Laurson and Alava
Journal of Materials Science: Materials Theory (2024) 8:10
https://doi.org/10.1186/s41313-024-00064-8

Journal of Materials Science: Materials Theory

REVIEW

Open Access

Dislocation-precipitate interactions in crystals: from the BKS model to collective dislocation dynamics

Lasse Laurson[1*] and Mikko J. Alava[2,3]

*Correspondence: lasse.laurson@tuni.fi

[1] Computational Physics Laboratory, Tampere University, P.O. Box 692, FI-33101 Tampere, Finland
[2] Aalto University, Department of Applied Physics, PO Box 11000, 00076 Aalto Espoo, Finland
[3] NOMATEN Centre of Excellence, National Centre for Nuclear Research, A. Soltana 7, 05-400 Otwock-Swierk, Poland

Abstract

The increase in the yield stress due to the presence of obstacles to dislocation motion such as precipitates is a multiscale phenomenon. The details on the nanoscale when an individual dislocation runs into a precipitate play an important role in determining plasticity on a macroscopic scale. The classical analysis of this phenomenon is due to Bacon, Kocks and Scattergood (BKS) from early 1970's and has been followed by a large body of work both developing the theory and applying it to real experiments and their understanding. Beyond the microscopic details the next level of complexity is met in the micrometer scale when the physics of the yielding and the yield stress depend on two mechanisms: the dislocation-precipitate interaction, and the collective dynamics of the whole ensemble of dislocations in the volume. In this review we discuss the BKS relation and collective dislocation dynamics in precipitation-hardened crystals in the light of recent research, including large-scale discrete dislocation dynamics simulations, statistical physics ideas, and machine learning developments.

Keywords: Precipitation hardening, Dislocation dynamics

Introduction

On the occasion of Professor Nasr Ghoniem's retirement, it is appropriate to remind ourselves of what we have learned about his research field – the mechanics and physics of defects in crystals – during the last couple of decades. One key problem where Prof. Ghoniem has made important contributions is that of dislocations in crystals interacting with precipitates (Takahashi and Ghoniem 2008). Precipitate strengthening is an important mechanism allowing one to design alloys with desirable strength characteristics. It is based on the second phase precipitates in the alloy's matrix acting as obstacles for dislocation motion, resulting in significant increases in the yield strength and hardness of the alloy.

Here, we'll present our viewpoint, in the form of a short review, of recent developments and current trends in this field. We focus especially on the theory and development of multiscale computational methods for plasticity of alloys with precipitates, as well as on what the resulting multiscale models tell us about the complex nature of plasticity in precipitation-hardened crystals on a larger scale. More specifically, on the one hand we discuss “microscopic” theories such as the Bacon-Kocks-Scattergood (BKS) relation (Bacon et al. 1973) and its various extensions connecting the obstacle hardening to the yield stress, along with numerical tests of these theories, e.g., by means of molecular dynamics (MD) simulations in the case of small, nanoscale precipitates. Typically such studies consider a single dislocation line driven by an applied stress through a regular array of precipitates; in MD simulations this is equivalent to considering a dislocation interacting with a single precipitate with periodic boundary conditions. An important aspect here is the influence of the lattice type. As is well-known on the atomistic scale Face-Centered Cubic (FCC) and Body-Centered Cubic systems have very different features. In the FCC case the dislocation splits into two partials and in the BCC one the most important mechanism is thermally activated kink propagation.

In general, one can distinguish two well-known mechanisms via which a dislocation may overcome a precipitate if the former is driven with a large enough stress, i.e., a stress exceeding the critical resolved shear stress (CRSS): Either the dislocation cuts through the precipitate by shearing it by a shearing stress τ_p due to the formation of an antiphase boundary, or it overcomes the precipitate via the Orowan looping mechanism. In addition to this, the physical properties of the precipitate compared to the matrix are important (Hu and Curtin 2022, 2021). This includes two effects, elastic misfit for coherent precipitates and the mismatch of the elastic constants as discussed below. Finally the precipitate is changed by shearing and an atomic surface step is formed. In what follows, we concentrate on spherical precipitates, as they are the most evident test case for the BKS idea. However, there is spectrum of other cases, where the precipitates are needle or plate-shaped (Zhang and Sills 2023) or even cubic (Ni-based superalloys). In these cases the basic Orowan bow-out mechanism may fundamentally change simply due to the geometry of the dislocation-precipitate interaction, and many of the ideas we present below for the case of many dislocations interacting among themselves and a precipitate field might need to be reconsidered.

On the other hand, on a larger scale a large number of dislocations interact not only with the randomly positioned precipitates but also with each other via their long-range stress fields (the effect of the latter, with the exception of dislocation self-interactions, is typically neglected in the BKS type theories). These interactions result in intriguing collective dynamics of dislocations manifested as critical-like features such as power-law distributed strain bursts, better captured by larger-scale models such as discrete dislocation dynamics (DDD) simulations; we note that Prof. Ghoniem has played a central role in the introduction and development of the DDD method (Amodeo and Ghoniem 1990a, b; Ghoniem et al. 2000). The DDD codes take all into account the microscopic detail (FCC or BCC symmetry or some other, and the resulting character of dislocation junctions, interactions, and climb). Then, related to such collective effects, we highlight recent DDD simulations including precipitates (which may use parameters obtained from MD in the spirit of multi-scale modelling (Lehtinen et al. 2016)), and how these simulations have revealed the manner in which the nature of this critical-like, intermittent deformation process is controlled by the presence or absence of static, or quenched, obstacles to dislocation motion (Salmenjoki et al. 2020): The competing effects of dislocation-precipitate and dislocation-dislocation interactions result in collective dislocation dynamics governed by either pinning of dislocations by the precipitates or by dislocation jamming, respectively (Ovaska et al. 2015).

Finally, we also briefly highlight recent machine learning (ML) approaches relevant for such issues, including, e.g., a confusion algorithm shown to be able to distinguish the systems into two separate phases where dislocation dynamics is governed by pinning and jamming, respectively (Salmenjoki et al. 2020.) We discuss also the prospects of applying related techniques such as Bayesian optimization to automatically design alloys with desirable mechanical properties (Sarvilahti and Laurson 2022).

Collective dislocation dynamics in precipitation hardened crystals

One should note that the BKS theories (to be discussed in more detail later) are essentially single-dislocation descriptions. Real plastically deforming crystals, however, always include a large number of dislocations interacting not only with the precipitates but also with each other. The usual approach employed in the materials science literature to account for this is to employ various rules of mixture to combine contributions from different hardening mechanisms, such as precipitate hardening and strain hardening due to dislocation-dislocation interactions (Queyreau et al. 2010; Monnet et al. 2011). While such approaches tend to be successful in accounting for the resulting material strength, the employed rules of mixture are by nature somewhat phenomenological, and do not necessarily imply much physical insight as to how the different strengthening mechanisms might be related. This raises the question if there are effects of interest related to collective dislocation dynamics that arise due to a large number of dislocations interacting with the time-independent (quenched) pinning field due to a random distribution of precipitates within the matrix? Indeed, while much of the literature on the effect of precipitates for dislocation dynamics in precipitation hardened crystals has focused on estimating the CRSS and the ensuing yield stress due to adding precipitates into the matrix, typically using single-dislocation descriptions not capturing full complexity due to mutual interactions of a large number of dislocations, recently also other, more subtle effects due to precipitates have been discovered. These are related to the precise nature of critical-like collective dislocation dynamics which gives rise to phenomena such as power-law distributed strain bursts in micron-scale crystals and acoustic emission in larger samples.

Precipitates in 2D DDD

In order to present the main ideas, we start by discussing recent studies of simple, single-slip 2D DDD systems with a quenched pinning field mimicking the effect of precipitates (Ovaska et al. 2015). While such systems treating dislocation lines as point particles (cross sections of straight parallel dislocation lines) are not fully physical especially in the present context as bending of the dislocation lines due to interaction with localized precipitates is not described, these systems nevertheless serve as useful minimal models for the study of the relative importance of dislocation-dislocation and dislocation-precipitate interactions. Concerning the effects of precipitates and other quenched (time-independent) obstacles to dislocation motion on the nature of criticality of dislocation dynamics, the picture emerging from recent works is that of a competition between two mechanisms of dislocation arrest: *jamming* of dislocations due to other dislocations (Ispánovity et al. 2014; Miguel et al. 2002), and *pinning* of dislocations by obstacles such as precipitates (Ovaska et al. 2015). This idea is schematically summarized in Fig. 1a in the case of a simple 2D DDD model with quenched pinning centres, illustrating how the no pinning/weak pinning case is expected to be governed by dislocation jamming, while stronger pinning should lead to a depinning transition of the dislocation assembly interacting with the quenched pinning field created by the obstacles.

In the jamming-dominated regime, the dislocation systems behave similarly to glassy systems in that no clear critical value of the external stress can be identified. Instead, the system in the thermodynamic limit has been argued to be "critical at any stress". This is evident by considering the time-dependence of the strain rate at a fixed external stress which exhibits a power-law decay largely independently of the external stress value (Ispánovity et al. 2011), the exponential increase of the cutoff avalanche size s_0 with the external stress σ_{ext} (Ispánovity et al. 2014) (rather than a power-law divergence at a critical point as in depinning), as well as the observation that power-law distributed dislocation avalanches can be observed even at zero applied stress in response to small localized perturbations (Janićević et al. 2015).

This "glassy" behavior can be contrasted with what happens when the pinning strength is increased from zero such that the dislocation-obstacle interaction becomes comparable in strength to the dislocation-dislocation one. The stronger pinning breaks down the "generic scale invariance" of the pure dislocation system, and results in a transition between pinned and moving phases of the dislocation assembly which exhibits the usual characteristics of depinning phase transitions of elastic manifolds in random media (Ovaska et al. 2015). For example, the relaxation of the strain rate in a dislocation system subject to a constant external stress now depends on the stress value such that a temporal power law decay is observed only at a specific, critical value of the external stress [see Fig. 1b]. Moreover, the strain burst (or "dislocation avalanche") size distributions are power laws terminated at a cutoff, with the cutoff scale s_0 diverging at the critical external stress value as in standard depinning phase transitions, i.e., $s_0 \propto (\sigma_{\mathrm{c}} - \sigma_{\mathrm{ext}})^{1/\sigma}$, where $1/\sigma \approx 1.9$ is a critical exponent [see Fig. 1c and d]. These features - divergent spatial and temporal scales at a σ_{c} with power-law distributions whose cutoffs in accordance also diverge upon approach - are a definition of "true criticality".

The above scaling picture including glassy jamming of pure dislocation systems and depinning criticality for systems with obstacles of "intermediate" strength was first discovered in simple 2D DDD simulations (Ovaska et al. 2015), but has more recently been found also in 3D DDD simulations with flexible dislocation lines interacting with spherical precipitates (see below for more details on 3D DDD with precipitates) (Lehtinen et al. 2016). For the specific case of 2D DDD, it was also demonstrated that even stronger pinning results in a third "phase" of dislocation behavior characterized by the lack of collective, critical dislocation dynamics as the dislocation-obstacle interactions completely dominates over the dislocation-dislocation interactions, resulting in exponentially distributed avalanche size distributions (Ovaska et al. 2015). It remains an open question if this phase exists also in 3D DDD.

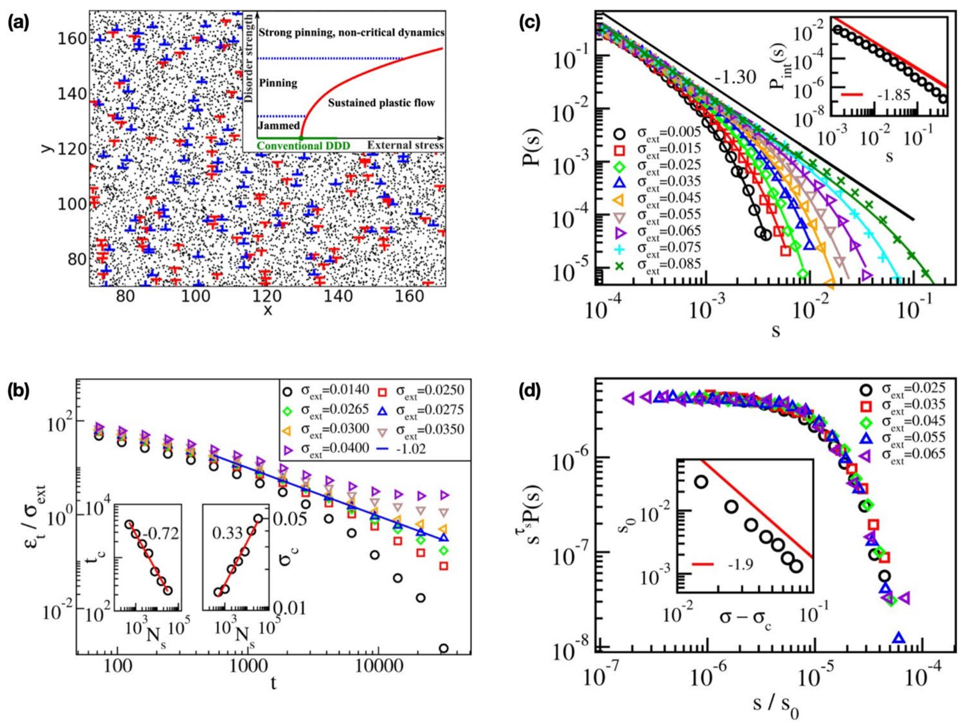

Fig. 1 2D complexity: **a** Dislocations present a phase diagram (inset), and **b** exhibit "true" critical behavior with a critical stress that scales in scale-free way with the precipitate field. The resulting bursts [size distributions shown in (**c**)] can be scaled as in critical phenomena [a data collapse shown in (**d**)]. Figure reproduced from Ovaska et al. (2015)

Precipitates in 3D DDD

In order to get a more realistic picture of effects of precipitates on collective dislocation dynamics, 3D DDD simulations with precipitates included are necessary, including a multiscale modelling step (Kubin 2013; Monnet 2015). Various approaches to include precipitates in 3D DDD have been proposed, of which we here consider our recent model (Lehtinen et al. 2016) where precipitates are modelled by employing a Gaussian potential $U = A\exp[-(r/R)^2]$, generating a normal force acting on the dislocation segments parameterized by the strength A and radius R of the precipitates, see Fig. 2. For a specific alloy/precipitate, these parameters can be fixed via a multiscale handshake of single-dislocation DDD simulations with the corresponding molecular dynamics (MD) simulations, by comparing the CRSS and the manner in which the dislocation bypasses the precipitate in MD and DDD. One should note that this approach leads to an isotropic field, which cannot deal with the size mismatch effect, leading to an anisotropic stress field.

Such a handshake was performed for BCC iron with spherical cementite (Fe_3C) precipitates, of sizes 1 nm, 2 nm, and 4 nm, interacting with an edge dislocation (Lehtinen et al. 2016). Later, this model was applied to study effects of precipitates, together with dislocation loops, on the yield stress of irradiated iron with a large number of interacting dislocations (Lehtinen et al. 2018). As is obvious from snapshots of these simulations (see Fig. 3 for an example), the dislocation line network becomes quite complex, especially after finite strains have been reached.

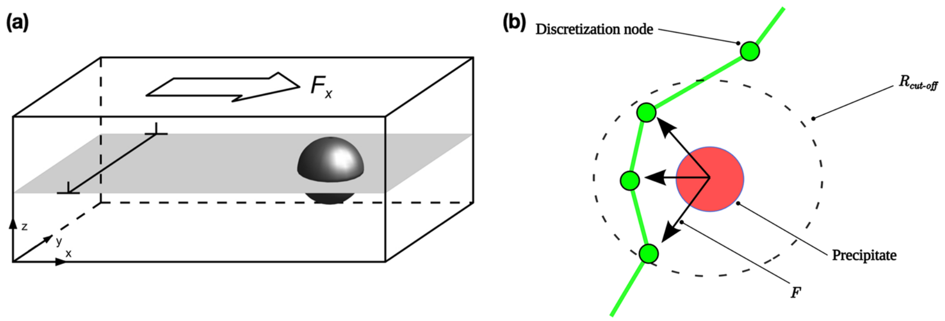

Fig. 2 Multiscale handshake from MD to DDD: **a** In the typical test scenario one runs MD simulations of the dislocation - precipitate collision and works out how the resulting behavior can be parameterized into the DDD simulation. **b** illustrates what this means in terms of the ParaDis code with precipitates. Figure reproduced from Lehtinen et al. (2016)

The Bacon-Kocks-Scattergood relation and beyond

Here we take a different, more microscopic viewpoint to dislocation-precipitate interactions by considering the BKS relation (Bacon et al. 1973), which is an extension of the formula for the classical Orowan stress for a dislocation driven through a regular array of impenetrable spherical obstacles, $\tau_{\mathrm{Orowan}} = Gb/L$, where G is the shear modulus, b the Burgers vector, and L the obstacle spacing. The BKS relation is obtained as an extension of the above formula by considering the effect of mutual self-interactions of bowing dislocation loops around an obstacle with a finite diameter D. Typically one expects such interactions to reduce the CRSS from that given by τ_{Orowan} due to the attraction between opposite dislocation segments bowing around

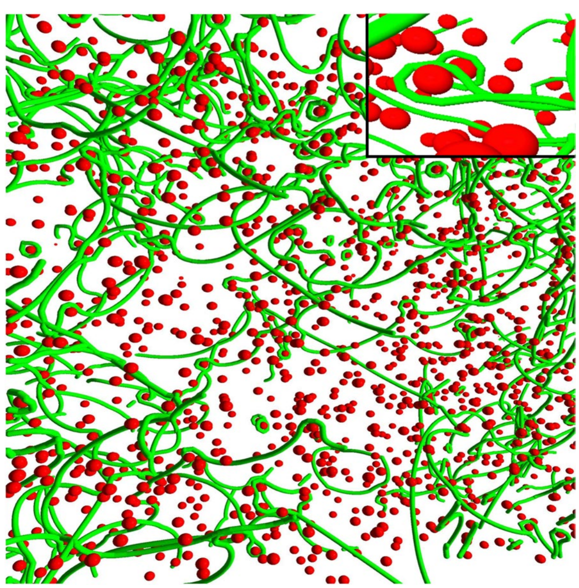

Fig. 3 An example of the dislocation-precipitate system configuration at a finite strain of 0.68 % in BCC Fe. Dislocations (green lines) that have bypassed precipitates (red spheres) have left Orowan loops around some of the obstacles. The inset shows a twisted noose where the edge arms of the loops are on different glide planes and hence cannot annihilate each other. Figure reproduced from Lehtinen et al. (2018)

the precipitate. As a result of the self-interactions, the Orowan stress was argued to be of the form (Bacon et al. 1973)

$$\tau_{\mathrm{BKS}} = \frac{Gb}{L} A \left[\ln \left(\frac{\bar{D}}{b} \right) + B \right], \tag{1}$$

where A is either $1/2\pi$ for an edge dislocation or $1/2\pi(1-\nu)$ for a screw dislocation (ν is the Poisson's ratio), B is a constant of the order 1 (about 0.7 based on fitting the model predictions with DDD simulations), and $\bar{D}$ is the harmonic mean of D and L, i.e., $\bar{D} = (D^{-1} + L^{-1})^{-1}$. Equation (1) has been extended to the case of a random distribution of spherical impenetrable precipitates (Bacon et al. 1973; Santos-Güemes et al. 2022),

$$\tau_{\mathrm{BKS,rand}} = \frac{1}{2\pi\sqrt{1-\nu}} \frac{Gb}{\langle L \rangle} \frac{[\ln(2\bar{D}/b)]^{3/2}}{[\ln(\langle L \rangle/b)]^{1/2}}, \tag{2}$$

with $\langle L \rangle$ the mean inter-precipitate distance and the constant A in Eq. (1) is chosen to represent a mixture of edge and screw dislocations. An expression similar to Eq. (2), with $\langle L \rangle$ within the glide plane estimated from the 3D precipitate number density, was shown to reproduce 3D DDD simulation results with spherical precipitates reasonably well, assuming a linear rule of mixture of the "pure" system yield stress, due to dislocation jamming, and the strengthening effect due to precipitates (Lehtinen et al. 2018). Analogous descriptions of non-spherical (e.g., rod or disc-shaped) impenetrable precipitates have also been proposed (Nie 2003; Nie and Muddle 2008).

The above descriptions are constructed for impenetrable precipitates which the dislocations bypass via the Orowan looping mechanism. Shearable point-like precipitates have been described with the rather obvious idea that there is a finite maximum force that the precipitate can withstand before shearing takes place, which should be related to a critical angle θ_c between the two dislocation "arms" around the precipitate. Employing such ideas, Friedel (1964) derived an expression of the form

$$\tau_{Friedel} = \frac{Gb}{\langle L \rangle} \frac{\ln(\langle L \rangle/b)}{2\pi}, \tag{3}$$

which was argued to be valid for a random distribution of weak point-like precipitates. Effects due to shearable precipitates of a finite size have been modelled, e.g., via the introduction of a friction stress acting on the dislocations inside the precipitate (Monnet 2018), as well as via a simple Gaussian potential modelling the dislocation-precipitate interaction (Lehtinen et al. 2016).

More recently, a "generalized" line tension model including the effect of the elastic mismatch between the matrix and the precipitates has been proposed (Santos-Güemes et al. 2022). Precipitates that are either stiffer or more compliant than the matrix were studied, and both shearable and impenetrable precipitates were considered (hence the generalized nature of the resulting line tension model). In particular, formulae were derived to describe the experimentally relevant case of strengthening due to random precipitate distributions. In the case of impenetrable precipitates, the starting point is the BKS equation, Eq. (2), which was modified by employing averaged geometrical descriptors to read

$$\tau_{\text{BKS,rand}} = \frac{1}{2\pi\sqrt{1-\nu}} \frac{Gb}{\langle L_{\text{eff}} \rangle} \frac{[\ln(2\overline{\langle D \rangle}/b)]^{3/2}}{[\ln(\langle L_{\text{eff}} \rangle/b)]^{1/2}}, \tag{4}$$

where the average effective distance is given by $\langle L_{\text{eff}} \rangle = \langle L \rangle (1 - \alpha \langle D \rangle / \langle L \rangle)$, and $\overline{\langle D \rangle} = (\langle D \rangle^{-1} + \langle L \rangle^{-1})^{-1}$ is the harmonic average of the mean planar diameter $\langle D \rangle = \pi D/4$ and the average inter-precipitate distance $\langle L \rangle = \langle L_{\text{ctc}} \rangle - \langle D \rangle$, where the average center-to-center distance between precipitates is $\langle L_{\text{ctc}} \rangle = D/2\sqrt{2\pi/3f}$, with f the precipitate volume fraction.

The shearable precipitate case requires a different treatment, and the outcome depends on details such as the elastic mismatch $\Delta G = G^P - G^M$, where G^M and G^P are the shear moduli of the matrix and the precipitate, respectively, and on the friction stress τ_p. The resulting CRSS $\tau_{\text{sh,rand}}$ reads

$$\tau_{\text{sh,rand}} = K_1 |\Delta G| \left(\frac{\langle D \rangle}{\langle L_{\text{ctc}} \rangle} \right)^{K_2} + \left(\frac{\langle G^M \rangle}{\langle G^P \rangle} \right)^{K_3} \tau_p \frac{\langle D \rangle}{\langle L_{\text{ctc}} \rangle}, \tag{5}$$

where K_i are constants that depend on the dislocation character and on whether the precipitate is stiffer or more compliant than the matrix (Santos-Güemes et al. 2022). Equation (5) can also be expressed in terms of the precipitate volume fraction f instead of $\langle D \rangle / \langle L_{\text{ctc}} \rangle$. Equations (4) and (5) were validated via DDD simulations including a random distribution of 12 spherical precipitates with very good results, even if the formula for impenetrable precipitates, Eq. (4), overestimates slightly the DDD results for screw dislocations. It was also found that in agreement with the model predictions, for a fixed f and τ_p the CRSS is (within error bars) independent of the precipitate diameter D for shearable precipitates, while it decreases with increasing D for impenetrable precipitates (Santos-Güemes et al. 2022).

BKS in the light of DDD studies

Next we look at attempts to use the BKS theory in more practical cases. Figure 4 shows this in two cases, where multi-dislocation DDD simulations with spherical precipitates included are considered. For Fe (BCC) and two different precipitate sizes the density of precipitates is varied (Lehtinen et al. 2018). Thus the typical precipitate distance changes, and the data allows reasonable BKS-style fits. The Al (FCC) case is more interesting. The question here is a more accurate one, since from other simulations for the same system we know that the yielding is characterized by two regimes: one where dislocation-dislocation interactions dominate, so that the precipitates are a perturbation, and one where dislocation-precipitates interactions rule (Salmenjoki et al. 2020). Even though there is a transition at some precipitate density (Ovaska et al. 2015) nevertheless a BKS fit may be applied. The inset of the figure demonstrates that there is an effective renormalization of the scales: how close the dislocations are to precipitates is a self-organized process. It can be fit from the simulations. Notice that in the systems with multiple interacting dislocation considered here, the fits also include the pure system yield stress as a constant, an addition to the single-dislocation BKS formula.

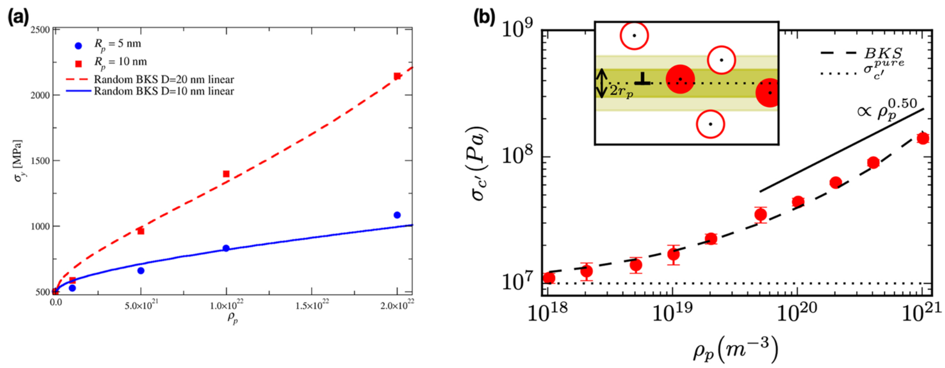

Fig. 4 Two examples of how the BKS relation can be used to fit DDD data. **a** The case of a BCC metal (Fe, figure reproduced from Lehtinen et al. (2018)). **b** FCC (Al, figure reproduced from Salmenjoki et al. (2020)). The inset of (**b**) illustrates how it is crucial how the dislocations (here, edge dislocations) explore their neighborhood and that the true precipitate-dislocation interaction shall depend on the strength of the microscopic repulsion, but also on the geometry including the presence of other dislocations

We finally point out how the BKS theory can be used for "material design". One can either lean on the theory itself and by using precipitate-related parameters such as the precipitate elastic modulus (G^P) and shearability (τ^P) consider the impact of the precipitates on strengthening (Santos-Güemes et al. 2022). As in Fig. 4, we see here in Fig. 5a and b that quite large improvements are possible within the necessary assumptions and that they depend on the precipitate properties. In particular the prediction is that in general the yield stress is improved, and that more tough precipitates (measured by τ^P) lead to a bigger increase. Figure 5c shows a (non-linear, actually) relation of the yield stress to the precipitate volume (applying the results of Lehtinen et al. (2018)) for 10 nm size precipitates.

Collective phenomena in 3D DDD with precipitates

Now that we have discussed the 3D DDD method with precipitates, it is time to examine to what extent the picture of collective dislocation dynamics emerging from the competition between dislocation jamming and pinning due to precipitates, outlined above for the 2D DDD case, is applicable in 3D DDD. To this end, we'll discuss the recent 3D

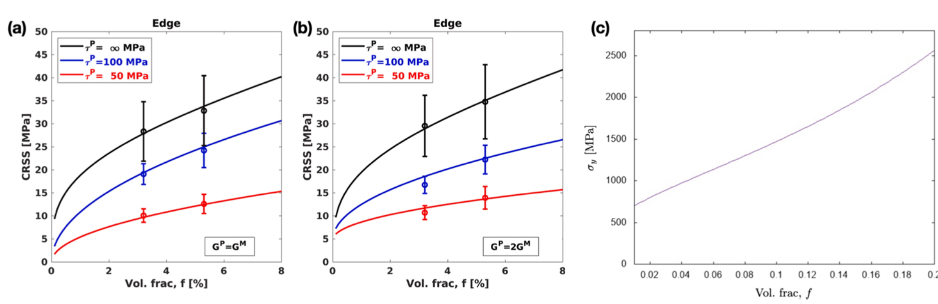

Fig. 5 **a** and **b** The BKS relation (Santos-Güemes et al. 2022) and assumptions about how random precipitate geometries influence the yield stress results in concrete predictions about the yield stress. **c** Likewise, the DDD results can be parameterized to show how "to design materials" by controlling the precipitate volume fraction in the system

DDD simulation study with precipitates included (Salmenjoki et al. 2020), and compare the findings with earlier simulations of a similar system where precipitates were absent (Lehtinen et al. 2016). First of all, we note again that from the 2D modelling (Ovaska et al. 2015) we know that it is expected that there are two phases as long as the dislocations interact: the no/low disorder phase where as above noted the precipitates act essentially as a perturbation. In this case, the avalanche picture may be called "extended criticality": the burst size distributions appear scale-free from zero stress on, but no critical point (in stress/strain) exists such that the cut-off would diverge there. We note that the above-mentioned papers consider the avalanche-like response of the dislocation systems to quasistatically increasing external stress, and that imposing a high enough deformation rate has been shown to result in an intermittent-to-smooth transition (Sparks et al. 2019). Also, the 3D DDD simulations discussed below are performed for fcc crystals; on the other hand, for bcc Nb, the long-range and scale-free dynamics at room temperature has recently been shown to get progressively quenched out with decreasing temperature (Rizzardi et al. 2022), highlighting the temperature-dependent nature of bcc plasticity. Moreover, the simulations reported below consider the rather minimal description of the precipitates via the Gaussian potential, such that, e.g., the elastic stress fields of the precipitates which could be computed from Eshelby's inclusion theory are not included (Ringdalen et al. 2017).

Figure 6a from Ref. (Salmenjoki et al. 2020) illustrates the difference between these phases. DDD simulations of creep relaxation indicate that precipitate pinning accelerates the decay of the creep rate and in particular, that the power-law ("primary creep") exponent depends on the parameters. In the weak disorder phase, it is close to 0.3, but above a threshold (e.g., in precipitate density) starts to increase. Likewise [Fig. 6b] these effects are accompanied by an increase in dislocation density, and the forest hardening this implies creates an internal degree of freedom, that must be at least partly the cause for the varying exponent. We have also addressed the problem as to whether the two phases can be identified already in the relaxed dislocation structures at zero stress (Salmenjoki et al. 2020). It turns out that dislocation configurations are correlated with the precipitate density (or the strength of interaction with those) and these correlations match with the resulting response, that is creep behavior.

Figure 6c and d show finally, that for a high enough density of strong enough precipitates the yield stress is in fact a critical point. The usual picture of a data collapse of the distributions $P(s, \sigma)$ as a function to the critical stress σ_c as at a depinning transition works well. The avalanche size exponent that results here (for two cases only) is about 1.25-1.3. To complete the picture, the σ_c value found by these simulations of stress-strain curves by a quasi-static ramp agrees well with what can be determined by creep studies, where a pure power-law response emerges at the critical point (whereas below that there is a transition to exponential decay, and above the system reaches a state of constant flow). When looking at correlations between subsequent events along the stress-strain curve, the presence of precipitates has been shown to lead to another signature of a depinning phase transition: the correlations between subsequent avalanches tend to push the stress-strain curves towards the average curve at large strains (i.e., close to $\sigma = \sigma_c$), while for "pure" samples such correlations were observed in the small strain region (Salmenjoki et al. 2021).

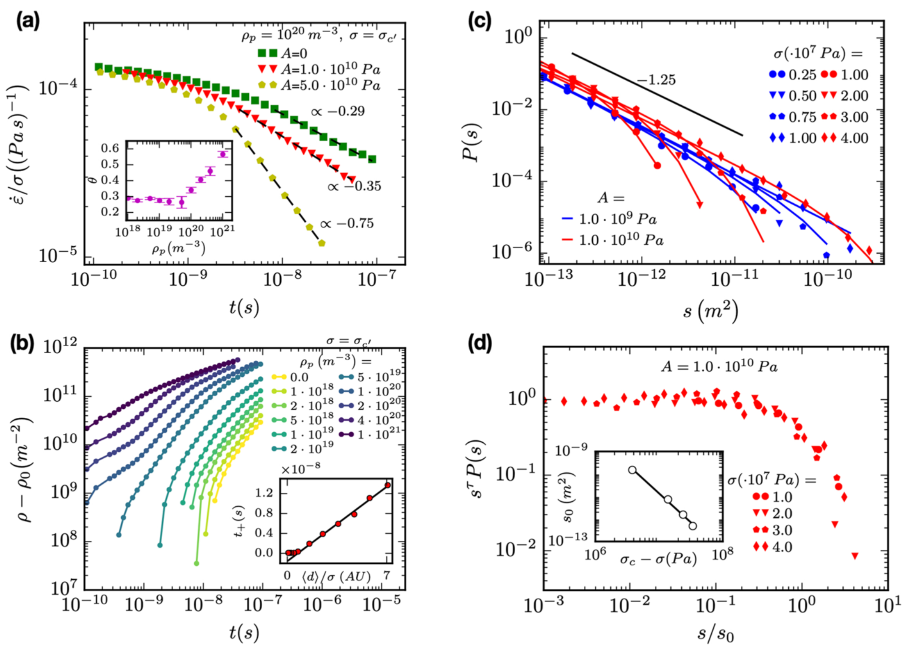

Fig. 6 The collective phenomena in 3D DDD simulations when the precipitates dominate the physics of the yielding can be seen both in creep modelling and in shear-tests. **a** illustrates how the power-law creep becomes quite complex: the decay of the strain rate exhibits a power-law exponent that varies with the strength of the precipitate-dislocation interaction. **b** shows how the dislocation density increases during creep. In **c** we illustrate the fact that a true "critical point" of statistical mechanics ensues such that the approach towards the σ_c and the associated yield strain is accompanied with strain bursts the distribution of which ($P(s)$) follows a data collapse shown in **d**. This in turn indicates an increasing correlation length. Figure reproduced from Salmenjoki et al. (2020)

Discussion and conclusions

Based on the above, it is evident that there are two main theoretical/numerical approaches to study the effects of precipitates on plastic deformation mediated by dislocation motion in crystals: (i) BKS-type theories (and related MD and DDD simulations) addressing in detail the magnitude of the CRSS and the microscopic mechanisms via which *individual* dislocations overcome precipitates, and (ii) larger scale multi-dislocation modelling of plasticity of precipitation-hardened crystals describing the *collective* dynamics of a large number of interacting dislocations. Here, we have highlighted some key aspects of both approaches.

To summarize, we started by illustrating the formation of a "true critical point" by the example of 2D DDD, by the addition of pinning points such as precipitates. For the 3D case, the FCC case reproduces this but leaves open a number of questions: what happens for BCC which has not been looked at in detail. Our own work presented above did not consider the yield strength or avalanche behavior from the depinning perspective. Our main point in the FCC case that has been resolved is that the depinning is more complex than that of individual dislocations interacting with disorder (Geslin 2024) and with a hint of lack of universality as the pinning strength due to precipitates changes the creep exponent. For low disorder, what is observed is a slightly increased yield stress but otherwise the dislocation system seems to not qualitatively change even though the similitude principle does not apply due to the length scale from precipitate density. These two regimes, with and without collective depinning, lead to the question whether a rule of mixture could be found to describe the alloy yield stress, as we discuss below.

Our take is that a key challenge worth future research efforts in this field has to do with integrating the two levels of description mentioned above. One may ask for instance a question of immense practical relevance: how to compute the yield stress of a precipitation-hardened crystal with a large number of interacting dislocations? Above, we have presented ideas suggesting that it might be possible to approximate this as a simple sum (or some other rule of mixture) of the pure system yield stress due to dislocation jamming and the contribution due to precipitates, with the latter estimated from BKS-type theories. However, it is not clear if such a simplistic approach should work in the general case. This is because the presence of precipitates affects the structure of the dislocation network in the crystal, and hence the "jamming component" of the yield stress might not be independent from the "pinning component" due to precipitates.

Another timely issue has to do with a key goal of metallurgy, i.e., designing materials with desirable mechanical properties by tuning the precipitate content of the alloy. Here, we have illustrated that BKS-type theories may be used as a theoretical guideline in designing materials with suitable strength characteristics. We note that an alternative approach is given by black box optimization algorithms such as Bayesian optimization, which can be exploited, e.g., to find optimal precipitate size distributions (optimizing a given mechanical property of interest), subject to the constraint of a fixed precipitate volume fraction (Sarvilahti and Laurson 2022). Overall, machine learning and data science approaches show great promise in the study of the plastic deformation (Salmenjoki et al. 2018; Mińkowski et al. 2022; Mińkowski and Laurson 2023) in a wide range of contexts, e.g., on the granular level in polycrystalline alloys (Salmenjoki et al. 2023), suggesting that machine learning can assist in optimising material properties across the scales, ranging from microscopic interactions of dislocations with individual point defects to granular and microstructural properties to achieve desired material properties.

From a more theoretical point of view, one may also outline several open questions that have to do with understanding phenomena such as the statistics of strain bursts - a key manifestation of collective dynamics of dislocations in plastically deforming crystals. In crystals with precipitates or other obstacles to dislocation motion of varying strength and density, one may envisage a number of different scenarios for critical-like dislocation dynamics. Above, we already discussed the pinning dominated case of the dislocation ensemble interacting with precipitates, and contrasted that to dislocation jamming occurring in "pure" dislocation systems without precipitates. We pointed out the possibility of critical exponents that vary continuously, as seen in the precipitate dominated case for the creep (or order parameter relaxation, in the depinning language) exponent. In addition, in a system of low dislocation density and high precipitate density, (de)pinning of individual dislocation lines might become the dominating mechanism. Moreover, in 2D DDD simulations it was found that very strong pinning disorder might completely quench critical behaviour. It remains to be seen if this is observable also in 3D systems. Finally, the crossovers between these different regimes of avalanche-like dislocation plasticity remain to be properly characterized.

Acknowledgements
See Funding.

Authors' contributions
LL and MJA wrote the manuscript.

Funding
Open access funding provided by Tampere University (including Tampere University Hospital). LL acknowledges the support of the Research Council of Finland via the Academy Project COPLAST (project no. 322405). MJA acknowledges support from the European Union Horizon 2020 research and innovation programme under grant agreement No 857470 and from European Regional Development Fund via Foundation for Polish Science International Research Agenda PLUS programme grant No MAB PLUS/2018/8.

Availability of data and materials
The data that support the findings of this study are available from the corresponding authors on reasonable request.

Declarations

Competing interests
The authors declare no competing interests.

Received: 4 October 2023 Accepted: 2 May 2024
Published: 13 May 2024

References

R.J. Amodeo, N.M. Ghoniem, Dislocation dynamics. i. a proposed methodology for deformation micromechanics. Phys. Rev. B. **41**(10), 6958 (1990)
R. Amodeo, N. Ghoniem, Dislocation dynamics. ii. applications to the formation of persistent slip bands, planar arrays, and dislocation cells. Phys. Rev. B. **41**(10), 6968 (1990)
D. Bacon, U. Kocks, R. Scattergood, The effect of dislocation self-interaction on the orowan stress. Philos. Mag. **28**(6), 1241–1263 (1973)
J. Friedel, *Dislocations*, vol. 3 (Pergamon Press, Oxford, 1964)
P.-A. Geslin, Modeling of solid solution strengthening in fcc alloys: Atomistic simulations, statistical models and elastic continuous approaches. Comput. Mater. Sci. **232**, 112624 (2024). https://doi.org/10.1016/j.commatsci.2023.f112624
N. Ghoniem, M., S.-H. Tong, L. Sun, Parametric dislocation dynamics: a thermodynamics-based approach to investigations of mesoscopic plastic deformation. Phys. Rev. B. **61**(2), 913 (2000)
Y. Hu, W.A. Curtin, Modeling peak-aged precipitate strengthening in Al-Mg-Si alloys. J. Mech. Phys. Solids. **151**, 104378 (2021). https://doi.org/10.1016/j.jmps.2021.104378
Y. Hu, W.A. Curtin, Modeling of precipitate strengthening with near-chemical accuracy: case study of al-6xxx alloys. Acta Mater. **237**, 118144 (2022). https://doi.org/10.1016/j.actamat.2022.118144
P.D. Ispánovity, I. Groma, G. Györgyi, P. Szabó, W. Hoffelner, Criticality of relaxation in dislocation systems. Phys. Rev. Lett. **107**(8), 085506 (2011)
P.D. Ispánovity, L. Laurson, M. Zaiser, I. Groma, S. Zapperi, M.J. Alava, Avalanches in 2d dislocation systems: Plastic yielding is not depinning. Phys. Rev. Lett. **112**(23), 235501 (2014)
S. Janićević, M. Ovaska, M.J. Alava, L. Laurson, Avalanches in 2d dislocation systems without applied stresses. J. Stat. Mech. Theory Exp. **2015**(7), 07016 (2015)
L. Kubin, Dislocations, Mesoscale Simulations and Plastic Flow, vol 5 (Oxford University Press, 2013)
A. Lehtinen, G. Costantini, M.J. Alava, S. Zapperi, L. Laurson, Glassy features of crystal plasticity. Phys. Rev. B. **94**(6), 064101 (2016)
A. Lehtinen, F. Granberg, L. Laurson, K. Nordlund, M.J. Alava, Multiscale modeling of dislocation-precipitate interactions in fe: From molecular dynamics to discrete dislocations. Phys. Rev. E. **93**(1), 013309 (2016)
A. Lehtinen, L. Laurson, F. Granberg, K. Nordlund, M.J. Alava, Effects of precipitates and dislocation loops on the yield stress of irradiated iron. Sci. Rep. **8**(1), 6914 (2018)
M.-C. Miguel, A. Vespignani, M. Zaiser, S. Zapperi, Dislocation jamming and andrade creep. Phys. Rev. Lett. **89**(16), 165501 (2002)
M. Mińkowski, L. Laurson, Predicting elastic and plastic properties of small iron polycrystals by machine learning. Sci. Rep. **13**, 13977 (2023)
M. Mińkowski, D. Kurunczi-Papp, L. Laurson, Machine learning reveals strain-rate-dependent predictability of discrete dislocation plasticity. Phys. Rev. Mater. **6**(2), 023602 (2022)
G. Monnet, Multiscale modeling of precipitation hardening: Application to the fe-cr alloys. Acta Mater. **95**, 302–311 (2015). https://doi.org/10.1016/j.actamat.2015.05.043
G. Monnet, Multiscale modeling of irradiation hardening: Application to important nuclear materials. J. Nucl. Mater. **508**, 609–627 (2018)
G. Monnet, S. Naamane, B. Devincre, Orowan strengthening at low temperatures in bcc materials studied by dislocation dynamics simulations. Acta Mater. **59**(2), 451–461 (2011)
J.F. Nie, Effects of precipitate shape and orientation on dispersion strengthening in magnesium alloys. Scripta Mater. **48**(8), 1009–1015 (2003)

J.F. Nie, B.C. Muddle, Strengthening of an al-cu-sn alloy by deformation-resistant precipitate plates. Acta Mater. **56**(14), 3490–3501 (2008)

M. Ovaska, L. Laurson, M.J. Alava, Quenched pinning and collective dislocation dynamics. Sci. Rep. **5**(1), 1–8 (2015)

S. Queyreau, G. Monnet, B. Devincre, Orowan strengthening and forest hardening superposition examined by dislocation dynamics simulations. Acta Mater. **58**(17), 5586–5595 (2010)

I. Ringdalen, S. Wenner, J. Friis, J. Marian, Dislocation dynamics study of precipitate hardening in al-mg-si alloys with input from experimental characterization. MRS Commun. **7**(3), 626–633 (2017)

Q. Rizzardi, C. McElfresh, G. Sparks, D. Stauffer, J. Marian, R. Maaß, Mild-to-wild plastic transition is governed by athermal screw dislocation slip in bcc Nb. Nat. Commun. **13**(1), 1010 (2022)

H. Salmenjoki, M.J. Alava, L. Laurson, Machine learning plastic deformation of crystals. Nat. Commun. **9**(1), 5307 (2018)

H. Salmenjoki, A. Lehtinen, L. Laurson, M.J. Alava, Plastic yielding and deformation bursts in the presence of disorder from coherent precipitates. Phys. Rev. Mater. **4**(8), 083602 (2020)

H. Salmenjoki, L. Laurson, M.J. Alava, Probing the transition from dislocation jamming to pinning by machine learning. Mater. Theory. **4**(1), 1–16 (2020)

H. Salmenjoki, L. Laurson, M.J. Alava, Avalanche correlations and stress-strain curves in discrete dislocation plasticity. Phys. Rev. Mater. **5**(7), 073601 (2021)

H. Salmenjoki, S. Papanikolaou, D. Shi, D. Tourret, C. Cepeda-Jiménez, M. Pérez-Prado, L. Laurson, M. Alava, Machine learning dislocation density correlations and solute effects in mg-based alloys. Sci. Rep. **13**(1), 11114 (2023)

R. Santos-Güemes, J. Segurado, J. LLorca, A generalized line tension model for precipitate strengthening in metallic alloys. Eur. J. Mech.-A/Solids. **93**, 104540 (2022)

M. Sarvilahti, L. Laurson, Bayesian optimization of discrete dislocation plasticity of two-dimensional precipitation-hardened crystals. Phys. Rev. Mater. **6**(12), 123801 (2022)

G. Sparks, Y. Cui, G. Po, Q. Rizzardi, J. Marian, R. Maaß, Avalanche statistics and the intermittent-to-smooth transition in microplasticity. Phys. Rev. Mater. **3**(8), 080601 (2019)

A. Takahashi, N.M. Ghoniem, A computational method for dislocation-precipitate interaction. J. Mech. Phys. Solids. **56**(4), 1534–1553 (2008)

Y. Zhang, R.B. Sills, Strengthening via orowan looping of misfitting plate-like precipitates. J. Mech. Phys. Solids. **173**, 105234 (2023). https://doi.org/10.1016/j.jmps.2023.105234