - (2\pi y/L)\sinh(2\pi y/L)] \left[\cosh(2\pi y/L) - \cos(2\pi x/L)\right]^2.$$  \hspace{1cm} (1.12)

To accommodate periodicity also perpendicular to the glide plane, the final stress field $\sigma_{xy}^{PBC}$ is obtained by summing $\sigma_{xy}^{PBC}'$ over one periodic image in the $y$-direction, so that every dislocation sees a copy of all other dislocations both below and above itself.

The motion of dislocations is driven by the Peach-Koehler force (Eq. (1.2)) which, when assuming over-damped dynamics, leads to equation of motion for $i$th dislocation

$$\frac{v_i}{\chi b} = s_i b \left[ \sigma_{ext} + \sum_{i \neq j} s_j \sigma_{PBC}^{xy} (x_i - x_j, y_i - y_j) \right],$$  \hspace{1cm} (1.13)

where $\chi$ denotes the dislocation mobility, $v$ the velocity, $s$ and $b$ the sign and magnitude of the Burgers vector, respectively, and the sum is taken over all
other dislocations in the system. For convenience, parameters of the model, i.e. \( D, \chi \) and \( b \) are set to unity in the simulations of this dissertation. The moving dislocations then accumulate strain with rate \( \dot{\varepsilon} = \frac{b}{L^2} \sum_i s_i v_i \). As a final remark, the divergence of the stress field of Eq. (1.12) at \( r = 0 \) is handled by dislocation annihilation: dislocation pairs with opposite Burgers vectors are deleted from the system if their distance becomes less than \( 2b \).

The most notable shortcoming of this 2D DDD model is the lack of dislocation sources: With dislocation annihilation, the amount of dislocations can only decrease during the loading. Therefore, the model does not produce the important effect of dislocation multiplication leading to work hardening where increasing dislocation density affects the plastic deformation as new dislocations block and jam dislocation motion [42]. But despite the simplified system, the 2D model still captures many features encountered in crystal plasticity. Most importantly, it produces the crackling noise behaviour [23, 24, 8]. Therefore, 2D DDD simulated systems are a good starting point in the challenge of predicting the plastic deformation process by the initial dislocation structure in Publication I.

### 1.3.2 Discrete dislocation dynamics in 3D

The 3D DDD simulations of this dissertation are performed with ParaDiS (Parallel Dislocation Simulator) which is a software implemented in Lawrence Livermore National Laboratory [43]. With ParaDiS, line-like dislocations are simulated in a \( L \times L \times L \) box of single crystal. Compared to the 2D DDD model, ParaDiS enables simulation of more realistic dislocation structures.

Generally in 3D DDD, dislocation lines are discretized as a set of nodes and segments connecting the nodes. In ParaDiS, the interaction forces are computed for the discretization nodes separating the segments. Similarly as in 2D DDD, the dislocations interact through their linear elastic stress fields. For nearby segments, the interactions are computed with line integrals while for further dislocations – including the dislocations in periodic images enabling PBC – the forces are calculated by multipole expansion. At dislocation core, ParaDiS avoids the divergence of interaction force due to the elastic theory by using results from molecular dynamics simulations.

From the stress field, the force (per unit length) \( f \) acting on a discretization node is obtained again by the Peach-Koehler equation (Eq. (1.2)). Finally the nodal velocities \( v \) are computed using mobility function \( M(\cdot) \) which ensures that the dislocations prefer their corresponding glide planes,

\[
v = M(f).
\]

In practice, ParaDiS has separate mobility functions for BCC (Body-Centered-Cubic) and FCC.

One fundamental property of dislocations captured in 3D DDD simulations is the evolution of the dislocation density. Unlike in 2D DDD where only dislocation
annihilation is enabled, 3D dislocations can bow and bend which leads to forming of new dislocations and, therefore, 3D simulations can reproduce the work hardening behaviour [42]. In practice, dislocation multiplication occurs as dislocations encounter for instance other dislocations that block the motion at some points along the dislocation line, while the segments between the blocked points are able to continue motion which leads to the formation of a Frank-Read source [7]. In ParaDiS, the nodes manage dislocation annihilation and multiplication processes which are implemented by deleting old and creating new nodes. Example dislocation structures from a ParaDiS simulation are illustrated in Figure 1.6.

To include static pinning field mimicking the effect of alloying, a modified version of ParaDiS has been implemented to enable inclusion of spherical precipitates [44]. The precipitates are assumed fully coherent and they generate isotropic short-range interaction between the precipitate and dislocation. The interaction arises from a Gaussian potential $U(r)$ pinning the dislocations, causing a radial outward force $F(r)$

$$F(r) = -\nabla U(r) = \frac{2Ab^3re^{-r^2/r_p^2}}{r_p^2},$$

where $r_p$ is the precipitate radius and $A$ is a scaling factor to adjust the strength of the precipitates. In Chapter 3, these precipitates are used to evoke and study jamming-depinning transition of dislocation systems.

### 1.3.3 Simulations at the quasistatic limit

As a final step to produce crackling plastic deformation, a loading scheme is chosen to mimic favourable conditions of micropillar compression. In the simulations of this dissertation, this is achieved by carrying majority of the simulations with quasistatic stress ramp [37, 19].

The implementation follows the same idea in both 2D and 3D DDD simulations: First, the system is initialized with preset number $N$ of randomly located dislocations. Then, a relaxation period follows, during which the dislocations form a meta-stable state with minimal dislocation motion. In 2D, the dislocations stop all motion ($v_i \approx 0$ to the floating point precision) but in 3D, some small
motion and oscillations exist due to instabilities of the numerical scheme. However, the stability of the formed 3D microstructure is confirmed by the eventual loading as the ensuing stress-strain response behaves as expected without large avalanches right in the start of the loading (e.g. in Section 2.2). If simulating 3D systems with precipitates, precipitates are added after the first relaxation period and this is followed by a second relaxation period. Once the system reaches the meta-stable state (referred to as the initial state), the external loading starts.

The loading stress is increased with a rate $\dot{\sigma}$ while measuring the velocity signal $V(t)$ of the dislocation ensemble. In 2D, the velocity is computed as the average of absolute values of single dislocation velocities

$$V_{2D}(t) = \frac{1}{N} \sum_{i}^{N} |v_i|,$$

(1.16)

and in 3D as the extensive dislocation velocity

$$V_{3D}(t) = \sum_{i} l_i |v_{\perp,i}|,$$

(1.17)

where the sum is taken over every segment, and $l_i$ is the length of segment $i$ and $v_{\perp,i}$ is the velocity of segment $i$ perpendicular to its line direction. When the signal $V(t)$ exceeds a preset threshold $V_{\text{thres}}$, an avalanche starts and loading is paused until the motion ceases below the threshold. The produced signal is the type illustrated in Fig. 1.3 where the signal comes from a 2D DDD simulation. The eventual avalanche size can be measured by the integral of the signal during the avalanche,

$$s = \int_{0}^{T} [V(t) - V_{\text{thres}}] \, dt,$$

(1.18)

where $T$ is the avalanche duration or, alternatively, by the accumulated plastic strain during the avalanche [37]. Both definitions are encountered throughout the dissertation and, on each occasion, it will be stated which one is used.

### 1.4 Machine learning in the study of crystal plasticity

Machine learning (ML) has conquered a foothold in many fields of physics and materials science is no exception [45, 46, 47]. The ever growing whopping popularity of machine learning arises mainly from two facts: Firstly, ML encompasses a large range of different methods – from the classic Principal Component Analysis to sophisticated neural network models – sharing the basis of mathematical processing of data [48, 49]. Secondly, ML is supported by the boom of increasing computational capacity and data collection, combined with easy-to-use libraries like scikit-learn [50] and Keras [51] that enable fast implementation. In crystal plasticity, possible applications of ML are numerous and results have already been obtained in various studies on both simulated and experimental dislocation structures [52, 53, 54, 55, 56, 57].

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Generally ML can be divided into two main categories, *supervised* and *unsupervised* ML. In supervised ML, the goal is to find a mapping from a set of features corresponding to a sample combined into a feature vector $\mathbf{x}^h$ of sample $h$, to a target $y^h$. The target can be for instance a single value or a vector (regression) or a category (classification). Conversely in unsupervised ML, the target is unknown and the aim is to find a mapping that reveals regularities such as clusters in the data. As a way of brief introduction to ML, the next sections discuss the methods (both supervised and unsupervised) encountered in this dissertation.

### 1.4.1 Neural networks for supervised learning

For supervised ML, arguably the most popular method is the artificial neural network (NN). It is a network built of nodes that are loosely based on the operating principles of neurons in human brains and follow the concept of Rosenblatt’s perceptron [58, 59]. In NNs, perceptrons are generalized to artificial neurons which combine a set of input signals to create an output and, to form a NN, neurons are repeated and stacked in layers. The simplest architecture is the multi-layered feed-forward NN where the output from the neurons in the previous layer is used as the input for the neurons in the next layer. To elucidate, Fig. 1.7 illustrates a regression NN with three layers. As depicted by the figure, every connection in the network is given a weight $w_{n,j}^{i,j}$ (the $i$th connection for a neuron $n$ in layer $j$) that multiplies the passing value and, inside the neuron, all the incoming signals are then summed and passed to activation function $f_{\text{activ}}$. By using a non-linear, continuous activation function, the NN is able to learn a non-linear mapping from the input $\mathbf{x}^h$ to the output $y^h$ [60].

The iterative process of finding optimal weights $w$ is called training. It requires some training data, that is fed to the NN while measuring the loss $\mathcal{L}$, i.e. the error between the true values $y^h$ corresponding to the data and the network output $y_{\text{pred}}^h$. For instance in regression a typical loss function is the mean squared error between the two. During training, the weights of the NN are updated by back-propagating the loss from the output layer to the previous layers and changing the weights accordingly [59]. Simple algorithm to find the weight update is gradient descent which states that the change in weight $\Delta w_{n,i}^{j}$ is given by

$$\Delta w_{n,i}^{j} = -\eta \frac{\partial \mathcal{L}}{\partial w_{n,i}^{j}}, \quad (1.19)$$

where $\eta$ is the learning rate parameter and $w_{n,i}^{j}$ refers to the weight associated to connection between $n$th neuron in the $j$th layer and $i$th neuron in the previous layer. One way to decide whether to continue training is to observe the loss. To avoid overfitting, the loss is measured for validation data which is not used in the computation of the updated weights. Once the validation loss stops decreasing, training is stopped and the generalisability of the NN, meaning the success...
Figure 1.7. A schematic showing the working principle of a feed-forward regression NN. The input signal, namely a vector of various descriptors, goes through three fully connected hidden layers, with e.g. 20 neurons in each layer, before arriving at the output which represents the mapped value. To clarify the process, the lower box depicts the passing of the signal through $n$th neuron in the second hidden layer. Input for the neuron consists of the values coming from the previous, first hidden layer, and they form the vector $y_1$. Elements of $y_1$ are multiplied with the weights of the corresponding connections which form the $n$th row of matrix $w_2$ of all connection weights in the second layer. The sum of the products is then added to the bias of the neuron and passed to an activation function $f_{activ}$. Finally, the output is the value from the activation function and it is passed to every neuron of the subsequent hidden layer. This NN architecture was used in Publication I.

of the mapping that the NN has learned between input and output, can be measured by computing the loss for test data that is unseen during the training process.

NNs enable establishing a non-linear mapping of multiple input parameters to desired output if a mapping and enough training data exist. One such problem is encountered in crystal plasticity: Given an initial dislocation structure, can a NN predict its mechanical response once it is deformed with external force? This was studied in Publication I.
1.4.2 Unsupervised learning of phase transitions

The study of different phases of matter and transitions between them is one of the fundamental questions of statistical mechanics [61]. This goes beyond the elementary school level understanding of the basics – solid, liquid, gas – as hundreds of phases exist. Generally, phase transitions can be recognized by defining an order parameter that measures the symmetries inside the matter. During a phase transition, the order parameter changes either abruptly or continuously (second-order phase transition).

Conveniently unsupervised ML is a handy tool in identifying different phases: With no pre-coded information of any transition, unsupervised methods can extract phases by independently detecting symmetries and the proper order parameter. This has been demonstrated with for instance well-known many-body systems such as the Ising model and the classical XY model [62, 63, 64] but generally any continuous phase transition should work [65].

A clever confusion method to discover the critical point of a phase transition with no prior knowledge was developed by van Nieuwenburg et al. [66]. It starts by assuming that there exists a critical point \( k_c \) inside a range of control parameter \( k \), \([k_0,k_1]\) (e.g. temperature in case of Ising model). Then, by collecting observations of the system throughout the range with various values of \( k \), one can train some (supervised) ML classifier (e.g. NN; so one could arguably call confusion scheme semi-supervised) with labels defined by a trial value \( k^* \): Observed data with \( k < k^* \) is given label 0 and \( k > k^* \) label 1. By repeating the training for multiple values of \( k^* \) and measuring the success \( S' \) (correctly classified samples / all samples) of the ML classifier, the resulting curve of \( S' \) vs. \( k^* \) becomes \( W \)-shaped in the control parameter range. The high success near \( k_0 \) and \( k_1 \) is an artifact of uneven number of samples with the artificial labels which leads to easy task for the classifier as it succeeds by predicting always the majority label. But the maximum at an intermediate \( k^* \) arises because the ML classifier succeeds at \( k^* \approx k_c \) where the observations are truly distinguishable.

As discussed earlier in Section 1.2.2, a transition between dislocation jamming and depinning exists in dislocation systems with quenched disorder. Therefore, there must be some critical density of disorder where the dynamics change. In Publication IV, the confusion scheme was used to study the transition in 3D DDD systems with precipitates and the results are presented in Section 3.2.
2. Predicting single sample response and effect of avalanche correlations

At this point, the bursty nature of crystal plasticity has become evident: Dislocations travel mostly in collective avalanches leading to a stochastic-like response to external loading on micron-scale. This Chapter focuses on this "stochastic" aspect of crystal plasticity. First in Section 2.1, which presents the results of Publication I, machine learning was used to predict the stress-strain response of dislocation systems simulated with 2D DDD. Then in Section 2.2, where results of Publication II are summarised, avalanches from 2D and 3D DDD simulations were analysed to reveal correlations between subsequent events.

2.1 Machine learning single sample stress-strain curves

Using ML to predict non-linear complex phenomena such as earthquakes or solar flares has been widely pursued but has not lead to any groundbreaking, long-term forecasting [67, 68]. With crystals, one such question is material yielding: Knowledge of yield stress of different metals on macro-scale and bracing for stochastic-like yielding on micron-scale are crucial in manufacturing. For the former, ML offers a new aspect on materials design and a possibility to optimise e.g. the mechanical properties [69, 70]. But for the latter the question remains: Can one predict the yielding or the single avalanches?

Ultimately, yielding and accumulation of plastic strain are governed by the dislocation motion which is (especially in room-temperature) highly deterministic as dislocations prefer to move in their glide planes. Therefore, knowledge of the initial dislocation microstructure should contain information about the eventual yielding of the sample. Here we aimed to exploit this: we used ML, or more specifically NNs, to predict the plastic deformation process of quasistatically loaded dislocation structures simulated with the simple 2D DDD model.

First we simulated 5000 systems with each initial dislocation amount from \( N = 50 \) to \( N = 400 \) (except for \( N = 50 \), for which we had 10000 simulations) and the system size was set to result in constant dislocation density \( \rho = 0.04 \frac{1}{b^2} \) (e.g. \( L = 100b \) for \( N = 400 \)). For every simulation, we saved the initial (relaxed,
metastable) dislocation structure and proceeded to measure the stress-strain curve arising from a quasistatic stress ramp. For comparison, we prepared also a second dataset of systems that had had an initial deformation (ID), i.e. we took the previously driven systems at strain \( \varepsilon = 0.2 \) and let them relax before performing a second quasistatic loading. This way we were able to induce pre-existing dislocation structures which can be measured by the pair-wise dislocation correlation

\[
d(x, y) = \left( \frac{1}{\rho_0} \sum_i \rho_i(x, y) \right) - 1,
\]

where \( \rho_0 \) is the average dislocation density and \( \rho_i(x, y) \) is the dislocation density at \((x, y)\) relative to dislocation \( i \). The different sets of initial snapshots of systems (basic and ID; different \( N \)) were given as input to a NN that would then predict the stress-strain curve of the following stress ramp.

Next step was to engineer a set of features that would convey information about the initial dislocation setup to the NN. Because the straightforward position vectors of dislocations are not sufficient to describe the system (due to the periodic boundaries), we settled on three different approaches.

First, we computed the coarse-grained field of Geometrically Necessary Dislocation (GND) density. In 2D, this is depicted by the net sum of Burgers vectors inside the computational cell, i.e. \( \rho_{GND} = \rho_+ - \rho_- \) where \( \rho_+ (\rho_-) \) is the density of dislocations with positive (negative) direction of Burgers vector [71, 72]. To encode the effect of the periodic boundaries into the descriptors, the GND density field was represented by its three first Fourier coefficients in both \( x \)- and \( y \)-directions. Second, we calculated the stress field induced by the initial dislocations inside the simulation volume and computed related statistics such as average and variance. Third, we counted the number of initially present dislocation walls inside the systems. Finally for ID systems, also the value of stress at the end of the pre-loading was considered. These three (four for ID) sets of parameters were collected to a vector of size 19 (20) and associated to corresponding samples. Summary of the described workflow is presented in Fig. 2.1.

For the NN, the architecture followed the one presented in Fig. 1.7. The NN training was implemented with stochastic gradient descent, i.e. as a modification to gradient descent of Eq. 1.19 the weight update included randomness by computing gradients on subsets of training data so that the algorithm was able to avoid getting stuck to local optima. The data was split to 80% training, 10% validation and 10% test sets to apply early-stopping and to find optimal learning rate (which was chosen randomly from uniform distribution \([5 \cdot 10^{-5}, 10^{-4}]\) for different training realisations) by measuring the validation loss during training. Results discussed in this section consider the predictions for the test set obtained with the NN with smallest measured validation loss.

Fig. 2.1g depicts some hand-picked predictions of stress-strain curves for
Figure 2.1. The scheme of predicting the plastic deformation of 2D DDD systems. (a) The initial state of the system is described by for instance the (b) GND density and (c) stress fields. For comparison, part of the systems were first initially deformed to produce states with stronger initial dislocation correlations, as seen in (d) and (e) that show the pair-wise dislocation correlation function $d(x, y)$ of basic and ID systems, respectively. (f)(g) The characterization of the initial systems was then fed to a neural network that predicted the system’s response under loading.

test samples after training the NN. As the figure shows, the NN captures the overall shape and relative strength of the single stress-strain curves but fails to predict individual avalanches. More generally, the goodness, or score, of the NN predictions can be measured by the coefficient of determination $S$, defined by

\[ S = 1 - \frac{\sum_h (y^h - y^h_{\text{pred}})^2}{\sum_h (y^h - \langle y \rangle)^2}, \]

where $y^h$ is the true value for sample $h$ and $y^h_{\text{pred}}$ is the NN output for the same sample. The score parameter is illustrated in Fig. 2.2 for both basic and ID systems. The figure shows that the success of prediction is high with small $\varepsilon$ but deteriorates quickly to a minimum. However after the minimum at larger strains, $S$ recovers and predictions become modest – even more so with ID systems that reach $S \approx 0.7$ opposed to basic systems with $S \approx 0.5$. Notably here the largest systems seem to produce the best scores.

2.1.1 Perspectives on the stress response predictability

The high success at small strains where the systems are close to the initial state is no surprise but the non-trivial, non-monotonic behaviour is. This can be explained by looking at the burst events that the NN failed to predict: Fig. 2.3 shows the distribution of avalanche starting strains $\varepsilon_{\text{aval}}$ plotted on the same logarithmic axis of strain as the $S$ curves from the previous figure. As is evident from the figure, the minimum of the prediction score coincides well with the
Figure 2.2. Score $S$ according to Eq. (2.2) of the NN predictions as a function of strain for (a) basic systems and (b) ID systems of different sizes. The insets show example of predictions versus target values for a single value of $\sigma$.

Figure 2.3. Upper axes show the avalanche starting strain distribution and lower axes show the score $S$ on logarithmic $\varepsilon$-scale for (a) basic systems and (b) ID systems.
Predicting single sample response and effect of avalanche correlations

Figure 2.4. Pair-wise correlation functions of (a) all and (b) positive dislocations in the initial systems with different amount of initial deformation strain. The inset of (a) shows the exponent $\beta$ of the power-law fit $d(0, y) = \alpha y^{-\beta}$ versus the average score ($S$) in the range $\varepsilon \in [0.15, 0.2]$. Similarly, the inset of (b) shows $\alpha$ of the power-law fit $d_{++}(0, y) = \alpha y^{-\beta}$ versus the average score in the range $\varepsilon \in [0.15, 0.2]$, as the exponent $\beta \approx 1.5$ with every different ID.

avalanche activity, thus leading to an observation that the system response is hardest to predict when the systems exhibit most strain bursts.

The effect of the initial deformation is clear from the dislocation-dislocation correlation functions shown in Figs. 2.1d-e: The correlations get stronger especially in the $y$-direction, i.e. initial deformation increases the amount of dislocation walls, and also the number of dislocation dipoles increases. As these dislocation walls are quite stable in the sense that dislocations inside walls tend to move collectively, their effect on the stress-strain predictability is apparent. For further evidence, we trained the NN with datasets of varying amount of ID strain $\varepsilon_{ID}$. Fig. 2.4 illustrates the correlation functions $d(x = 0, y)$ of all dislocations and $d_{++}(x = 0, y)$ of positive dislocations in the direction of walls with different amount of $\varepsilon_{ID}$. The correlations decay as a power-law $\alpha y^{-\beta}$. Both the cases of $d(0, y)$ and $d_{++}(0, y)$ conclude that stronger (in the form of larger $\alpha$) and further carrying (smaller $\beta$) correlations indeed improve the predictability as shown in the insets of the figure: with $d(0, y)$, larger $\beta$ leads to a decrease in NN score, while with $d_{++}(0, y)$ larger $\alpha$ leads to an increase.

The score functions also exhibited an interesting size effect – larger systems were more predictable. Fig. 2.5a shows a distribution of avalanche sizes measured by the accumulated strain $s$ for avalanches starting in a strain-bin close to the beginning of the simulation. So on the one hand, the smaller systems exhibit larger strain bursts already with smaller starting strains $\varepsilon_{aval}$, thus causing larger aberration to the stress-strain curves. Fig. 2.5b presents also a plot of linear correlation of several single descriptors with the stress at $\varepsilon = 0.1$ measured with $r^2$. There some of the used descriptors – especially GND density in the $y$-direction (the first Fourier coefficient $f_{y1}$) – become more informative in the larger systems due to the system containing more dislocations (Fig. 2.5b). Because the dislocation motion is restricted to glide in the model, GND density in the $y$-direction is conserved through out the simulation and, therefore, it is a
Predicting single sample response and effect of avalanche correlations

Figure 2.5. (a) Probability distribution of avalanche sizes (accumulated strain) in different sized systems without initial deformation. The avalanches come from a bin of relatively small strain shortly after the onset of the stress ramp. (b) Single feature correlation with $\sigma(\varepsilon = 0.1)$ for different systems sizes. Single features here are the average of the absolute stress field $\langle |\sigma_{sf}| \rangle$, kurtosis of the stressfield $\text{kurt}(\sigma_{sf})$, the first and second Fourier coefficients in the x-direction $f_{x1}$ and $f_{x2}$ respectively, and the first Fourier coefficient in the y-direction $f_{y1}$.

fundamental parameter in predicting the large strain behaviour as shown also by its high $r^2$. 
Predicting single sample response and effect of avalanche correlations

0.0
0.025
0.050
0.000
0.1
0.2

Figure 2.6. A stress-strain curve with the staircase shape is made of subsequent avalanches and stress increments. For analysis of subsequent avalanches 1 and 2, relevant parameters are the starting strains $\varepsilon_1, \varepsilon_2$; starting stresses $\sigma_1, \sigma_2$; their sizes $s_1, s_2$ and the stress increment between the avalanches $\Delta \sigma$.

2.2 Avalanche correlations and deviation from average response

As the previous section showed, the stress-strain response of the 2D DDD systems could be well predicted except for the individual avalanches. Additionally, the parts of stress ramp, where the systems exhibited the most avalanches, led to the minimum score so the strain bursts are a nuisance for the predicting algorithm.

But the dislocation avalanches can not be totally random: Considering a staircase-like stress-strain curve such as the one in Fig. 2.6, the curve is made of repeating strain increments during avalanches (of size $s$) and somewhat linear parts between avalanches with stress and strain increments $\Delta \sigma$ and $\Delta \varepsilon$, respectively, [73]. If the stress-strain curves were then constructed by subsequently randomly choosing these building blocks (from the corresponding distributions), the resulting curve would be unpredictable and independent of the initial dislocation positions contrariwise to the results in the previous section. Kapetanou et al. proved this by a statistical analysis which showed that randomly drawn curves have larger scatter around the average curve than DDD simulated curves [74]. In addition to the computational study, dislocation avalanches in single crystal ice have displayed also spatial correlations [75].

In the quest of finding avalanche correlations from our DDD simulations, the first thing to look at were all the subsequent avalanche pairs, such as the example illustrated in Fig. 2.6. We concentrated our analysis on both 2D and 3D DDD simulations: The 2D DDD data is from the simulations presented in Section 2.1 with $L = 100b$, while 250 3D DDD simulations were carried with same details as in [37], i.e. material parameters are those of FCC aluminum and the systems with size 1.43$\mu$m were initialised with 40 mixed dislocations in the $\frac{1}{2}(110)(111)$ slip system. The stress rate was set to $\dot{\sigma} = 2.5 \times 10^{13}$ Pa/s in the
direction [010] and the simulations were conducted without cross slip.

As shown by Fig. 2.7, the strain-binned avalanche sizes from both 2D and 3D follow the distribution of Eq. (1.9) with the exponential cutoff. Here avalanche sizes were measured by the change in the plastic strain during the event. We obtained the fitted curves by using the maximum-likelihood method [76]. Because most encountered avalanches are small with no visible effect on the stress-strain curves, we neglected them and focused on the avalanches with \( s > c \cdot s_0 \) where \( s_0 \) is the strain-dependent fitted value of the cutoff avalanche size and \( c < 1 \) is a parameter ensuring a sufficient number of subsequent avalanche pairs (approximately few per system).

Fig. 2.8 shows the Spearman correlation coefficient \( \rho_{\sigma_1, \Delta \sigma} \) between the first avalanche starting stress \( \sigma_1 \) and the stress increment after the avalanche \( \Delta \sigma \), and \( \rho_{\Delta \sigma, s_2} \) between \( \Delta \sigma \) and the second avalanche size \( s_2 \). Moreover, the correlations are plotted as a function of the first avalanche starting strain \( \varepsilon_1 \). As is evident from the figure, both 2D and 3D systems display correlated avalanches with small strains, where the larger \( \Delta \sigma \) implies larger size for the following avalanche \( s_2 \) with \( \rho_{\Delta \sigma, s_2} > 0.5 \). Similarly 3D systems show clearly negative

![Figure 2.7](image-url)
correlation between $\sigma_1$ and $\Delta \sigma$ (i.e. large first avalanche stress implies smaller increment in stress before next avalanche) again with small strain. In 2D, this correlation is also negative but weaker.

### 2.2.1 Impact of the discovered avalanche correlations

Interestingly, both of the found correlations ($\rho_{\sigma_1,\Delta \sigma}$ and $\rho_{\Delta \sigma,s_2}$) affect the ensuing stress-strain curve in a similar manner: Both correlations push the stress-strain curve towards the average curve. If $\sigma_1$ is large, the following increment in stress is smaller and the stress-strain curve 'waits' for the average response to catch up. Correspondingly if $\sigma_1$ is small, the curve tries to take a larger increment before the next avalanche, i.e. now the single curve is trying to catch up the average. Similarly with positive $\rho_{\Delta \sigma,s_2}$, large increment between avalanches leads to larger avalanche (as one could expect) which, in turn, lets the average curve to catch up. As these correlations decay with increasing strain, this push towards the average curve can be seen only with small strain.
Predicting single sample response and effect of avalanche correlations

The push towards the ensemble average becomes evident in Fig. 2.9 which shows example single system stress-strain curves shifted by the average curve. In the small strain region, the curves cross \((\sigma - \langle \sigma \rangle = 0)\) the average much more often than with larger strains. To quantify the tendency of a single system to approach the ensemble average, we defined the rate of intersections with the mean curve, \(\frac{N(\sigma - \langle \sigma \rangle = 0)}{d\varepsilon}\). So in practice, the rate is taken with respect to accumulating strain. The rate along the simulated strain interval is shown in Fig. 2.10 for both 2D and 3D. It is plotted with the probability distribution of avalanche starting strains (both all avalanches and avalanches above the set threshold \(s > c \cdot s_0\)) and, in case of 2D, additionally the prediction score of the stress obtained with a NN in the previous section (Fig. 2.2).

In 2D, the rate follows almost exactly the confined peak of starting avalanche distribution observed at small strains and, therefore, it matches also with the dip in the NN score. Therefore, we can deduce that, to large extent, the drop in the predictability is caused by the uncertainty in the systems’ relative strength as the systems cross the average response while trying to decide their eventual position compared to it. On the other hand in 3D, \(\frac{N(\sigma - \langle \sigma \rangle = 0)}{d\varepsilon}\) is not peaked but it decays throughout the simulated strain interval. This difference in the small
strain regime arises from the model details as the meta-stable initial state with ParaDiS does not achieve perfectly relaxed state ($V_{3D} \neq 0$ at $\sigma_{\text{external}} = 0$) unlike in 2D which can cause instabilities and avalanches already at minimal stresses. But most importantly, the large strain behaviour of decreasing $\frac{N(\sigma - \langle \sigma \rangle = 0)}{dt}$ and ‘fixed’ stress-strain response in relation to the average is shared in 2D and 3D.

![Diagram](image)

**Figure 2.10.** The rate of intersecting the average response $\frac{N(\sigma - \langle \sigma \rangle = 0)}{dt}$ in (a) 2D and (b) 3D DDD. Additionally the figures include the distributions of avalanche starting strain $\varepsilon_{\text{aval}}$ of both all and threshold avalanches. For 2D, also the stress-strain curve prediction score of Fig. 2.2 is plotted for comparison.

What helps the systems anchor their position relative to the average is the evolution of the stress increments. Fig. 2.11 presents the strain-resolved complementary cumulative distributions of stress increments between all avalanches in 2D and 3D systems. In 2D, the distributions do not change notably per se but, as the stress-strain curves become more spread and their standard deviation grows, less stress increments cause a sufficient change with respect to the average response. In 3D, the standard deviation stays approximately constant after the initial jump (Fig. 2.7b), but the tails of the distributions move towards smaller and smaller $\Delta \sigma$ which ultimately leads to the same effect as in 2D.
Figure 2.11. Complementary cumulative distributions of stress increments between all avalanches in (a) 2D and (b) 3D systems. The dashed lines in (a) depict the standard deviation of the stress-strain curves at the corresponding strain.
3. Dislocation ensembles in systems with coherent precipitates

In the previous chapter, the results were obtained for pure dislocation systems that exhibit extended criticality and the yielding is governed by a ever continuous process of successive avalanches near an unreachable critical point. But situation changes as quenched disorder is added to the system. This Chapter discusses results from extensive 3D DDD simulations of dislocation systems with coherent precipitates. The system dynamics were studied by varying the level of disorder many orders of magnitude, as illustrated in Fig. 3.1, to enable the transition from dislocation jamming to depinning. First Section 3.1 considers Publication III where the yielding of these systems was analysed from the perspective of its statistical nature and the changes in the yield stress. Then in Section 3.2, which presents the results of Publication IV, unsupervised machine learning was used to extract the critical point of the jamming-depinning transition from the dislocation structures.

3.1 Avalanche statistics and yielding

Previous results of 2D DDD simulations have brought forth the disparity between systems of pure, obstacle free dislocation motion and systems where dislocations move in a static field of disorder [36, 40]. Essentially, only the latter type of systems goes through a non-equilibrium phase transition at $\sigma_c$, between states of dislocations stuck to the pinning points and free-flowing dislocations. In pure dislocation systems, no pinning points exist and the dislocation ensemble recedes in the state of extended criticality without distinct critical point [37].

However, the two types of dynamics, jamming and depinning, share some similarities in the response to creep with constant applied stress (or creep-like loading in case of DDD simulations, as one could argue that time-scales are short and temperature-dependent phenomena, such as dislocation climb, are mostly neglected). Originally, Andrade established experimental law for time-evolution of strain during creep that can be formulated as

$$\dot{\varepsilon} \propto t^{-\theta},$$  \hspace{1cm} (3.1)
Figure 3.1. Initial dislocation ensembles from 3D DDD simulations with the density of precipitates $\rho_p$ (a) $1 \times 10^{19} \text{ m}^{-3}$, (b) $1 \times 10^{20} \text{ m}^{-3}$ and (c) $1 \times 10^{21} \text{ m}^{-3}$. Same systems are plotted both with (left) and without (right) the precipitates.
Dislocation ensembles in systems with coherent precipitates

where $\dot{\varepsilon}$ is the strain rate and $\theta = 2/3$ [77]. 2D DDD studies have shown that both pure systems [8, 78] and systems with quenched disorder [40] exhibit this power-law relaxation during constant loading, although possibly with $\theta \neq 2/3$. With quenched disorder, the power-law emerges with a stress $\sigma_{c'}$ ($\sigma_{c} = \sigma_{c'}$ expected with pinning) while for stresses below or above $\sigma_{c'}$ the strain rate decays exponentially or settles for a constant value, respectively. On the other hand in pure systems, the eventual decay / constant flow starts after a period of power-law relaxation [8] which is again another sign of extended criticality as the systems exhibit criticality regardless of the external loading [78].

We studied the transition of dislocation dynamics from jamming to pinning by both quasistatic and constant, creep-like loading. Material parameters were again set to those of FCC aluminum and the initial number of dislocations was 24 in the $\frac{1}{2}(110)(111)$ slip system which led to initial dislocation density of $\rho_0 \approx 2 \times 10^{12} \text{m}^{-2}$ inside a simulation box of size $L = 4 \mu\text{m}$. With precipitates, the aspect defining the type of system dynamics is the competition between dislocation-dislocation and dislocation-obstacle interactions. To control the latter, two options remain: One can change either the strength or the density of the obstacles. With the modified version of ParaDiS, we explored both as the former is controlled by the precipitate force scaling parameter $A$ of Eq. (1.15) and the latter by the number of precipitates in the system. The precipitate radius was set to $r_p = 100b = 2.86 \times 10^{-8} \text{m}$.

3.1.1 Quasistatic loading

For the stress ramp simulations, we fixed the precipitate density to $\rho_p = 1 \times 10^{20} \text{m}^{-3}$ and varied their strength from weak (force scaling parameter $A = 1 \times 10^{9} \text{Pa}$) via intermediate ($A = 1 \times 10^{10} \text{Pa}$) to strong ($A = 5 \times 10^{10} \text{Pa}$). Although for strong precipitates, the computational cost of simulations became overwhelming and the reached maximum strains were smaller than for other precipitate strengths. The number of simulated systems was 100 for each $A$ and we also prepared a control set with no precipitates (i.e. $A = 0$). The loading was conducted with stress rate $\dot{\sigma} = 1 \times 10^{14} \text{Pa/s}$ in the direction $[100]$ and cross slip was enabled. The ensuing avalanche sizes were measured by the integral of the dislocation velocity signal above the threshold.

The evolution of mean dislocation avalanche size and the resulting stress-strain curves are presented in Fig. 3.2. First, $\langle s \rangle(\sigma)$ shows the sought transition from one type of dynamics to another. With weak or no precipitates, mean size grows exponentially $\langle s \rangle \propto e^{\sigma/\sigma_0}$ with $\sigma_0 = 3.4 \times 10^{6} \text{Pa}$ for the fitted solid line of weak precipitates. But with intermediate precipitates, the typical depinning behaviour emerges and $\langle s \rangle$ diverges at some $\sigma_c$. By fitting $\langle s \rangle \propto (\sigma_c - \sigma)^{-\gamma'}$, we obtained $\sigma_c = 4.4 \times 10^{7} \text{Pa}$ and $\gamma' = -1.7$. For strong precipitates, a possible critical point is still far from the attained stress values.

The effect of precipitates and evolution of $\langle s \rangle$ transmit to the stress-strain
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Figure 3.2. (a) The mean avalanche size during quasistatic loading for different precipitate strengths. The solid line shows the fitted function of $\langle s \rangle \propto e^{\sigma/\sigma_0}$ and dashed line of $\langle s \rangle \propto (\sigma_c - \sigma)^{-\gamma}$. (b) The average stress-strain curves from the same simulations. The inset shows the curves scaled by the corresponding values at $\sigma(\varepsilon_0) = 0.005\%$.

curves averaged for each precipitate strength in Fig. 3.2b. As one would expect, the stronger the precipitates, the larger the required stress to reach any amount of plastic strain. If, for instance, we define a strain $\varepsilon_0 = 0.005\%$, every increase of $A$ increases also $\sigma(\varepsilon_0)$. Additionally, the divergence of the mean avalanche size changes the shape of stress-strain curve. When scaling the curves by $\sigma(\varepsilon_0)$ in the inset of the figure, the curve becomes more flattened for $\varepsilon > \varepsilon_0$ with intermediate (and strong precipitates that share the shape up to the point of attained strain), while with weak or no precipitates it continues its sharper increase.

To same extent, the stress-resolved avalanche size distributions $P(s)$ of Fig. 3.3a imply a depinning-like transition with intermediate precipitates. There the distributions are again fitted with the power-law with exponential cutoff, Eq. (1.9). Unlike with weak precipitates, intermediate precipitates produce a diverging cutoff of the distributions. As shown in Fig. 3.3b, this yields the collapsing curves when scaling $P(s)$ with $\tau_s$ of the distribution and $s$ with $1/s_0$. The inset shows the diverging cutoff $s_0 \propto (\sigma_c - \sigma)^{-1/\Sigma}$, where the fit gives $\Sigma = 2.6$. Notably neither of the fitted exponents obtained here (nor other exponents explored in
Figure 3.3. (a) Stress-resolved avalanche size distributions from the simulations with weak and intermediate precipitates. (b) The data collapse for the distributions with intermediate precipitates. The inset shows the divergence of the distribution cutoff $s_0$.

Publications III) comply with the ones of mean-field depinning (which states e.g. $\tau_{s}^{MFD} = 3/2$ and $\Sigma^{MFD} = 2$).

### 3.1.2 Critical relaxation and stress in creep simulations

In the constant loading, creep-like simulations, the critical stress was deduced by first performing 19 simulations for each combination of control parameters ($A$, $\rho_p$, and $\sigma$) and averaging the obtained relaxation curves $\dot{\varepsilon}$ vs $t$. Then we chose the $\sigma_c'$ as the stress that produced approximate power-law relaxation.

In our simulations, the magnitude of disorder changed both the stress of critical relaxation $\sigma_c'$ and the exponent of power-law relaxation. The latter is seen in Fig. 3.4a. There the averaged critical relaxation is plotted for systems of fixed $\rho_p = 1 \times 10^{20} \text{m}^{-3}$ and increasing precipitate strength $A$ (main figure) and the exponent $\theta$ of the power-law as the function of $\rho_p$ for fixed $A = 1 \times 10^{10} \text{Pa}$ (inset).

By adjusting both control parameters $A$ and $\rho_p$, the effect on the power-
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Figure 3.4. (a) Average relaxation curves scaled with $\sigma_c'$ for systems with varying precipitate strength $A$ and fixed $\rho_p$. The inset shows how the power-law exponent depends on $\rho_p$ with fixed $A = 1 \times 10^{10}$ Pa. (b) The increase in dislocation density from the start of constant stress loading with $\sigma = \sigma_c'$ for different $\rho_p$ and fixed $A$. The inset shows the time scale $t_s$ of positive $\rho - \rho_0$ with the characteristic obstacle length divided by the loading, $\langle d \rangle / \sigma$ as explained in the text.

law exponent is the same. Increasing the precipitate strength from $A = 0$ via intermediate precipitates $A = 1 \times 10^{10}$ Pa to strong precipitates $A = 5 \times 10^{10}$ Pa increases the exponent from $\theta = 0.29$ via $\theta = 0.35$ to $\theta = 0.75$, respectively. Similarly seen in the inset with varying $\theta(\rho_p)$ and fixed $A = 1 \times 10^{10}$ Pa, the exponent is approximately constant $\theta \approx 0.3$ with small $\rho_p$, until it starts to increase after $\rho_p^0 \approx 5 \times 10^{19}$ m$^{-3}$. Notable here is that the depinning-like system with intermediate precipitate strength and $\rho_p = 1 \times 10^{20}$ m$^{-3}$ ($A = 1 \times 10^{10}$ Pa in Fig. 3.2) belongs to the regime of faster relaxation. Thus, with the depinning-dominated dynamics, $\theta$ increases and the power-law relaxation becomes more rapid.

The dependence of $\theta$ on $\rho_p$ demonstrated the transition in the dominant dynamics: After a certain density $\rho_p^0$, the relaxation becomes more rapid as the added disorder overcomes the dislocation-dislocation interaction. This can be also observed in the evolution of the dislocation density $\rho$. Generally, when a dislocation encounters any obstacle – precipitate or other dislocation – it pins
and starts to bend leading to increase in $\rho$. Fig. 3.4b shows the evolution of dislocation density during our creep simulations, $\rho - \rho_0$ where $\rho_0$ is the (system dependent) dislocation density in the initial state after relaxation. Clearly the systems with larger precipitate densities (and increased $\theta$) exhibit instant and more significant increase in dislocation density.

The time when the dislocation density starts to increase (positive $\rho - \rho_0$) gives a time scale $t_+$ for each $\rho_p$. In the inset of Fig. 3.4b this time scale is shown to be linearly correlated with another time scale $\langle d \rangle / \sigma$, obtained from the characteristic obstacle-obstacle distance $\langle d \rangle$ divided by the ‘dislocation velocity’ which is here taken to be proportional to the driving stress. Both precipitates and dislocation are considered as obstacles, yielding

$$\langle d \rangle = \left( d_p^{-3} + d_d^{-3} \right)^{-1/3},$$  \hspace{1cm} (3.2)

where $d_p = \rho_p^{-1/3}$ and $d_d = \rho_0^{-1/2}$.

Finally, Fig. 3.5 shows $\sigma_c'$ or the ‘yield stress’ as a function of the precipitate density $\rho_p$. For the systems exhibiting depinning, i.e. $\rho_p = 1 \times 10^{20} \text{m}^{-3}$, the obtained $\sigma_c' \approx 4.5 \times 10^7 \text{Pa}$ is same as the fitted value in Fig. 3.2. As the figure shows, $\sigma_c'$ follows closely the Bacon-Kocks-Scattergood (BKS) equation for the strengthening of a dislocation driven in a field of randomly distributed obstacles \[79\]

$$\sigma_{c'}(\rho_p) = \sigma_{c'}^{\text{pure}} + \frac{Gb}{2\pi \alpha} \left[ \ln \left( \frac{(2r_p \rho_p)^{-1/2}}{r_{\text{core}}} \right) \right]^{-\frac{1}{2}} \left[ \ln \left( \frac{D}{r_{\text{core}}} \right) + 0.7 \right]^{\frac{3}{2}},$$  \hspace{1cm} (3.3)

where $\sigma_{c'}^{\text{pure}}$ is the critical stress of a system with $\rho_p = 0$, $\alpha$ is the Schmid factor, $r_{\text{core}}$ the dislocation core radius and $D = \frac{2r_p(2r_p \rho_p)^{-1/2}}{2r_p + (2r_p \rho_p)^{-1/2}}$. Notable in using the BKS equation here is that $(2r_p \rho_p)^{-1/2}$ is the inter-obstacle distance in the glide plane as explained in the inset of Fig. 3.5, and the proper value can vary with the used precipitate strength [80]. On the other hand with large $\rho_p$ in the depinning regime, there could be also power-law dependence $\sigma_{c'} \propto \rho_p^{0.5}$ and no clear evidence of superiority between the power-law and BKS can be seen in the data.
Figure 3.5. The dependence of $\sigma_{c'}$ on the precipitate density with fixed strength $A = 1 \times 10^{10}$ Pa. The dotted line shows $\sigma_{c'}^\text{pure}$ of pure systems, the dashed line the BKS equation, Eq. (3.3), and the solid line the square root evolution $\sigma_{c'} \propto \rho_p^{0.5}$. The inset shows a schematic of the precipitates considered as obstacles for glide in the plane marked by the dotted line for dislocation $\perp$. Here, the coloured precipitates in the darker shaded sector are included.
3.2 Machine learning the transition from dislocation jamming to pinning

In the previous section, systematic tuning of the disorder produced a transition from one type of dynamics to another. In constant stress simulations, the transition manifested as a quickened critical relaxation and larger exponent $\theta$ for systems with disorder-dominated dynamics. This is illustrated also in Fig. 3.6 where the power-law relaxation with $\sigma_c'(\rho_p)$ is plotted for systems of varying precipitate density.

Clearly, there exists a critical precipitate density $\rho_p^c$ that separates the response to constant loading to those of $\theta \approx 0.3$ and increasing $\theta$ with shorter transient time before the start of the power-law relaxation. Thus, $\theta$ is an order parameter describing the dynamics of the system. As the dynamics change from dislocation-dislocation dominated jamming to dislocation-obstacle dominated depinning, the question of structural differences remains: how is the change in dominating interaction reflected on the dislocation structure and its evolution? To address this, we studied the transition in the constant loading simulations with the unsupervised confusion algorithm which was discussed in Section 1.4 [66].

3.2.1 Descriptors of dislocation structure

The first step in applying the confusion scheme was same as in Publication I: how to characterise the dislocation structures as a feature vector. Here, as the dislocation structures were 3D, it enabled the use of dislocations’ line properties.

One way to look at the dislocation structure is the distribution of dislocation junctions, i.e. segments that connect intersection nodes of more than two ending segments. These junctions have an important effect on strain hardening of
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Moreover with larger amount of objects as pinning points for dislocations, the segments connecting the dislocation junctions can start to increase in length as the dislocation expands at the non-pinned parts. Therefore, we defined a measure $J$ of ‘junction length difference’ between the segments connecting the intersection nodes $l_{\text{along}}$ and the shortest possible length between the nodes $l_{\text{shortest}}$,

$$J = l_{\text{along}} - l_{\text{shortest}},$$

(3.4)

and used the collected distribution of values of $J$ from a system as one characterisation of the microstructure.

Another approach was to re-use the idea of GND density that worked well in the 2D DDD stress response prediction. In 3D, the GND density $\rho_{\text{GND}}$ is calculated from the Nye tensor $\alpha$, which is defined by [81, 71, 53]

$$\alpha = \frac{1}{V_{\text{voxel}}} \sum_i b_i \otimes \xi'_i,$$

(3.5)

where $V_{\text{voxel}}$ is the volume of the volume element (or voxel) for which $\rho_{\text{GND}}$ is computed, the sum is taken over all dislocation segments inside the voxel and $\xi'$ is the line direction vector with length equal to the segment length. Then $\rho_{\text{GND}} = ||\alpha||$. To assess the evolution in the dislocation structure, we computed the change in GND density, namely $\Delta \rho_{\text{GND}} = \rho_{\text{GND}}(t) - \rho_{\text{GND}}(0)$ and, to reduce effect of periodic boundaries, used Fourier transform of $\Delta \rho_{\text{GND}}$ as one descriptor.

As a third approach, we extracted the dislocation spacing correlation by [82]

$$C(r) = \left( \frac{d}{dr} L'(r) \right) / \left(4\pi r^2 \rho \right),$$

(3.6)

where $L'(r)$ is the average sum of dislocation length inside a sphere centered at dislocation core and radius $r$. Fig. 3.7 summarises the used descriptors. For every simulated system, three distinct feature vectors (one corresponding to each descriptor) were compiled by collecting the system structure at up to 30 time steps separated by $1 \times 10^{-9} \text{s} = 2.6 \times 10^5 \text{GM}$ where the latter unit of shear modulus $G$ multiplied by the dislocation mobility $M$ was defined to represent time. We then used the feature vectors to first extract few of their top principal components that were then passed to a simple classifier based on linear discriminant analysis [48] with 2-fold cross-validation, according to the confusion scheme.

3.2.2 Critical precipitate density and descriptor properties

The confusion curves, i.e. the classification score according to trial values $\rho_p^*$, for each descriptor are presented in Fig. 3.8 along with the exponent of power-law relaxation $\theta$. All three curves exhibit the expected $W$-shape, with a distinct maximum of $S > 0.95$ at the same $\rho_p$ value. More importantly, the maximum
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Figure 3.7. (a) Histogram of $J$ in single systems at time $t = 1 \times 10^{-9}$ s. The left-most bin includes all the values down to $J = 0$. (b) A single system $\rho_{GND}$ at $t = 1 \times 10^{-9}$ s with $10^3$ voxels. (c) Dislocation spacing correlation functions computed for single systems at time $t = 1 \times 10^{-9}$ s according to Eq. (3.6).
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is positioned at approximately same $\rho_c \approx 3 \times 10^{19} \text{m}^{-3}$ where the dynamics change to faster power-law relaxation and increasing $\theta$. Therefore, the confusion algorithm is indeed capable of finding the critical point of the transition from jamming to depinning with any of the used descriptors.

![Confusion curves for each of the used descriptor set resulting from 2-fold cross validation. The number of principal components was five for junctions and GND density (computed in 253 voxels), and ten for correlation. The number of components was chosen by taking the confusion curve that had the highest maximum excluding the ending points of the $\rho_p$ range. (b) The exponent of power-law relaxation with $\sigma_c(\rho_p)$.]

The success of all three descriptors reveals that the dislocation structures differ in the jamming and depinning phases on both short and long length-scales. From the used features, especially spacing correlation considers the long-range structures as it is computed up to $\sim 1\mu$m. The change in GND density, e.g. with the $25^3$ computational voxels, is more short-range with voxel size $\sim 0.1\mu$m. To highlight the indifference of learned transition on the length scale of the characterized dislocation structures, Fig. 3.9 depicts the confusion curves obtained by varying the voxels from $50^3$ to $4^3$ when computing the GND density. Regardless of the number of voxels, the transition is established and the discovered critical density is identical with any voxelisation.

Finally to obtain view on how the structures and their distinguishability
evolves during the loading, we performed the confusion learning on single
snapshot image data instead. Fig. 3.10 presents the distinct W-curves for the
30 time steps for each of the three descriptors. First in Fig. 3.10a, the junction
lengthening of single snapshot dislocation structure appears to capture the
transition after only short time and the curves quickly converge to the shape
seen in Fig. 3.8.

Conversely with change in GND density with $25^3$ voxels (Fig. 3.10b), first
time steps show the same observed transition but the maximum of $W$-curve
weakens fast and the curve is closer to $V$-shape. Of course here the GND density
difference was calculated with respect to the initial state of the system and,
because the $25^3$ voxels represents short-range structures, the information gets
lost at longer times. Moreover, neither the raw GND density (without removing
the initial state) nor subsequent time step change did show the transition at all.

The single snapshot spacing correlation (Fig. 3.10c) has similar evolution as
junction lengthening where the confusion curve converges to same $W$-shape
after a transit period (although longer than with junction lengthening). Notable
here is that the right-hand notch of the confusion curve is quite flat. That is,
the spacing correlation for systems with any $\rho_p$ in the depinning phase shows
distinct features which is not too surprising as after all there the relaxation
becomes more and more rapid with increasing $\rho_p$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Figure3.9.png}
\caption{Confusion curves obtained with GND density computed in varying number of voxels.
}\label{fig:3.9}
\end{figure}
Figure 3.10. Confusion curves for single snapshot dislocation structure characterized by (a) junction lengthening, (b) change in GND density and (c) spacing correlation. The confusion algorithm was run with top two principal components of each descriptor. The number of simulated systems (i.e. data points) starts to decrease after $t = 4.7 \times 10^6$ GM as some of the systems ran out of their allocated computing time.
4. Conclusions

This dissertation focused on two themes of crystal plasticity: Dislocation avalanches that produce stochastic-like accumulation of plastic strain. And the competition between dislocation-dislocation and dislocation-disorder interactions in crystals with added obstacles. These were studied with extensive DDD simulations and machine learning methods.

The results presented in Chapter 2 revealed the interplay between dislocation system predictability and the avalanches they exhibit. In Publication I, we used neural networks to predict the avalanche-dominated stress response of 2D DDD systems using the systems’ initial dislocation structure as input. The predictability showed a non-monotonic strain-dependence meaning parts of the stress-strain curve with intermediate strains were harder to predict than the ultimate large strain behaviour. Although the general shape of the ensuing stress-strain curves was reproduced by the neural networks, single avalanches were not.

The observed non-monotonic predictability was then further studied in Publication II. There we analysed avalanches from both 2D and 3D DDD simulations that exhibited correlations with small strains that pushed the single system stress response towards the ensemble average. So at small to intermediate strains the stress-response oscillates around the average and is, therefore, harder to predict than the eventual large strain ‘yield stress’ where the single systems have fixed their position with respect to the average curve.

Natural direction to continue the work on predicting the plastic deformation would be to move from the simple 2D DDD model to more realistic and complex systems such as the 3D DDD simulations. In view of the discovered avalanche correlations, that shared similarities in 2D and 3D, 3D systems could possess some predictability at large strains because the systems’ large strain response ceases to oscillate around the average response like in 2D. In 2D, the predictability benefited from the conserved dislocation density perpendicular to the single-slip direction but correspondingly 3D systems can retain some structures on inactive slip-systems too. However with 3D DDD, the challenge is to build a feasible data set: a thorough description of dislocations in 3D can
require more parameters than in 2D which complicates the machine learning process and increases the amount of needed data points. This leads to problems with computational cost as 3D simulations require significantly more resources.

Although the 2D and 3D DDD simulations were conducted in more bulk-like setting with the periodic boundary conditions, extending the study to micropillars is another intriguing direction. Imaging techniques such as electron backscatter diffraction enable extraction of dislocation structures at least on the surface of the samples, so mapping these structures before loading to the mechanical response would be a direct generalization of the results described here. But again, the required amount of experiments to accomplish sensible predictions can be overwhelming. In any case, it would also be interesting to analyse avalanches from some micropillar compression experiment to study if the discovered avalanche correlations exist in real crystals too.

Chapter 3 focused on simulations of 3D DDD with coherent precipitates. In Publication III, we observed the transition from dislocation-dislocation dominated jamming to dislocation-disorder dominated depinning-like phase by systematically changing both the precipitate strength and density. The transition was evident through diverging avalanche sizes emerging with quasistatic loading and accelerated power-law relaxation during constant stress loading. The results on systems in the depinning regime were consistent with respect to the critical stress encountered in the diverging avalanche size and the stress leading to critical relaxation with constant loading. The critical stress also followed closely the Bacon-Kocks-Scattergood equation with varying precipitate density.

Then in Publication IV, we further studied the transition encountered in constant loading simulations. We passed characterisations of the evolving systems with varying precipitate densities to an unsupervised machine learning algorithm. The algorithm was able to distinguish two phases of dislocation structures that were separated at a critical density that was close to the point of change in the relaxation dynamics. Moreover, the transition was captured by both short- and long-range descriptors of the microstructure.

The future prospects of the study of jamming-depinning transition are similar as with the stress response predictability: Any type of experimental investigation would be interesting to see. There of course exist challenges with the systematic control of disorder and, again, collection of sufficient statistics. Additionally, the question of universality class of dislocation-disorder dominated systems remains: the overall behaviour with the critical stress $\sigma_c$ encountered here shared a lot of similarities with the depinning theory, but the critical exponents differed from the mean-field depinning values.

Finally, the findings of the dissertation can be concluded with two more general remarks. Firstly, machine learning enabled here an alternative way of focusing on the plastic deformation and yielding of single dislocation systems instead of ensemble statistics. Extending its use from simulated to physical systems is restricted mostly by the bottleneck of obtaining valid experimental data and, once
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that is overcome, machine learning could be used to help metallurgical materials
design and even some production chains of e.g. micron-scale components. And
secondly, the results here highlighted one of the fundamental questions on the
interface of computational statistical physics and materials science: how do the
observed statistical aspects of avalanches, including the changing criticality with
disorder and subsequent avalanche correlations, manifest in physical systems?


References


References


