Abnormal subgrain growth in a dislocation-based model of recovery

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Abstract
Simulation of subgrain growth during recovery is carried out using two-dimensional discrete dislocation dynamics on a hexagonal crystal lattice having three symmetric slip planes. To account for elevated temperature (i) dislocation climb was allowed and (ii) a Langevin type thermal noise was added to the force acting on the dislocations. During the simulation, a random ensemble of dislocations develops into a subgrain structure and power-law type growth kinetics are observed. The growth exponent is found to be independent of the climb mobility, but dependent on the temperature introduced by the thermal noise. The in-depth statistical analysis of the subgrain structure shows that the coarsening is abnormal, i.e. larger cells grow faster than the small ones, while the average misorientation between the adjacent subgrains remains nearly constant. During the coarsening Holt’s relation is found not to be fulfilled, such that the average subgrain size is not proportional to the average dislocation spacing. These findings are consistent with recent high precision experiments on recovery.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

During the initial stages of annealing of a highly deformed metal, dislocations organize into low angle grain boundaries (LAGBs) that enclose cells (subgrains) with low dislocation content [1]. At elevated temperatures these walls are mobile leading to the gradual coarsening of the subgrains. This phenomenon, known as recovery, has a particularly important role, for instance in the nucleation of recrystallization [1].

The experimental investigation of recovery is rather difficult, since it is obscured by the early onset of recrystallization, and usually only a relatively small amount of subgrain growth can be observed [2–4]. Recently, however, measurements were carried out on specimens
of certain orientation and deformation modes, where the recrystallization is suppressed, and much more subgrain growth occurs [5–7]. Due to the development of precise orientation measurement techniques [8], these new experimental results shed new light on the physics of recovery. The most important findings revealed the abnormality of growth, with large subgrains growing faster than small ones [5, 6], and that the coarsening obeys type 2 kinetics [1, 6, 7]. The latter means that the time dependence of the average subgrain diameter \( D \) is well approximated by a power law

\[
D^n - D_0^n = ct,
\]

with \( D_0 \) being the cell size at \( t = 0 \) and \( c \) being an appropriate constant. The growth exponent \( n \) was found to depend strongly on the annealing temperature and on the initial microstructure with values in the range \( \sim 2–7.5 \) [1, 6]. Additionally, the size distribution of the grains was observed to be close to lognormal, and its variance was found to increase faster than its average in time [5, 7].

Several methods have been proposed to model subgrain growth. Molecular dynamics offers the possibility of investigating the dynamical aspects of recovery at the microstructural scale of individual atoms; however, computationally such simulations are too expensive [9, 10]. For example in the MD simulations performed in [9] with a volume of \( 70 \times 70 \times 1.5 \text{ nm}^3 \) and containing 25 subgrains of 15 nm diameter, the portion of grain/subgrain growth within the timeframe of 7 ns is quite limited. Such a simulation is at the limit of both time and length scales possible with MD simulations. To overcome these constraints several mesoscopic models have been proposed, including Monte Carlo Potts models (e.g. [11, 12]), the phase-field method (e.g. [13]) and vertex simulations (e.g. [14–16])—all of them relying on input parameters such as grain boundary mobility or energy.

During recovery mainly LAGBs are moving, where the misorientation between adjacent subgrains is less than \( \sim 15^\circ \). In this case the dislocation cores do not overlap, thus it is completely justified to study the properties of LAGBs within the framework of dislocation theory (see [17] or [18] for reviews). However, only a few results have been published concerning dislocation-based modelling of cell formation and coarsening. They either focused on LAGB mobility measurements (e.g. [19]) or on a limited ensemble (e.g. [20]). Recently, a new algorithm was developed by Bakó et al., which, due to a certain multipole method, made it possible to study a much larger number of dislocations than before [21, 22]. It was shown that enabling climb leads to cell formation and subsequent subgrain growth with the description of this growth given in terms of power laws [21, 22].

In this paper this two-dimensional (2D) discrete dislocation dynamics (DDD) technique is developed further. As described in section 2, the modifications are undertaken in order to increase the computational precision, include thermal noise and use core regularized stress fields to account for dislocation core effects. Due to the improvements, the maximum number of dislocations increases to \( N = 200\,000 \) in a single simulation run. A method is also developed in this work to obtain the corresponding orientation field and the reconstructed subgrain structure. In section 3 a detailed analysis of the observed subgrain growth is carried out in terms of experimentally measurable quantities. The comparison of the model predictions with the experimental findings is given in the second part of section 3 before concluding.

2. Applied methods

2.1. Two-dimensional DDD

The simulation of the motion and interaction of individual dislocations is carried out using DDD in two dimensions. The main features of the method are summarized as follows.
The system consists of parallel edge dislocations which are perpendicular to the plane of the square-shaped simulation area of size $L \times L$. Three possible Burgers vector directions $\pm (\cos(m\pi/3), \sin(m\pi/3))$, $m = 0, 1, 2$ are considered, emulating a hexagonal underlying lattice. Periodic boundary conditions are applied and overdamped dynamics are assumed for the dislocation motion.

The stress field of the dislocations is long-range, and therefore at every time step all the pair interactions have to be taken into account, which results in an $O(N^2)$ algorithm, where $N$ is the total number of dislocations. This time complexity makes it impossible to study a large number of dislocations ($N \geq 10000$). To be able to consider a larger ensemble of dislocations Bakó et al used coarse grained stress fields instead of the analytical ones, which allows the direct calculation of the pair interactions to be skipped [21]. The main idea is to build up a coarse grained discrete Burgers vector density field $(\alpha_x(l, m), \alpha_y(l, m))$ defined on an $M \times M$ mesh. Let $\alpha_x(l, m)$ and $\alpha_y(l, m)$ denote the $x$ and $y$ coordinate of the net Burgers vector divided by the box area in the box indexed by $(l, m)$. From this field the coarse grained stress field can be determined on the same mesh using a discrete convolutional integral. The approximation here is that the stress field is calculated as if each dislocation was at the centre of its cell, so it corresponds to a first-order multipole approximation. For further details of the method, of the used periodic stress fields and of the convolution procedure the reader is referred to [21]. The most important feature of the method is the reduction of the computational demand which allows the inclusion of a much larger number of dislocations than previously (now up to 200000 compared with a few thousands).

In this paper the numerical precision of the $O(N^2)$ algorithm and the more advantageous time complexity of the coarse grained method is combined. To this end, the following modifications have been included:

(i) In contrast with the previous method of [21] where, when determining the $\alpha_i(l, m)$ fields, each dislocation only contributed to the cell which contained it, here the Burgers vector is distributed between the four closest cells weighted with a bilinear approximation term. With the notations of figure 1, if the dislocation is positioned between the mesh points $(x_i, y_j)$ and $(x_{i+1}, y_{j+1})$, then the weight for the $(i, j)$ node is $w_{i, j} := (1 - \Delta x)(1 - \Delta y)/\delta^2$, for the $(i + 1, j)$ node $w_{i+1, j} := \Delta x(1 - \Delta y)/\delta^2$, etc, where $\delta := 1/M$. As a result, when a dislocation moves from one cell to a neighbour cell, there will be no sudden jumps in the $\alpha_i(l, m)$ field, and therefore, also in the coarse grained stress field.
(ii) After performing the convolution, the calculated coarse grained shear stress field is given on the $M \times M$ discrete mesh $\tau_{cg}(i, j)$. To obtain a smooth (continuous) stress field $\tau_{cg}^{\text{intp}}(x, y)$ we introduce an other bilinear interpolation between the cells as

$$
\tau_{cg}^{\text{intp}}(x, y) := w_{i,j} \tau_{cg}(i, j) + w_{i,i+1,j} \tau_{cg}(i+1, j) + w_{i,j,j+1} \tau_{cg}(i, j+1) + w_{i+1,j+1} \tau_{cg}(i+1, j+1)
$$

with the same weighting factors $w_{i,j}$ as in the previous point. The same is done for the $xx$ and $yy$ component of the stress tensor. The forces acting on dislocations are then computed using these continuous stress fields.

(iii) To decrease the inaccuracy introduced by the method a length parameter $R_e$ is introduced. If two dislocations are closer to each other than $R_e$, their interaction is calculated analytically and not through the coarse grained field\(^3\). The value of $R_e$ is chosen to be much larger than the average dislocation spacing and the grid point distance $1/M$.

(iv) To account for the fact that close to the dislocation core the generated stress field does not diverge as $1/r$, the core regularized stress fields described in [23] are implemented. In this case a new parameter, the core radius $r_c$ is introduced which is of the order of the Burgers vector. In figure 2 the behaviour of the regularized fields is demonstrated by plotting the $xy$ component of the stress field induced by a dislocation in its glide plane.

This modified method is completely continuous, and introduces some approximation only at the interaction of far dislocations. To test the level of the error, the dependence of the results on $R_e$ has been studied. It was found that if $R_e \gtrsim 2 \rho^{-0.5}$, then this dependence is negligible (here $\rho$ stands for the total dislocation density and $\rho^{-0.5}$ is the average dislocation spacing). In the rest of this paper this criterion is always fulfilled.

To mimic the effect of temperature, dislocation climb is allowed using the simplest possible mobility rule:

$$
v_g = M_g F_g \quad \text{and} \quad v_c = M_c F_c,
$$

\(^3\) This means that in practice first the stress contribution of each close dislocation in the coarse grained field has to be subtracted. To this end the double interpolation scheme of point (i) and (ii) has to be evaluated separately for these dislocations. Then the analytical stress field is added.
where \( v_g \) and \( v_c \) are the glide and climb velocity of the dislocation, \( F_g \) and \( F_c \) are the glide and climb components of the acting Peach–Köhler force, \( M_g \) is the glide and \( M_c \) is the climb mobility. Since the magnitude of the mobilities can be absorbed into the time scale [24], the only parameter that affects the dynamics is the ratio \( \eta := M_c/M_g \) between the two mobilities.

In addition to enhancing dislocation climb, temperature has another important effect on dislocation motion: it induces a random movement due to the thermal noise. This should be introduced into the model. Usually it is accounted for by adding a stochastic component to the force acting on the dislocation segments [25–27]. In this work, when the dynamics are overdamped, it is equivalent to adding a stochastic component to the position (Langevin dynamics). This means that after every time step all the dislocations are shifted with \( \Delta x_g \) in the glide, and with \( \Delta x_c \) in the climb directions. The \( \Delta x_g, c \) values are independent, normally distributed random variables with zero mean and, according to the description of Langevin dynamics [28], a half width of

\[
\Sigma^2_{g,c} = \frac{2 M_{g,c} k_B T \Delta t}{\Delta l},
\]

where \( T \) is the temperature, \( k_B \) is the Boltzmann factor, \( \Delta t \) is the actual time step and \( \Delta l \) is the length of the dislocation segment. Note that this half width is the same as in [27], but slightly different from the results reported in [25, 26].

The equation of motion (3) is solved by a fifth-order Runge–Kutta method [29]. Annihilation events are introduced if two or three dislocations with zero net Burgers vector are closer to each other than a certain predefined value \( d_{\text{annih}} \).

2.2. Simulation parameters and dimensionless variables

The simulations are started from random distributions of \( N = 200,000 \) dislocations. The initial number of dislocations is equal on all three slip planes, and the net Burgers vector is zero. The core radius is set to \( r_c = L/2000 \), which is around 20% of the initial average dislocation spacing, and decreases to around 5% during a typical simulation. For the coarse graining mesh \( M = 512 \) is chosen. The parameter \( \eta \) is varied between 0.02 and 0.25. The annihilation distance \( d_{\text{annih}} \) was set to be equal to the core radius \( r_c \).

According to the equation of motion (3), the material parameters can be absorbed into the time scale [24]. In contrast to the situation in [24], here the dislocation density is not constant and a new length scale \( r_c \) has been introduced, so it is advantageous to use \( L \) as the normalizing length scale instead of the average dislocation spacing. The dimensionless variables (denoted with prime (‘)) are, therefore, defined as

\[
x' := x/L \quad \text{and} \quad t' := t M_g b^2 / L^2,
\]

where \( b \) is the magnitude of the Burgers vector and \( G = \mu/[2\pi(1-\nu)] \), with \( \mu \) and \( \nu \) being the shear modulus and Poisson’s ratio, respectively.

With the above definitions it is convenient to introduce the dimensionless temperature as

\[
T' := \frac{4\pi(1-\nu) k_B T}{\mu b^2 \Delta l},
\]

in order to get

\[
\Sigma^2_g = T' \Delta t' \quad \text{and} \quad \Sigma^2_c = \frac{M_c}{M_g} T' \Delta t'.
\]

The dimensionless temperature \( T' \) estimates the ratio between \( k_B T \) and the energy of an edge dislocation of length \( \Delta l \). To approximate \( T' \) in 3D crystals, one might consider the elastic
 constants and the Burgers vector of aluminium at $T = 600$ K. The average segment length $\Delta l$ is approximated by the average local dislocation distance, the only length parameter present in the system at this scale. In small angle grain boundaries as a typical value $\Delta l = 10^{-8}$ m is taken. With these data $T' = 2.6 \times 10^{-2}$ is obtained. In this paper $T'$ varies between 0 and 0.2, because pronounced effects were observed in this range. One should be careful, however, with comparing temperature values of 2D and 3D systems, as thermal effects can be rather different in the two cases.

2.3. Characterization of the subgrain structure

During the simulations subgrains form and then grow, in agreement with earlier investigations [20, 21]. A typical sequence of dislocation configurations observed (if dislocation climb is present) is plotted in figure 3. Although subgrain formation is apparent, it is not straightforward to define the distinct subgrains from the position data of the individual dislocations. The method applied is now described (and is similar to the one of [20]). According to the Kröner–Kosevich continuum theory of dislocations, in the present case, the orientation field $\omega(r)$ is connected to the dislocation density tensor $\alpha$ as [30]

$$\partial_x \omega = \alpha_x \quad \text{and} \quad \partial_y \omega = \alpha_y,$$

(8)

where the notations $\alpha_x := \alpha_{31}$ and $\alpha_y := \alpha_{32}$ are introduced. These quantities are the continuum versions of $\alpha_{x,y}(l, m)$ defined in section 2.1. Equations (8) can be transformed into

4 In the Kröner–Kosevich continuum theory a quantity called the ‘dislocation part of the relative rotation’ is introduced, which is the non-elastic component of the rotation field, and is denoted by $\theta$. The introduced $\omega$ field corresponds to the $z$ component of this field.
a Poisson equation

$$\Delta \omega = \partial_x \alpha_x + \partial_y \alpha_y,$$  \hspace{1cm} (9)

which can be solved efficiently on a discrete grid iteratively by a multigrid method [29]. Consequently, periodic boundary conditions are automatically fulfilled. Thus from the dislocation positions the discrete $\alpha_{x,y} (l, m)$ fields can be constructed, and then $\omega(l, m)$ follows from (9). This procedure can be performed on an arbitrarily smooth $K \times K$ mesh. Figure 4(b) shows the orientation map corresponding to the configuration of figure 4(a) for $K = 512$. It is important to note that without the introduction of core regularized stress fields it is not possible to define $b$ in a straightforward manner, and therefore, the $\theta \approx b/d$ misorientation cannot be defined. In the present setup, however, one can assume $b := r_c$, leading to defined $\omega$ values in figure 4(b). Hence, the misorientation values are directly comparable to the experiments.

The subgrain structure is then derived by locating close to constant orientation regions on the $\omega$ field. Figure 4(c) shows the structure derived from figure 4(b), the colours referring to the average orientation in the subgrain. According to figure 4(c), the large subgrains are determined confidently, while there is some arbitrariness in the definition of the small ones. This is the direct reflection of the unavoidable uncertainty of the subgrain definition. After the subgrain structure has been reconstructed the average area $\overline{A}$ and the standard deviation $\delta A$ can be measured. The linear size is then $D := \sqrt{\overline{A}}$ and $\delta D := \sqrt{\delta A}$.

The subgrain sizes are of course not uniform, they obey a certain distribution $P(A)$, where $A$ denotes the area of a subgrain. From the reconstructed structure of figure 4(c)
$P(A)$ is easily obtained. For better numerical accuracy the cumulative distribution function $F(A)$ of $P(A)$ was constructed and then averaging was performed over statistically equivalent realizations of the system. In figure 4(d) $F(A)$ is plotted, and one can conclude from the fit that the distribution is close to lognormal (just like in experiments [5, 7]). Note that here and in the rest of the paper, ensemble averaging is always performed over 16 independent simulation runs.

2.4. Possible effects of 2D modelling

Two-dimensional mesoscopic methods are rather usual for grain/subgrain growth modelling and provide excellent qualitative comparisons with experiments, enabling an insight into the mechanisms at play which cannot be deduced from experiment. They mostly assume relations for the subgrain boundary mobility or energy. The model described above is microscopic, as it is based on individual dislocations, the basic component of subgrain boundaries. As such, no assumption has to be made on mesoscopic properties like subgrain boundary mobility. It is planned, however, to extract such properties in a forthcoming publication.

The 2D dislocation model lacks a few features present in 3D dislocation structures. The most important among them is that in 2D the evolving subgrain boundaries consist of an array of parallel edge dislocations, contrary to a complex network of edge and screw dislocations in 3D. This simplification might affect the mobilities of the boundaries, and, consequently, the properties of growth. According to figure 3, however, the boundary directions seem to be quite isotropic, not preferring the slip plane orientations (having a 0°, 60° and 120° angle with the $x$ axis). This means that the boundaries contain dislocations from different slip planes, and, therefore, climb is always needed for them to move. Hence, despite the difference in the boundary structure, the mobility-misorientation relation is not expected to show fundamental differences between 2D and 3D. It is noted that the main advantage of this model is that it incorporates properly the long-range stress fields of the dislocations, and also the stress screening phenomenon, found to be very important in the physics of dislocation systems [31]. A quantitative agreement with the experiments is, of course, beyond the capabilities of this model.

It is important to add that there is another practical relevance of 2D modelling, namely, that it is directly comparable to real 2D crystals with a triangular lattice. Examples include dusty plasmas [32, 33], vortex lattices in type II superconducting films [34, 35], colloidal crystals [36, 37] and foams [38]. Recently, grain coarsening was studied experimentally and by simulations in dusty plasmas [39], and the observed growth was quite similar to the results of this paper.

3. Results

3.1. Power-law growth

First the effect of the climb mobility is investigated, whereby simulations with different $\eta$ values have been performed at $T' = 0$. As seen in figure 5, the average subgrain size $\bar{D}'$ follows power-law kinetics. Since the smallest identifiable subgrain is limited by the resolution of the mesh on which (9) is solved, at small $t'$ values a higher average is obtained than the real value. On the other hand, when $\bar{D}' \approx 0.1$, the size of the largest subgrains is already in the order of the system size $L$, which biases the average in the other direction. Nevertheless, the power-law regime lasts for more than 1.5 decades in time, which confirms that the coarsening obeys type
The average subgrain size evolution at $T' = 0$ and different climb mobilities. The values were plotted against $t' \eta$.

Figure 5.

The average subgrain size as a function of time at $\eta = 0.1$ and different $T'$ values.

Figure 6.

2 kinetics. From the fit $n = 2.9 \pm 0.2$ is obtained, which is not far from the experimentally observed low-temperature values [1, 6].

The other consequence of figure 5 is that the power-law exponent does not depend on $\eta$. More precisely, a slight deviation is only seen when $\eta$ is larger than 0.1. This is consistent with the results of Hartmaier et al [40] who studied the creep properties of thin films. Therefore $\eta = 0.1$ is implemented in the rest of the work presented in this paper. Moreover, the curves almost overlap when they are plotted versus $t' \eta$ indicating that the climb rate only modifies the time scale of the simulation but not the nature of the dynamics.

The constancy of the power-law exponent contradicts experimental findings which report decreasing $n$ with increasing temperature [1, 6]. However, the addition of thermal noise to the dislocation motion (as described in section 2.1) leads to the expected increase in the power-law exponent, that is, to the decrease in $n$. This is demonstrated in figure 6, where it is seen that the exponent of $n = 2.9 \pm 0.2$ decreases to about $2.2 \pm 0.2$. The numerical values of the exponents are different from the experimental values, which is one of the limitations faced by a 2D model studying a 3D phenomenon. In addition, several mechanisms that hinder boundary motion,
such as dislocation-point defect interactions, are not considered. The tendency observed, however, is in good agreement with the experiments [1, 6].

The exponent was found to depend on the initial number of dislocations $N_0$ as well as on the core radius $r_c$. As seen in figure 7, $n$ increases as the core radius and the initial density grow and as expected, only the $r_c/\rho_0^{-0.5}$ ratio, i.e. the ratio between the core radius and the average dislocation spacing, is important. A possible reason for this dependence could be that the mobility of a dislocation wall increases with decreasing core radius. However, for a thorough explanation further studies are required.

It is also instructive to look at the evolution of the average misorientation between adjacent subgrains. Starting from the reconstructed subgrains of figure 4(c) the mean misorientation $\bar{\theta}$ was measured which is by definition the mean misorientation between all possible neighbour subgrain pairs. As seen in figure 8, a slowly growing average misorientation was found which is non-sensitive to the climb mobility and its growth rate decreases with increasing temperature. In experiments $\bar{\theta}$ was found to be nearly constant [6]. In this work the growth rate is low, and is even decreasing at high temperatures, thus providing good qualitative agreement.

The discussion now returns to growth exponents. It was found above that the exponents $n$ are slightly below the experimentally obtained values. They are surprisingly high, however, if compared with the predictions of the existing models of subgrain growth kinetics. Models based on dislocation climb predict parabolic subgrain growth, i.e. $n = 2$ [1, 4, 41, 42]. As a possible solution for the discrepancy it was suggested that the thermally activated migration of the ledges is the rate controlling mechanism [4], or the gradual decrease in the average misorientation is responsible for the increased exponent [6] and not the climb. According to these simulation results it is evident that a simple climb model is able to account for an exponent of $n = 3.3$, even with a slightly increasing average misorientation. Thus it is likely that some important feature of subgrain growth is missing from the existing climb-based models, which should, therefore, be revised.

3.2. Discontinuous subgrain growth

During discontinuous (or abnormal) subgrain growth large cells grow faster than small ones, which leads to an inhomogeneous subgrain distribution during annealing. This type of growth
was confirmed by recent experiments [5, 6]. A simple consequence of this behaviour is that the subgrain structure is not self-similar, and the scaled size distribution of subgrains broadens with time.

From the reconstructed subgrain structures the average linear size of the subgrains ($D'$) and its standard deviation ($\delta D'$) were measured as described in section 2.3. In figure 9 the evolution of the relative scattering $\delta D' / D'$ is plotted at various simulation parameters, and figure 10 plots the evolution of subgrain size distributions. It is evident that the growth is discontinuous, and that neither the temperature nor the climb rate has any effect on it.

3.3. Length scales in the microstructure

It is commonly assumed that in large dislocation systems there is only one length parameter: the average dislocation spacing $\rho^{-0.5}$. This means that dislocation structures are scalable, which in the case of cell sizes $D$ is expressed by Holt’s relation [43]

$$D = K \rho^{-0.5},$$

(10)
Figure 10. The evolution of the subgrain size $A'$ distribution at $T' = 10^{-1}$, and the lognormal fits (dashed lines). At other simulation parameters the evolution looks rather similar.

Figure 11. The average cell size ($\bar{D}$) versus the average dislocation spacing $\rho^{-0.5}$. Holt’s relation would imply a linear dependence.

where $K$ is a suitable constant. Relation (10) was proven experimentally for example on deformed iron [43], on crept LiF [44] or more recently on doped GaAs [45]. It is surprising, therefore, that Holt’s relation (10) contradicts the observed abnormal nature of subgrain growth. Namely, if there is only one length parameter (the system is scalable) only self-similar, i.e. normal growth, is possible. But in the present case to describe the size distribution at least two length parameters are needed (its mean and its deviation) since the observed relative scattering of cell sizes increases, and therefore the growth rate cannot be normal.

It was already mentioned that in these simulations together with the core regularized stress fields a new length parameter, the core radius $r_c$ was introduced. Since Holt’s scaling argument only assumes a $1/r$ type dislocation stress field, this could solve the contradiction. Hence, the simulations were repeated with different core radii, and the average cell diameter $\bar{D}$ dependence on the average dislocation distance $\rho^{-0.5}$ was investigated. Figure 11 shows that the effect of $r_c$ is negligible on the $\bar{D} = \rho^{-0.5}$ relation. This is understood as the average distance of dislocations in the LAGBs was found to be at least 3 times larger than the core
radius \( r_c \), even at the highest value of \( r_c \). Hence, it is not the introduction of core regularized fields that breaks Holt’s relation.

The contradiction can be removed if the initial dislocation density rather than the instantaneous dislocation density is considered in the scaling relation (10). In figure 12 the average misorientation \( \bar{\theta} \) was plotted as a function of the average subgrain size \( \bar{D} \) at different initial dislocation densities \( \rho_0 \). The latter simply indicates the different number of initial dislocations in the \( L \times L \) simulation box. In addition, the misorientation was divided by the initial average dislocation spacing. The curves fully overlap revealing \( \bar{\theta} = K\rho_0^{-0.5} \), with \( K \) depending on time, average subgrain size, etc.

It is reasonable to assume, therefore, that during the initial stages of the simulations, when the first dislocation walls are formed from the random arrangement of dislocations, the average distance of the dislocations within the walls must scale with \( \rho_0^{-0.5} \). According to this discussion, this distance, which is directly related to \( \bar{\theta} \) through Frank’s formula, remains nearly constant throughout the growth process. To understand the slight increase observed, which cannot be explained by simple energy considerations\(^5\), requires further studies.

Note that contrary to the present investigations, in the previous work of Bakó et al. [21], Holt’s relation was found to be satisfied throughout the growth process. After the more precise analysis of this paper, the conclusion obtained is that those results were due to numerical noise. The latter is similar to thermal noise, such that those results should be regarded as if very high temperature was applied (see figure 6).

The next question to be addressed is why Holt’s relation is valid in a wide range of systems with cell structure. The possible reason is that in those cases subgrain formation is induced by external stress, rather than being a simple growth phenomenon. It is well known that during creep, the subgrain structure is characterized by a dynamic equilibrium, that is, the plastic strain is produced by the moving subgrain walls, but still, the average subgrain size remains constant [46]. In this state, the net dislocation annihilation must be balanced by creation mechanisms. The latter is absent in this model and also during recovery. In summation, from

\(^5\) The energy of a subgrain boundary increases with misorientation [1], therefore one may expect that higher angle boundaries would disappear with higher probability than lower angle ones.
this investigation it is evident that dislocation creation is the key to the dynamic equilibrium during creep, and to the fulfilment of Holt’s relation.

4. Conclusions

Cellular dislocation patterning and its growth phenomenon have been investigated within a simple 2D DDD model. The effects of the climb rate, the thermal noise and the size of the dislocation core radius on the kinetics of growth have been studied. The main results of the paper are as follows:

(i) The coarsening follows power-law kinetics, with a growth exponent not depending on the dislocation climb mobility but rather on the thermal noise and core radius.
(ii) The size distribution of the subgrains was close to lognormal, which broadened with time. This means that growth is abnormal (discontinuous).
(iii) Holt’s relation is not fulfilled in the conventional way—the average subgrain size is proportional to the initial dislocation spacing not to the temporal spacing.
(iv) The average misorientation between the adjacent subgrains slightly increases throughout the growth process.
(v) Despite the simplicity of this model, all of the above results are in qualitative agreement with the experiments.
(vi) In contrast to previous dislocation climb-based models, our simulations yield growth exponents considerably larger than $n = 2$.

These results indicate the success of using 2D DDD in modelling subgrain coarsening.

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References

[1] Humphreys F J and Hatherly M 2004 Recrystallization and Related Annealing Phenomena 2 edn (Oxford: Pergamon)
[2] Sandström R, Lehtinen E, Hedman B, Groza I and Karlsson J 1978 Subgrain growth in Al and Al–1% Mn during annealing J. Mater. Sci. 13 1229–42
[3] Varma S K 1986 Effects of the amount of prior cold work and annealing temperature on subgrain growth in Al–0.2Mg alloy Mater. Sci. Eng. 82 L19–L22
[4] Furu T, Ørsund R and Nes E 1995 Subgrain growth in heavily deformed aluminium-experimental investigation and modelling treatment Acta Metall. Mater. 43 2209–32
[5] Ferry M and Humphreys F J 1996 Discontinuous subgrain growth in deformed and annealed \{110\} (001) aluminium single crystals Acta Mater. 44 1293–308
[6] Huang Y and Humphreys F J 2000 Subgrain growth and low angle boundary mobility in aluminium crystals of orientation \{110\}(001) Acta Mater. 48 2017–30
[7] Ferry M and Burhan N 2007 Structural and kinetic aspects of continuous grain coarsening in a fine-grained Al–0.35c alloy Acta Mater. 55 3479–91
[8] Humphreys F J 2001 Grain and subgrain characterisation by electron backscatter diffraction J. Mater. Sci. 36 3833–54
[9] Haslam A J, Philpott S R, Wolf D, Moldovan D and Gleiter H 2001 Mechanisms of grain growth in nanocrystalline fcc metals by molecular-dynamics simulation Mater. Sci. Eng. A 318 293–312
[10] Haslam A J, Moldovan D, Yamakov V, Wolf D, Philpott S R and Gleiter H 2003 Stress-enhanced grain growth in a nanocrystalline material by molecular-dynamics simulation Acta Mater. 51 2097–112
[11] Holm E A, Miodownik M A and Rollett A D 2003 On abnormal subgrain growth and the origin of recrystallisation nuclei Acta Mater. 51 2701–16
[12] Holm E A, Miodownik M A and Rollett A D 2004 A subgrain growth model for strain-free grain nucleation during recrystallisation Mater. Sci. Forum 467-470 611–6
[13] Ma N, Kazaryan A, Dregia S A and Wang Y 2004 Computer simulation of texture evolution during grain growth: effect of boundary properties and initial microstructure Acta Mater. 52 3869–79
[14] Humphreys F J 1992 Modelling mechanisms and microstructures of recrystallisation Mater. Sci. Technol. 8 135–44
[15] Weygand D, Bréchet Y and Lépineux J 1999 Zener pinning and grain growth: a two-dimensional vertex computer simulation Acta Mater. 47 961–70
[16] Hayes J S, Prangnell P B and Bate P S 2002 Modelling the microstructural evolution during annealing of a severely deformed Al–3% Mg alloy Ultrafine Grained Materials II ed Y T Zhu et al (TMS, Warrendale, PA) pp 495–504
[17] Sutton A P and Balluffi R W 2007 Interfaces in Crystalline Materials (Oxford: Oxford University Press)
[18] Gottstein G and Shvindlerman L S 1999 Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications (Boca Raton, FL: CRC Press)
[19] Lim A T, Srolovitz D J and Haataja M 2009 Low-angle grain boundary migration in the presence of extrinsic dislocations Acta Mater. 57 S013–22
[20] Argaman N, Levy O and Makov G 2001 When do 2-D dislocations form cellular structures? Mater. Sci. Eng. A 309–310 386–92
[21] Bakó B, Györgyi G and Zimányi G 2006 Dislocation patterning: the role of climb in meso-scale simulations Comput. Mater. Sci. 38 22–8
[22] Bakó B, Györgyi G and Zimányi G T 2007 Dislocation glasses: Aging during relaxation and coarsening Phys. Rev. Lett. 98 075701
[23] Groma I, Györgyi G and Ispányovity P D 2010 Variational approach in dislocation theory Phil. Mag. 90 3679–95
[24] Csikor F F, Zaiser M, Ispányovity P D and Groma I 2009 The role of density fluctuations in the relaxation of random dislocation systems J. Stat. Mech. P03036
[25] Rönnpelgel D, Streit Th and Pretorius Th 1993 Including thermal activation in simulation calculations of dislocation glide Phys. Status Solidi 135 445–54
[26] Raabe D 1998 Introduction of a hybrid model for the discrete 3D simulation of dislocation dynamics Comput. Mater. Sci. 11 1–15
[27] Hiranani M and Zhbi H M 2002 Stochastic dislocation dynamics for dislocation-defects interaction: a multiscale modeling approach J. Eng. Mater. Technol. 124 335–41
[28] Risken H 1989 The Fokker–Planck Equation 2nd edn (Berlin: Springer)
[29] Kröner E 1981 Continuum theory of defects Physics of Defects Proc. Les Houches Summer School, Session XXXV ed R Bian et al (North-Holland: Amsterdam) pp 215–314
[30] Groma I, Györgyi G and Kocsis B 2006 Debye screening of dislocations Phys. Rev. Lett. 96 165503
[31] Quinn R A and Goree J 2001 Experimental test of two-dimensional melting through disclination unbinding Phys. Rev. E 64 051404
[32] Novosel V, Zhdanov S, Iliev A V, Morfill G, Goree J and Piel A 2008 Heat transport in a two-dimensional complex (dusty) plasma at melting conditions Phys. Rev. Lett. 100 025003
[33] Blatter G, Feigel’man M V, Geshkenbein V B, Larkin A I and Vinokur V M 1994 Vortices in high-temperature superconductors Rev. Mod. Phys. 66 1125–388
[34] Miguel M-C and Zapperi S 2003 Tearing transition and plastic flow in superconducting thin films Nature Mater. 2 477–81
[35] Murray C A and Van Winkle D H 1987 Experimental observation of two-stage melting in a classical two-dimensional screened Coulomb system Phys. Rev. Lett. 58 1200–3
[36] Schall P, Cohen I, Weitz D A and Spaepen F 2004 Visualization of dislocation dynamics in colloidal crystals Science 305 1944–8
[37] Abd el Kader A and Earnshaw J C 1999 Shear-induced changes in two-dimensional foam Phys. Rev. Lett. 82 2610–13
[38] Hartmann P, Douglas A, Reyes J C, Matthews I S, Hyde T W, Kovács A and Donkó Z 2010 Crystallization dynamics of a single layer complex plasma Phys. Rev. Lett. 105 115004
[39] Hartmaier H G A and Buehler M J 2004 A discrete dislocation plasticity model of creep in polycrystalline thin films Defect Diffus. Forum 224–225 107–26
[41] Sandström R 1977 On recovery of dislocations in subgrains and subgrain coalescence Acta Metall. 25 897–904
[42] Sandström R 1977 Subgrain growth occurring by boundary migration Acta Metall. 25 905–11
[43] Holt D L 1970 Dislocation cell formation in metals J. Appl. Phys. 41 3197–201
[44] Reppich B 1971 Inhomogeneous dislocation distributions and the formation of dislocation cell structure J. Mater. Sci. 6 267–9
[45] Rudolph P, Frank-Rotsch Ch, Juda U and Kiessling F-M 2005 Scaling of dislocation cells in GaAs crystals by global numeric simulation and their restraint by in situ control of stoichiometry Mater. Sci. Eng. A 400–401 170–4
[46] Kassner M E 2009 Fundamentals of Creep in Metals and Alloys 2nd edn (Amsterdam: Elsevier)