The strength and dislocation microstructure evolution in superalloy microcrystals

Ahmed M. Hussein\textsuperscript{a,b,⁎}, Satish I. Rao\textsuperscript{c}, Michael D. Uchic\textsuperscript{b}, Triplicane A. Parthasarathay\textsuperscript{d}, Jaafar A. El-Awady\textsuperscript{a}

\textsuperscript{a} Department of Mechanical Engineering, Whiting School of Engineering, The Johns Hopkins University, Baltimore, MD 21218-2682, USA
\textsuperscript{b} Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433-7817, USA
\textsuperscript{c} Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland
\textsuperscript{d} UES Inc., 4401 Dayton-Xenia Road, Dayton, OH 45432-1894, USA

\textbf{ARTICLE INFO}

\textbf{Keywords:}
Superalloys
Dislocation microstructure evolution
Anti-phase boundary
Intrinsic size effects
Dislocation dynamics

\textbf{ABSTRACT}

In this work, the evolution of the dislocations microstructure in single crystal two-phase superalloy microcrystals under monotonic loading has been studied using the three-dimensional discrete dislocation dynamics (DDD) method. The DDD framework has been extended to properly handle the collective behavior of dislocations and their interactions with large collections of arbitrary shaped precipitates. Few constraints are imposed on the initial distribution of the dislocations or the precipitates, and the extended DDD framework can support experimentally-obtained precipitate geometries. Full tracking of the creation and destruction of anti-phase boundaries (APB) is accounted for. The effects of the precipitate volume fraction, APB energy, precipitate size, and crystal size on the deformation of superalloy microcrystals have been quantified. Correlations between the precipitate microstructure and the dominant deformation features, such as dislocation looping versus precipitate shearing, are also discussed. It is shown that the mechanical strength is independent of the crystal size, increases linearly with increasing the volume fraction, follows a near square-root relationship with the APB energy and an inverse square-root relationship with the precipitate size. Finally, the flow strength in simulations having initial dislocation pair sources show a flow strength that is about one half of that predicted from simulations starting with single dislocation sources. The method developed can be used, with minimal extensions, to simulate dislocation microstructure evolution in general multiphase materials.

1. Introduction

Thanks to their unique balance of structural, thermodynamic and kinetic properties as well as their excellent creep resistance properties, Ni-base superalloys are the state of the art materials used in the most demanding sections of gas turbine engines, which are subject to high temperature and stress levels (Reed, 2006). Embedded in the base Ni crystal (the $γ$ phase) is a distribution of secondary phase Ni$_3$(Al, Ti) precipitates (the $γ'$ phase) that have an $L1_2$ crystal structure. Unlike most metallic materials, the yield strength of Ni-base superalloys does not decrease with temperature up to 750–850 °C (Westbrook, 1957; Davies and Thornton, 1977; Veyssiere and Saada, 1996). On the other hand, Co-based superalloys typically exhibit a higher melting temperature and...
exhibit superior single-crystal solidification characteristics while maintaining compressive flow stresses comparable to their Ni-based counterparts (Eggeler et al., 2014). Similar to the Ni-based superalloys, the strengthening in these Co-based superalloys arises from the presence of Co$_3$(Al,W) secondary phase precipitates ($\gamma'$ phase having an L1$_2$ structure, embedded in the Co matrix ($\gamma$ phase) (Sato et al., 2006). As such, Co-based superalloys could potentially be of use for applications requiring higher operating temperatures than that accessible by Ni-based superalloys.

The shearing of $\gamma'$ precipitates by the glide of dislocations in the $\gamma$ phase is one of the dominant deformation mechanisms of Ni-based and Co-based superalloys at room temperature (Reed, 2006). A typical $\frac{1}{2}$〈110〉 dislocation gliding into the $\gamma'$ phase would disturb its local ordering forming an Anti-Phase Boundary (APB) surface that leads to an increase in the precipitate's energy. Thus, $\gamma'$ phase shearing is always resisted by a force proportional to the precipitate's APB energy, which for Ni-based superalloys is typically in the range of 0.12–0.4 J/m$^2$ (Sun et al., 1999; Rao et al., 2004). On the other hand, a $\frac{1}{2}$〈110〉 dislocation gliding on an already formed APB region would restore the local ordering back to the minimum energy state, hence, its glide is assisted by an APB force of the same magnitude and opposite direction of that during the APB formation. This alternation between resisting dislocation shearing and assisting it, makes the force acting on a dislocation in superalloys history dependent. A pair of identical dislocations gliding together on the same plane (i.e a superdislocation having twice the typical FCC Burgers vector $\frac{1}{2}$〈110〉) has no net effect on the local ordering of $\gamma'$. Thus, In the absence of coherency strains, the pair would experience no resistance as it approaches the precipitate surface locally compared to the case of a single dislocation approaching a precipitate in the absence of coherency strains. This is not to be confused with the global picture of a dislocation pair shearing through a distribution of precipitates where there is always a resisting force regardless of the presence of coherency strains. Pollock and Argon (1992) suggested that precipitate shearing by superdislocations requires the blockage of a leading dislocation at its surface until a two-dislocation pile-up forms. When $\Gamma_{APB}$ is too high and the formation of superdislocations is difficult, dislocations can glide in the narrower $\gamma$-channels when the resolved shear stresses are high enough, leading to the formation of loops around the precipitate. Alternatively, at high temperatures dislocations can overcome the precipitates by cross-slip and/or climb (Picasso et al., 1997). Finally, it should be noted that the shearing of a $\gamma'$ precipitate by a single $\frac{1}{2}$〈110〉 dislocation has not been observed in Ni- or Co-based superalloys, however, the predominant cutting process in Co-based superalloys containing 30–39 at% Ni is by a single $\frac{1}{2}$〈110〉 dislocation, leaving behind APBs with the same displacement (Eggeler et al., 2014).

Numerical simulations of the plastic response of superalloys can greatly facilitate the quantification of the underlying deformation mechanisms that affect their macroscopic mechanical properties, as well as expedite the design of the superalloy microstructure to achieve optimal strength and creep resistance. One suitable computational method that can handle all the physical dislocation-precipitate interactions with minimal ad-hoc assumptions is Discrete Dislocation Dynamics (DDD) (Kubin et al., 1992; Ghoniem et al., 2000; Verdier et al., 1998; Zhib et al., 2002; Weygand et al., 2002; Benzerga et al., 2004; Zhou et al., 2010). In this method, dislocations are explicitly modeled and their time evolution is calculated. Both two-dimensional (2D) (Rao et al., 2004, 2006; Devincre et al., 1999, 2012) and three-dimensional (3D) (Devincre et al., 1997; Mohles et al., 1999; Mohles, 2001a, 2001b, 2004; Kohl and Nembach, 2001; Shin et al., 2001, 2003, 2005, 2007; Yashiro et al., 2006; Vatré et al., 2009, 2010; Huang et al., 2012; Haghhighat et al., 2013; Liu et al., 2014; Yang et al., 2014; Gao et al., 2015) DDD simulations have been used in the past to study the behavior of Ni-base superalloys. However, most of these DDD studies have used simplified precipitate geometries (cubic or spherical) arrangements (a single precipitate or a regular array of precipitates), and simple precipitate shearing rules where the precipitate can either be unsharable or shearable only by superdislocations. A realistic superalloy simulation requires the capability of handling precipitates of geometries and distributions similar to those found in experiments. In addition, the formation of superdislocations in the simulation should take place only if the local stresses and precipitate resistance allow it to happen. This has been challenging for the DDD community in the past due to the geometric complexity of the problem.

To address these limitations, the target of the current study is to extend the DDD framework to model more realistic dislocation-precipitate interactions in small crystals. The paper is organized as follows, in Section 2, the necessary extensions to the 3D-DDD framework to model dislocation-precipitate interactions in superalloys are described. In Section 3, the parameters for the numerical simulations conducted are summarized. In Section 4, the results of the simulations are discussed and comparisons with analytical predictions and experimental observations. Finally, a summary and a conclusion of the work are given in Section 5.

2. Computational method

All simulations performed here are conducted using an in-house, modified version of the 3D-DDD open source code ParaDiS (Tang et al., 2007) that guarantees that all dislocation reactions are planar, and incorporates a set of atomistically-informed, physics-based cross-slip mechanisms, the details of which are described in Hussein et al. (2015). In addition, ParaDiS naturally accounts for dislocation reactions such as the formation of Lomer, Hirth and glide locks. The code was then extended as described below to model superalloys. Unlike pure single phase metals, the additional APB forces acting on dislocation segments in an L1$_2$ crystal structure depend on the history of the dislocation glide activity. The APB force per unit length is equal to $\Gamma_{APB} = \frac{2\pi\sigma}{\gamma}$ if the dislocation is gliding on a unsharable plane in the $\gamma$ phase (the negative sign indicates a repulsive force), or $\Gamma_{APB} = \frac{\pi\sigma}{\gamma}$ if it is gliding on a sheared plane in the $\gamma'$ phase. Since superdislocations do not create or destroy APB regions, no APB forces act on them. In order to handle the most general case, the state of being sheared or unsharable should be tracked for every point in the $\gamma'$ regions. This process amounts to tracking the APB fault regions as they are created and destroyed. The APB representation and tracking will be discussed next, however, an important prerequisite for APB tracking is a flexible precipitate geometry representation.
2.1. Precipitate geometry representation

To accurately model dislocation-precipitate interactions in 3D-DDD it is necessary to track the position of every dislocation segment every time step with respect to all precipitates in the simulation cell. This can add a significant computational overhead to the DDD simulations for a general complex precipitate structure. To mitigate this, the precipitate geometry should be chosen such that it would have a low memory footprint to enable the modeling of hundreds to thousands of precipitates efficiently, and the dislocation node containment check routine needs to be efficient. In addition, this should be achieved with minimum deviations from the experimentally observed precipitate geometries. Thus, in the current simulations the precipitate geometry is represented by the convex hull of a set of 3D points, which is defined as the smallest convex geometry that contains all the points in the set (O’Rourke, 1998). A convex geometry is a region \( H \) in \( \mathbb{R}^n \) such that for all points \( x, y \in H \), the set \( x + (y - x)n \in H \) for \( 0 \leq \eta \leq 1 \). That is, any two points inside \( H \) can be connected by a line segment that lies entirely inside \( H \). A convex geometry is also the intersection of a number of infinite half spaces in \( \mathbb{R}^n \). This latter property guarantees that the dislocation node containment check is robust since it reduces to checking the signs of a few vector dot products. An infinite half space \( L_i \) is the set of all points \( x \in \mathbb{R}^n \) such that

\[
L = x; (x_i - p_i)n_i \leq 0
\]  

where \( p_i \) is any point on the boundary of the half space, and \( n_i \) is the vector normal to the half space boundary in the outward direction. A convex geometry \( H \) is then the set defined by

\[
H = \cap_{i=1}^{N} L_i = \cap_{i=1}^{N} (x_i - p_i)n_i \leq 0
\]

where \( N \) is the number of intersecting half spaces that make up the convex geometry. The point \( x \) is outside \( H \) unless it is contained in every single half space \( L_i \) forming \( H \). Thus, the representation’s memory footprint is low since only 6N floating-point numbers are required to represent the entire precipitate (3 numbers for each \( p_i \) and another 3 for each \( n_i \)). In addition, the dislocation node containment check is fast because it is linear in the number of half spaces and the complexity of the half space containment check is constant and low.

It should be noted that the convex hull can represent any convex geometry exactly. For concave geometries, the accuracy of the representation depends on the degree of concavity. Extremely concave and self-intersecting geometries are the least accurately represented geometries using convex hulls. Nevertheless, in superalloys, precipitates typically have convex shapes of spherical or cuboidal geometries (Pollock and Argon, 1992; Ricks et al., 1983). Thus, in the current simulations all the precipitates are assumed to have convex geometries.

2.2. Tracking the APB region

The boundary of an APB region is either a \( \frac{1}{2}(110) \) dislocation curve that separates the sheared from the unsheared regions, the intersection curve of the precipitate that contains the APB region with the slip plane that the APB region is on, or a mixture of both. In the current method, at the beginning of the simulation, the crystal is assumed to be free of any APB regions. When a dislocation attempts to shear a precipitate, an APB plane that coincides with the dislocation slip plane is created and meshed into planar rectangular elements (termed hereafter APB plane cells). Each cell stores a shearing vector, \( v_i \), which is initially zero. An increase in the resolution of the APB plane mesh increases the accuracy of the tracking of the APB region, however, this leads to larger memory requirements. As a dislocation shears through the precipitate, each dislocation segment inside the precipitate is checked every time step to determine if it has swept the midpoint of any APB plane cells. For every dislocation segment that sweeps the midpoint of an APB plane cell, its Burgers vector is added to the shearing vector \( v_i \) of the APB plane cell it swept. Thus, any APB plane cell is considered unsheared if the cumulative shearing vector \( v_i \) sums up to an even integer multiple of a \( \frac{1}{2}(110) \) shifted by at most one \( (100) \) vector. In other words, the cell is considered unsheared if there is an integer \( k \) that satisfies the equation

\[
v_i - k(110) = \begin{cases} (000) \\ (100) \end{cases}
\]  

This corresponds to the case of two identical \( \frac{1}{2}(110) \) or three mutually different \( \frac{1}{2}(110) \) dislocations gliding in succession. If an integer \( k \) is found, the cell’s shearing vector \( v_i \) is reset to zero. This criterion is derived from the structure of an \( L_2 \) crystal where the translations with \( (100) \) or \( (110) \) vectors are symmetry operations.

The detection of segment-cell midpoint sweep requires a great deal of precision because any sweeping events that pass undetected would render the APB cell state wrong. For this reason, the 3D configuration is projected onto a 2D configuration where the sweeping detection depends on the sign of a dot product.

2.3. Computing the APB force

When a dislocation node is inside a precipitate, a hash search (Cormen et al., 2009) for the APB plane is performed to determine the APB plane cell this dislocation node belongs to. If this APB plane cell is already sheared, an APB force per unit length of magnitude \( F_{APB}lb \) is imposed on the dislocation node in the direction of the element’s midpoint (the APB region is attracting the dislocation). On the other hand, if this APB plane cell is unsheared, a repulsive force with the same magnitude is imposed on the dislocation node in a direction away from the element’s midpoint (the APB region is repelling the dislocation). This is shown...
schematically in Fig. 1 along with the sequence of events associated with the creation of the APB region during the shearing of a precipitate with a gliding dislocation.

It should be noted again that the accuracy of the method is strongly dependent on the APB plane cell size, and the dislocation segment maximum length. In general, the dislocation segment maximum length should be smaller than the smallest channel width in the simulations. The above implementation is validated by calculating the flow strength of an ideal configuration where an infinitely long superdislocation interacts with a cubic precipitate as discussed in Appendix A. Excellent agreement between the predicted flow strength from the current simulations and analytical predictions is found.

3. Numerical simulations

In the following, all simulation cells mimic rectangular shaped superalloy micropillars having square cross-sections. A uniaxial compressive load is imposed with a total strain rate of 500 s$^{-1}$ in the [001] direction. Due to the high computational complexity of DDD simulations, the use of high strain rates is necessary in order to achieve reasonable strain levels in a reasonable amount of simulation time. It is worth mentioning that experimental studies (Urdanpilleta et al., 2005) show that the strain rate exponent in superalloys is non-negligible, which is not addressed in the present study. Given that the shear moduli of the $\gamma$ and $\gamma'$ phases are not significantly different, the shear modulus and Poisson’s ratio in the simulations are taken to be 80 GPa and 0.31, for both the $\gamma$ and $\gamma'$ phases for simplicity. In the present simulations, the $\gamma - \gamma'$ lattice misfit stress is not accounted for and it is to be incorporated in the simulations in a future research effort. The height to edge-length ratio in all simulations is $L/D=3$, and the initial dislocation microstructure is introduced by randomly distributing Frank-Read (FR) sources uniformly on all twelve FCC slip systems in the $\gamma$ phase only with a total dislocation density of $10^{13}$ m$^{-2}$. Note that the first reported dislocation density value might be different that the initially generated dislocation density since the dislocation microstructure slightly relaxes initially before any stress application. This relaxation can cause dislocations to combine, annihilate or escape from the surface, which reduces the overall dislocation density. In all simulations, the precipitates have near cuboidal geometries with sides facing the matrix {100} planes, similar to those reported experimentally (Pollock and Argon, 1992).

In the following simulations, the effect of the precipitate volume fraction, APB energy, precipitate size, and crystal size, on the microcrystal strength and dislocation microstructure evolution are investigated. In each study, only one parameter is varied at a
time, and three different random initial configurations are simulated for each case to ensure that the results are statistically representative. The nominal values for the volume fraction, APB energy, average precipitate size, and crystal size are chosen as 0.7, 0.2 J/m², 0.3 µm, and 1 µm, respectively. To study crystal size effect, the simulations are performed for three different crystal sizes: \( D = 0.75, 1.0, \) and 2.0 µm. To study precipitate volume fraction effects, the simulations are performed for three different volume fractions: 0.25, 0.5, and 0.7. To study the APB energy effects, the simulations are performed for three different APB energies: 0.1, 0.3, and 0.5 J/m². Finally, to study the precipitate size effect, the simulations are performed for three different precipitate sizes: 0.2, 0.3, and 0.5 µm. A Simulation of a pure Ni single crystal micropillar having the same dimensions and initial dislocation density as the simulated superalloy crystals is also performed for comparison.

It should be noted that since the crystal size, precipitate size and its volume fraction are all related, one cannot control each of the three parameters independent of the other two. In all of the present simulations, the precipitates are distributed over a non-uniformly spaced three dimensional grid where each grid point is the center of a cuboid that contains the precipitates. The volume fraction is then defined to be the volume of the precipitate divided by the volume of the cuboid containing it, and the precipitate size is defined to be the ratio of the crystal volume to the number of precipitate containing cuboids inside it. The choice of nonuniform grid spacing was made so as to allow for a higher degree of statistical variation in the precipitates sampled by dislocations.

In the simulation setup discussed above, the initial dislocation network is composed of randomly distributed “single” FR sources. Furthermore, other than the imposed APB forces on the dislocations as they shear through precipitates, no conditions are imposed on whether precipitate shearing is by single dislocations or dislocation pairs. As will be discussed in details in Section 4, the predominant precipitate cutting process from these simulations is by single \( \langle 110 \rangle \) dislocations, leaving APB regions with the same displacement behind. Thus, the results qualitatively mimic deformation in Co-based superalloys containing 30–39 at% Ni (Eggeler et al., 2014). On the other hand, to shed light on the effect of precipitate shearing by pairs of dislocations, which mimics deformation in Ni-based superalloys, an extra simulation where the initial dislocation network was constructed by randomly distributing sources each composed of two identical FR sources on the same plane with a small separation between them was performed and its results are reported below. This final simulation is conducted for a crystal size of \( D = 1.0 \) µm, a precipitate volume fraction of \( f = 0.7 \), precipitate size of \( r = 0.3 \) µm, and an APB energy of \( \Gamma_{\text{APB}} = 0.2 \) J/m².

4. Results and discussion

4.1. Crystal size effects

The engineering stress-strain curves for crystals of three different sizes (\( D = 0.75, 1.0, \) and 2.0 µm) having the same precipitate volume fraction, APB energy, and precipitate size (i.e. same channel width) are shown in Fig. 2(a). It is apparent that the crystal size has a modest effect on crystal strength for the three crystal sizes modeled here. The predicted flow strengths compare favorably to the experimentally reported values for superalloy micropillars of similar sizes (Girault et al., 2010). This agrees well with microcompression experiments on René N5 microcrystals (Girault et al., 2010; Shade et al., 2012). Furthermore, the evolution of the dislocation density as a function of strain is shown in Fig. 2(b), and the crystal size effect on the dislocation density multiplication rate is negligible for the range of crystal size modeled and strain levels reached. The lack of crystal size effects for superalloy microcrystal arises from the existence of a smaller intrinsic length scale governed by the channel width. As long as this intrinsic length scale is sufficiently smaller than the crystal size, as is the case here, the crystal size effect will be negligible (Shade et al., 2012). This is in contrast with strong size-effects observed in single phase pure metals (Uchic et al., 2004; El-Awady, 2015). The yield strength scatter observed for larger samples (\( D = 2.0 \) µm) is due to the larger scatter in the initial FR source length distribution; as the

![Fig. 2. (a) Engineering stress, and (b) dislocation density, versus engineering strain for microcrystals of three different sizes having a precipitate volume fraction of 0.7, APB energy of 0.2 J/m², and precipitate size of 0.3 µm.](image-url)
crystal size increases, the standard deviation of the FR source length distribution increases. Two samples with the same initial dislocation density and crystal size might have FR sources which have very different activation strengths, giving rise to the observed variation in the yield strength.

4.2. Precipitate volume fraction effects

The effect of the precipitate volume fraction on the engineering stress-engineering strain response is shown in Fig. 3(a) for simulations having the same crystal size, precipitate size, and APB energy. Since one cannot simultaneously hold both the crystal size and precipitate size constant and vary the volume fraction arbitrarily, only here, the precipitate size is defined to be the average volume occupied by a single precipitate in the simulation. Thus, if one divides the crystal volume by the number of precipitates, the quotient is the same in all cases. The actual precipitate volume is then chosen such that its ratio to the volume occupied by a single precipitate is equal to the desired volume fraction. According to this choice of the precipitate microstructure parameters, precipitates in the higher volume fraction simulations will have larger sizes than those having smaller volume fractions.

The flow stress is observed to increase with increasing volume fraction following a linear relationship with a slope of 1800 MPa as shown in Fig. 4(a), in agreement with 3D-DDD simulations of a single pair of similar dislocations shearing a cubic precipitate in a simulation cell with periodic boundary conditions (Vattré et al., 2009). These results indicate the strong strengthening effects of precipitates even at low precipitate volume fractions. It should be noted that for microcrystals having a zero volume fraction (i.e. single phase Ni) the yield strength is not zero since there is a non-zero activation stress associated with the FR sources that depends on their lengths. The lengths of the FR sources used in these simulations are normally distributed with a mean of $\lambda = 0.6\mu m$ and a standard deviation of $\sigma = 0.03\mu m$ for all volume fractions, thus, the FR source strength represents a constant shift in the flow strength for all cases. Furthermore, the linear relationship between the strength and the volume fraction might be sensitive to the chosen simulation parameters (e.g. APB energy, shearing by single dislocations, precipitate size, and crystal size) and further experimental validation is required to confirm this behavior.

It is interesting to note that the average number of cross-slip events that took place by the end of the simulations were on average 112, 61 and 12 for simulations having $f=0.25$, 0.5 and 0.7 volume fractions, respectively. The significant decrease in the cross-slip frequency with increasing volume fraction, irrespective of the increasing flow stress, is because the probability of having screw-oriented dislocations in the channels decreases with increasing volume fraction (i.e. decreasing channel width).

The effect of the precipitate volume fraction on the evolution of the dislocation density is shown in Fig. 3(b). The dislocation density multiplication rate after flow commencement is observed to decrease with increasing precipitate volume fraction. The dislocation density evolution shows sharp increases followed by low multiplication rate intervals. The sharp increases correspond to the instances when dislocations glide in the channels while depositing dislocation segments at the $\gamma - \gamma'$ interface, while the low rate dislocation density multiplication corresponds to the trapping of the active dislocations at the precipitate interface, or when they are slowly shearing the precipitates. Representative dislocation microstructures at the onset of flow for simulations of the different volume fractions are shown in Fig. 5. For the low volume fraction cases ($f=0.25$), no precipitate shearing is observed for the strain levels reached since dislocations can easily loop around the precipitates by gliding through the wide channels, or by cross-slipping in the matrix to avoid the precipitate. For the intermediate volume fraction cases ($f=0.5$), deformation is dominated by dislocation glide in the channels with some shearing through precipitates. In the high volume fraction cases ($f=0.75$), precipitate shearing is typically the dominant mechanism. This transition in the dominant dislocation glide mechanism can be the reason behind the linear dependence of the strength on the volume fraction. The precipitate shearing is predominantly bowing assisted, in which a dislocation
stuck at the matrix-precipitate interface starts bowing in the channels around the precipitate corners inducing high attractive stresses between the nearby segments of the dislocation. The attractive stress brings the two segments together by shearing through the precipitate until they annihilate. The dislocation then advances through the precipitate and a similar bowed out configuration is recreated resulting in further advancements until the dislocation shears through the precipitate entirely. This bowing assisted shearing process is shown schematically in Fig. 6.

It should be noted that for the low volume fraction cases, the imposed strain rate can be sustained by the dislocation activity in the channels alone because of the larger area available for dislocation glide, thus, the crystal yields without any precipitate shearing and the strength depends mainly on the channel width. As the volume fraction increases, the yield strength increases since precipitate shearing dominates due to the now much narrower channels. In the absence of precipitate shearing, these observations can be quantified based on the dislocation source activation strength (Hirth and Lothe, 1982):

Fig. 4. The flow strength variation with the (a) precipitate volume fraction; (b) APB energy; and (c) precipitate size as predicted from simulations is compared to the (a) linear relationship discussed in Section 4.2; and power-law expressions given in (b) Eq. (8); and (c) Eq. (10) respectively.
\[ \sigma_f = \frac{\mu b}{Mw} \approx \frac{49}{w} \]

where \( \sigma_f \) is the axial flow stress, \( b=0.25\times10^{-9} \text{ m} \) is the magnitude of the dislocation's Burgers vector, \( w \) is the channel width and \( M=0.408 \) is the Schmid factor. Assuming a periodic cubic volume with edge length \( d \) and containing a single cubic precipitate, the volume fraction can be expressed as:
where \( r \) is the precipitate side length. The average channel width \( \pi \) is thus:

\[
\pi = d - r = d (1 - \frac{1}{f})
\]  

(6)

In the current simulations, there are approximately 192 cubic precipitates in a 1×1×3 \( \mu m^3 \) crystal, giving \( d=0.25 \). Thus, from Eqs. (6) and (4) the flow strength is given by:

\[
\sigma_f \approx \frac{196}{1 - \frac{1}{f}}
\]  

(7)

Eq. (7) estimates a flow strength of 530 and 950 for a 0.25 and 0.5 volume fractions, respectively. This is in good agreement with the predictions form the current simulations for the two lower volume fractions, in which deformation is dominated by precipitate looping. However, for a volume fraction of 0.7, Eq. (7) estimates a flow strength that is 34.5% higher than that predicted from the current simulations. This discrepancy for the highest volume fraction is mainly due to the fact that Eq. (7) predicts the strength based on dislocation bowing through the channels, while as shown in Fig. 5(c), the deformation is dominated by APB shearing.

It is worth noting that in the high volume fraction cases, very slight dislocation build-up takes place before dislocation shearing due to the size limitation imposed by the narrow channels. This size limitation, along with the absence of dislocation pile-ups, reduce the chance of dislocation cross-slip in \( \gamma \) phase.

4.3. The APB energy effects

The effect of the APB energy on the engineering stress-strain response of crystals having the same crystal size, dislocation density, precipitate volume fraction, and precipitate size is shown in Fig. 7(a). The flow strength versus the APB energy can be fitted by a power-law of the form

\[
\sigma_f = 2000(\Gamma_{APB})^{0.4} + 150
\]  

(8)

where \( \sigma_f \) is in MPa and \( \Gamma_{APB} \) is in J/m². It should be noted that previous simplified DDD simulations, where the initial dislocation microstructure consisted of one pair of identical dislocations, predict a square-root dependence on the APB energy (Rao et al., 2004; Vattré et al., 2009). However, in the current simulations, because dislocations are not initially paired and some of them, especially in the high APB cases, loop around the precipitates, there is a transition in the deformation mechanism from shearing at low APB energies to looping at high APB energies. This results in the slightly lower power law exponent of 0.4 predicted in this study. The average flow strength of the simulated pillars having different APB energies is compared to the relation given by Eq. (8) in Fig. 4(b).

For the case of an infinitely long dislocation shearing an infinitely large precipitate, the ideal shear stress for shearing is

\[
\tau_{\Gamma b} = \frac{\Gamma_{APB}}{d b}
\]

which leads to an ideal flow strength of

\[
\sigma_{\Gamma b} = \frac{\Gamma_{APB}}{M b} \approx 9.8\Gamma_{APB}
\]  

(9)

Thus, the ideal flow strength is 0.98, 1.96, and 4.9 GPa for APB energies of 0.1, 0.2, and 0.5 J/m², respectively. The predicted flow strength from the current DDD simulations for \( \Gamma=0.1 \) J/m² agrees well with this estimate, however, the flow strength deviates significantly from these estimates for the two higher APB energy cases. This is because in the current simulations, unlike the infinite
long straight dislocation case, dislocations glide in the channels. According to Eq. (7), the maximum flow strength for this volume fraction (via channel glide in the absence of precipitate shearing) is about 1.75 GPa. In addition, dislocation shearing is bowing assisted so an overall lower applied stress is required for precipitate cutting. However, bowing assisted cutting is still sensitive to the APB energy as the bowing angle should increase before cutting to provide enough attractive interaction stress for the shearing dislocation segments. As the APB energy increases, the yield strength is expected to plateau at 1.75 GPa when the APB energy becomes too high for any shearing to take place.

The effect of the APB energy on the dislocation density evolution is also shown in Fig. 7(b). The density multiplication rate after flow is observed to increase with increasing APB energy since more dislocations favor channel glide, which leads to an increase in the total dislocation length. Representative dislocation microstructures at the onset of yield for the different APB energies are shown in Fig. 8. In all three cases, the initial dislocation and precipitate microstructures were identical. The final dislocation microstructure consists primarily of many dislocations surrounding the precipitates in the highest APB energy cases, fewer loops in the intermediate APB energy cases, and none for the lowest APB energy case. These loops form when dislocations bow around a precipitate, fail to shear through it, and end up looping around the precipitate. These loops become immobile, which also partially explains the high strength observed. Moreover a dislocation loop deposited on the precipitate surface cannot be eliminated by a subsequent dislocation loop generated by the same FR source since the two loops have the same line direction. With fewer mobile dislocations, higher stresses are required to move the dislocation at a rate at which they can sustain the imposed plastic strain. Precipitate shearing takes place, even for the cases with higher energies for small precipitates due to the strong attractive force between dislocations on both sides of the precipitate. For low APB energies, the precipitate shearing stress is lower than the channel glide stress, thus, precipitate shearing dominates. As the APB energy increases, dislocations get stuck at channel entrances until the resolved shear stress is high enough for them to bow and glide into the channels. The accumulation of dislocation loops on the precipitate surfaces in the high energy case indicates the possibility of strain hardening at higher strain levels because the channels in which the loops accumulate would resist further dislocation glide through mutual repulsion.

When precipitate shearing is the dominant deformation mechanism (i.e in the high volume fraction or high APB energy cases), it was noticed that most dislocations shear the precipitates singly rather than in pairs. Shearing in pairs would reduce the applied resolved shear stress required by a factor of two. However, in these simulations dislocation pairs were not introduced initially in the γ phase. As the dislocation motion is integrated in time during the simulation, dislocation pairs can spontaneously form if their formation is energetically more favorable. At higher volume fractions or APB energies, dislocations get stuck at the γ − γ′ interface and effectively block all the inter-precipitate channels. This means that no further dislocations can be emitted by the FR sources until the already stuck dislocations either shear the precipitates or glide through the channels. In high volume fraction cases, channel glide
requires a high resolved shear stress that exceeds that required for a single dislocation precipitate shearing. As a result, it becomes energetically more favorable for dislocations to shear singly at twice the resolved shear stress required for pair shearing rather than glide through the narrow channels prior to forming dislocation pairs. It is important to note that this is a result of the choice of the simulation parameters in which the initial dislocation microstructure consisted of randomly distributed single dislocation FR sources rather than pairs of dislocations.

4.4. Precipitate size effects

A dislocation forming a loop around a smaller precipitate would require less applied stress to shear through it compared to another looping around a bigger precipitate. This is because the attractive stress between the dislocation segments on either side of the precipitate decreases the critical resolved shear stress required for shearing, and for the smaller precipitates, the segments are closer to each other. The whole, however, is not the sum of its parts when it comes to the effect of the precipitate size on the overall superalloy microcrystal strength. The effect of the precipitate size on the engineering stress-strain response for the same microcrystal size, precipitate volume fraction, and APB energy is shown in Fig. 9(a). It is observed that the flow strength decreases with increasing precipitate size and the relationship can be described by a power-law of the form

$$\sigma_f \approx 568 r^{-0.58} + 150$$

where $\sigma_f$ is in MPa and $r$ is the precipitate side length in microns. Eq. (10) agrees well with analytical predictions, which suggest that the shear strength required for defeating a regular array of precipitates is proportional to the inverse square-root of precipitate size (Reppich, 1993). A comparison of the strength predicted from the simulation and the power-law relationship given by Eq. (10) is shown in Fig. 4(c).

Furthermore, the dislocation density multiplication rate, after flow, increases with increasing precipitate size as shown in Fig. 9(b). The dislocation microstructures at the onset of flow are shown in Fig. 10. It is observed that a large number of dislocation loops develop in the simulations with 0.5 µm precipitate size compared to straight dislocations in simulations having smaller precipitate sizes. The dislocations pile up against the surface of the precipitates but do not shear them even though they effectively form a superdislocation. This is because it is energetically more favorable for the dislocations to remain separated in both $\gamma$ and $\gamma'$ phases. The leading dislocation in this case still needs a local resolved shear stress of $\tau = \frac{\Gamma b \Delta \theta}{2a}$ as described in Eq. (13) to penetrate the precipitate. Thus, while crystals having larger precipitates are weaker, the main flow mechanism is channel glide rather than precipitate shearing, while the opposite being true for crystals having smaller precipitates that show precipitate shearing but in a more difficult manner due to the narrower channels. The dislocations in crystals having the smallest precipitate sizes, $r=0.2$ µm, form complete or near complete loops surrounding a group of precipitates, rather than individual precipitates, as shown in Fig. 11, before they shear the precipitates and collapse. This explains the low density multiplication rate observed in crystals with smaller precipitates. There are two factors that can explain this behavior. First, the channel width is lower in the case of smaller precipitates, hence, a higher applied stress is required to cause the dislocations to bow inside the channels. Second, when a dislocation loops around a group of precipitates, as opposed to one precipitate, the loop radius is larger, which makes the attractive force between the dislocation segments on opposite sides of the loop weaker, resulting in them being unable to shear the precipitates. In this configuration, a weakest-link like mechanism takes place where two dislocation segments approach each other by gliding through the widest channels until they collide and pinch off, spawning a number of smaller loops that can collapse independently. This corresponds to a spike in the dislocation density where the total length increases instantaneously and then drops immediately after the loop collapses. It is interesting to note that unlike in the precipitate microstructures with narrow inter-precipitate channels, the
simulations having the largest precipitate size, which have wider channels, show pile-ups of two dislocations at the $\gamma - \gamma'$ interface which lowers the applied resolved shear stress for precipitate shearing. The two dislocation pile-ups form as a result of a single FR source pumping out a dislocation (the leading dislocation) that loops around the precipitate since it can easily glide in the wide channels, followed by pumping out another dislocation (the trailing dislocation) that loops around the first one forming the two dislocation pile-up.

4.5. Effect of shearing by pairs of dislocations

In the simulations discussed in Sections 4.1–4.4, dislocation pairing was not artificially introduced in the simulation cell, and the system was left to follow the evolution path that minimizes its overall energy. However, in order to probe the effects of precipitate shearing by dislocation pairs, as typically observed in Ni-based superalloys, one of the initial dislocation microstructures used in the simulations discussed earlier was modified such that every FR source was paired with an identical one placed close to it on the same slip plane. Thus, the initial dislocation density in this simulation is twice that of the single dislocations shearing case. The system was
then initially relaxed such that the dislocation pairs would reach their equilibrium spacing, then the crystal was loaded with the same strain rate. All the dislocation pairs were initially in the $\gamma$ phase and the $\gamma'$ phase distribution is identical to the one used in the single dislocation shearing case. In this simulation, the crystal size is $D=1.0$ µm, the precipitate volume fraction is 0.7, the precipitate size is $r=0.3$ µm, and the APB energy is $\Gamma = 0.2$ J/m$^2$.

A comparison between the stress-strain behavior and dislocation density evolution of the simulation starting with dislocation pairs and that starting with single dislocations is shown in Fig. 12. The flow strength in the pair simulation is about one half of that predicted from simulations starting with single dislocations. The dislocation density is initially twice that of the single dislocation case because of the dislocation pairing, and its evolution follows the same trend suggesting that most of the plastic strain was accommodated by dislocations glide inside the precipitates after shearing them. This is to be expected because at such a high volume fraction, inter-channel dislocation glide is considerably more difficult to sustain compared to precipitate shearing.

The dislocation microstructure at different strain levels for the simulation starting with dislocation pairs are shown in Fig. 13. The dislocations were observed to move only in pairs, and the inter-channel dislocation glide was minimal. The dislocation activity is intermittent due to the dislocation stop-and-go motion where the leading dislocation of the pair, under the combined effect of the interaction stress with the trailing dislocation and the applied stress, penetrates the precipitate and glides across it quickly to reduce the interaction stress imposed on it. The trailing dislocation which was originally held at equilibrium by the stress field of the leading dislocation, becomes unstable and due to the motion of the leading dislocation. Facing no APB resistance forces from the precipitates the trailing dislocation penetrates the precipitate and once inside, it is driven forward by the APB forces that aim to restore the local order in the $\gamma'$ phase. After exiting from the other side of the precipitate, the dislocation pair gets stuck at the interface of a different precipitate and the entire process is repeated.

It was also observed that unlike the single dislocation shearing case, only a few number of dislocation pairs are active within the range of strains reached here. Since the glide of a dislocation pair accommodates twice the plastic strain that can be carried by a single dislocation, it becomes sufficient for the system to move only the weakest dislocations (the one with the least resistance to motion) in order to sustain the imposed strain rate. Finally, the effects of pair shearing on the flow strength in lower volume fraction cases are expected to be smaller than that in the high volume fraction case studied here since precipitate shearing dominates at higher volume fractions as discussed in Section 4.2.

5. Summary and conclusions

In this work, the 3D-DDD framework has been extended to simulate the deformation of superalloy microcrystals by modeling the interactions between general dislocation microstructures residing initially in the $\gamma$ phase with an arbitrary distribution of $\gamma'$ precipitates that mimic experimentally observed precipitate microstructures. This framework is utilized to quantify the effect of the precipitate volume fraction, APB energy, precipitate size, and crystal size on the strength and dislocation microstructure evolution. In addition, the effect the initial dislocation network in terms of having randomly distributed single dislocation sources versus having initially random sources of dislocation pairs was also investigated. It was shown that the microcrystal strength varies linearly with the precipitate volume fraction, and at low volume fractions the dislocation density multiplication is faster and cross-slip in the $\gamma$ phase is more frequent. The strength-APB energy relationship follows a power law with an exponent of 0.4, close to the square-root dependence predicted previously from simplified planar DDD simulations. The strength-precipitate size relationship follows an inverse square-root law in agreement with analytical models (Reppich, 1993). The crystal size is shown to modestly influence the microcrystal strength for the crystal sizes modeled here, in good agreement with microcompression studies on René N5.
microcrystals (Shade et al., 2012). It is important to note that the functional form of these strength-microstructure relationships can be sensitive to the chosen simulation parameters and further investigations are required to confirm or rule out this possibility. The most influential factor on the crystal's strength was found to be the channel width. As the volume fraction increases or the APB energy decreases, the dominant dislocation glide mechanism shifts from channel glide to precipitate shearing. No strain hardening has been observed in all simulations up to the simulated strain levels. Finally, the flow strength in simulations having initial dislocation pair sources is about one half of that predicted from simulations starting with single dislocation sources. It should be noted that the developed framework can be extended with minimal modifications to track the formation and destruction of intrinsic and extrinsic stacking faults. Also it can be extended to study the formation of Kear-Wilsdorf locks and solid solution strengthening in the γ phase.

Acknowledgements

This research was sponsored by DARPA contract number N6600112-14229. MDU acknowledges support from the Air Force Research Laboratory, Materials and Manufacturing Directorate.

Appendix A. Validation of the APB tracking implementation

The implementation of the APB tracking algorithm described in Section 2.2 has been validated through a number of planar simulations where a pair of identical \(\langle 110\rangle\) dislocations are placed on the same plane outside a single cubic precipitate placed at the center of a cubic simulation cell as shown in Fig. 14. The simulations are conducted for the same configuration at different constant shear stress levels and the lowest resolved shear stress that allows the dislocation pair to shear through the precipitate is reported for simulations with different APB energies. Periodic boundary conditions are imposed along all directions to eliminate the effect of the dislocation length on strength.

In this configuration, a shear stress of \(\frac{\Gamma_{APB}}{b}\) on the leading dislocation is needed to shear through the precipitate. This stress arises from two sources, the applied shear stress, \(\tau_{\text{applied}}\), and the interaction shear stress, \(\tau_{\text{interaction}}\), with the trailing dislocation (which is repulsive). The latter is given by Hirth and Lothe (1982)
where $\alpha$ is a factor that depends on the dislocation orientation and $l$ is the distance between the two dislocations. At the same time, the distance $l$ depends on the applied shear stress $\tau_a$. At zero applied stress, the leading dislocation is blocked at the precipitate interface, as the applied stress increases the trailing dislocation is brought closer to the leading dislocation. Under any applied stress, the trailing dislocation is under static equilibrium due to the repulsion from the leading dislocation and the forcing of the applied stress, thus, the equilibrium distance $l_{eq}$ is given by

$$
\tau_l = \frac{\alpha \mu b}{l}
$$

Fig. 14. A pair of dislocations (black) shearing through a cubic precipitate (gray) at the center of a cubic simulation cell: (a) the pair is outside the precipitate; (b) when the applied stress is high the two dislocations combine to form a superdislocation since the leading dislocation is blocked at the surface of the precipitate; (c) the superdislocation shears into the precipitate; and (d) glides through it such that the pair bounds an APB region.

Fig. 15. The critical resolved shear stress for the case of a superdislocation shearing through a single precipitate spanning the entire crystal volume versus the precipitate's APB energy.
\[ \tau_{eq} = \frac{a_p b}{\tau_o} \]  \hspace{1cm} (12)

When the leading dislocation shears into the precipitate, the force equilibrium on the leading dislocation is the balance of the APB resistance on one hand, and the applied and interaction stresses on the other, such that:

\[ \frac{\tau_{APB}}{b} = \tau_a + \tau_i = \frac{a_p b}{\sigma_{eq}} + \tau_a = \frac{a_p b}{\tau_a} + \tau_a = 2\tau_a \]  \hspace{1cm} (13)

Hence, the condition for shearing the precipitate is that the applied resolved shear stress should be \( \tau_a = \frac{\tau_{APB}}{2} \). Fig. 15 shows the variation of the critical resolved shear strength with the APB energy for all the simulated cases. A linear variation can be observed in agreement with the prediction from Eq. (13).

References


