Dislocation Dynamics in polycrystals with atomistic-informed mechanisms of dislocation-grain boundary interactions

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Abstract

At the mesoscale, plastic deformation is facilitated by the motion of dislocations and is strongly dependent on the local crystallographic orientation. In polycrystalline materials, the mismatch between adjacent crystals inhibits the inter-granular dislocation mobility, reduces plastic strain homogeneity and significantly influences the hardening and softening stress-strain behavior. Studies have shown that inter-granular slip transmission is possible at high stresses, involving a complex combination of dislocation absorption, junction formation and nucleation interactions with the intrinsic grain boundary dislocations. These effects are thought to contribute significantly to the behavior of dislocation pile-ups and could explain the predominant mechanisms influencing the properties of nanocrystalline materials. Modelling the mesoscale microstructure-property relationships, observed in real materials, would be very useful to guide future developments in the field of grain boundary engineering.

Dislocation dynamics (DD) simulations are a promising framework for computational modelling to provide insights about phenomena that can only be explained from the intermediate scale between atomistic and macro scales. However, a robust framework for modelling dislocation interactions with internal microstructure such as grain boundaries (GBs) has yet to be achieved for 3D models of DD at the meso-scale. Atomistic studies have shown that GBs cannot be assumed to act purely as an inertial damper between two regions with identical crystallography [1], or as an impenetrable barrier [2, 3]. The primary aim of the present study was to establish a sufficiently ‘generic’ framework to enable the modelling of various GB structures, polycrystal geometries and crystallographic orientations. The framework described is effective for studying GB-dislocation interactions (including inter-granular effects) and the approach for partitioning the DD simulation domain also provides an ideal future basis for modelling precipitate-hardened materials.

To achieve a robust method to differentiate between crystal regions, the present framework utilizes a mesh-based partitioning system. The simulation domain is meshed and “region IDs” are assigned to individual mesh elements. GBs are recognized as internal surfaces separating regions with different “IDs”. This flexible construction allows modeling of an arbitrary number of grains and grain orientation. Within each grain, slip systems are determined by the grain orientation, and grain boundary dislocations are created to accommodate the grain misorientation. These special dislocations are either of sessile or glissile character, depending on the grain boundary structure. The glissile structure cases allow for grain boundary sliding. An algorithm was developed to re-position any dislocations which would otherwise cross the mesh-region interface to exactly intersect the GB plane. Dislocations in the GB are constrained to glide in the GB plane. Atomistically informed criteria for “slip transmission” are implemented. In particular, ‘Slip transmission’ was enabled by simulating dislocation nucleation in the adjacent crystal if the local Peach Koehler force on the secondary slip system exceeds the threshold value (obtained with atomistic studies).

GBs contain intrinsic dislocations (GBDs) which must be considered carefully, particularly when attempting to model inter-granular interactions with mobile lattice dislocations. A dislocation extraction algorithm was used to analyze the atomistic structure of a low angle grain boundary and identify the appropriate spacing of GBDs within the DD simulation bi-crystal model. This work provides a means to study multi-grain deformation processes governed by dislocations that “pile-up” at grain boundaries, in detail beyond feasible limits of experiments.

Keywords: Dislocation dynamics; Molecular dynamics; Slip transmission; Strain burst; Micro-pillar; Coincident-site lattice; Hall-Petch; Bi-crystal.

Introduction

Since the proposal of Taylor's theory of work hardening 1934 [4], the materials research sector has aimed to achieve a physics-based multi-scale model to non-empirically predict the non-linear (plastic) stress-strain behavior and properties of dislocation-hardened metals. Such models need to account for the dynamically evolving dislocation and grain boundary microstructure [5]. Dislocations are well-established to facilitate the bulk of irreversible crystal deformation due to their high mobility along specific crystallographic slip systems [6]. For this reason, the properties of polycrystalline materials are predicated by the orientation of the slip systems with respect to the loading direction, and by the microstructure which inhibits the dislocation mobility. Grain boundaries (GBs) are an intrinsic microstructural component of all metal (excluding single crystals) and contribute both a barrier to dislocation mobility and the transition between different slip-deformation systems [5]. GBs primarily inhibit dislocation motion; however, trans-granular 'slip transmission' can occur via a corresponding nucleation of new, re-orientated dislocations in the adjacent crystal [7]. The GB structure can facilitate dislocation nucleation, annihilation and/or recombination, which may be the rate-limiting effects in nano-crystalline materials [8-10]. For these reasons, the impact of dislocation dynamics on the non-linear stress-strain properties of polycrystalline materials can only be truly understood when interactions with the 3D network of grain boundary microstructures is accounted for. However, GBs remain significantly under-represented within the computational modelling and simulation research sector for studying defect-driven plastic deformation, below the empirical 'macro-scale' crystal plasticity simulations [11].

Dislocation dynamics (DD) simulations are widely acknowledged as a breakthrough meso-scale technique, with the capacity to establish a phenomenological link between fundamental atomistic studies and macro-scale continuum models useful for real-world material design [11-14]. However, DD remains in a development stage and has yet to be implemented in a way that can accommodate dynamic grain boundary interactions in 3D, which is necessary to understand effects of dislocation pile-ups and re-oriented slip transmission [11]. Previous attempts to model polycrystal DD with mesoscale simulations are mostly limited to 2D DD with impenetrable GBs [2, 15-17], which recently have included more complex interactions such as slip transmission through the GB interface [18]. These studies offer valuable insights about the effect of grain boundaries on the unimpeded motion along singular slip systems. However, 2D methods are incapable of modelling the evolution of dislocation density because dislocations are 'pseudo point defects'. Furthermore, the 2D systems are artificially constrained to only 1, 2 or (at best) 3 slip systems [16]. It is unlikely that such models will ever be capable of effectively capturing the complexity of cross-slip, multi-junction formation or more complex long-range dislocation force-field effects. In terms of 3D DD, rudimentary models have been created to evaluate the stress-fields in 'bi-crystals' containing of an array of impenetrable dislocations, akin to a low-angle GB [15]. However, this model did not account for changing crystallography at the interface, and no algorithms were provided to enable dislocation intersection with the GB interface. Hence, this dislocation array study is a good first step but does not provide a realistic representation of a GB interface. A more sophisticated model was established by Kubin et al. in 2009 [2], involving a truly polycrystalline, multi-textured simulation. However, the GBs were modelled with as impenetrable interfaces and the model was incapable of compensating for dislocation interactions with the intrinsic GB dislocations or reproducing inter-granular slip transmission. The present study establishes a 3D DD methodology which is robust for modelling multiple GB character and polycrystal geometries, and applies this for a rudimentary study of a bi-crystal with a 'penetrable GB',

The equilibrium atomistic structure of the GB core and the spacing and Burgers vectors of the intrinsic GB dislocations (GBDs) are entirely dependent on the misorientation angle and interfacial plane of the GB intersecting two adjacent crystals. Low angle GBs can be fully described as an array of 'grain boundary dislocations' (GBDs), and have been observed to occur with misorientation angles less than the 'transition angle' which is approximately between 10-15° [19]. The dislocation structure of higher angle GBs are generally more difficult to classify, however it is commonly believed that in this case, the GB core consists of overlapping dislocations. These are difficult to classify as dislocations, because the overlapped cores cannot be identified by forming a Burgers circuit according to the conventional methodology. Energetically favorable structures of GBs involve a repeated 'structural unit' of equi-spaced clusters of GBDs [20-22]. In situations with high local stress concentration such as near nanoindenters [23] and inside dislocation pile-ups [24], mobile lattice dislocations can 'penetrate' through the GB by interacting with the GBDs. Specifically, lattice dislocations can indirectly 'transmit' across the GB by forming junctions with GBDs, partially annihilating and re-nucleating a new dislocation with different orientation in the adjacent crystal. To establish an initial benchmark for the newly developed simulation methodology, the first case will involve a bi-crystal containing two low angle GBs, which were chosen because of the low GBD density. The bi-crystal was selected as the most simple benchmark geometry for comparison with MD simulations, and to isolate the influence of the GBDs on the mechanical properties [25].

The present study describes a novel modification of 3D DD simulation method, utilizing an array of co-planar intrinsic dislocations to model GB - dislocation interactions at the meso-scale. This will enable future studies of the intrinsically mesoscale effects of dislocation pile-ups and size-strength (Hall-Petch) relationships.

Framework of conventional mesoscale dislocation dynamics simulations

This study utilizes the Mechanics of Defects Evolution Library (MoDEL) code, based on the parametric DD approach described by Ghoniem et al [26] and recently modified to improve the description of the dislocation core by Po et al. [27, 28]. The 'parametric' DD approach is ideal for 3D modelling of multi-defect dynamics to achieve efficient modelling of curved dislocations of arbitrary shape, orientation and length. Although DD remains a 'state-of-the-art' method due to the nature of its ongoing development [13], there is a long history of development since the 1990's [13, 27-33] [34]. At its core, the procedure of evaluating the Peach-Koehler force interactions, discretizing the motion, network configuration and shape is well-established [13, 35]. The present study does not go into detail about the fundamental framework (refer to [13, 28]), but rather describes the novel implementation of polycrystalline effects and GB-dislocation interactions within the established 3D DD framework. However, first it is necessary to describe the elements of the present framework that are modified and which enable the description of grain boundaries in a constitutive linear elastic framework.

In this implementation, DD simulations are coded with object-oriented C++ programming to model the discretized motion of dislocation loops and Frank-Read sources [13]. In its most fundamental form, DD is a meshless-continuum method with 'infinite' dimensions; however a mesh can be utilized for the implementation of fixed surface boundary conditions. This contributes only a surface effect; and retains the single crystal orientation and isotropic elastic properties of the medium without simulation sub-domains. This 'conventional framework' for DD simulations can be decomposed into the following four fundamental elements:

a) Dislocation nodes (1D)

Nodes store discrete positions in the dislocation line at each timestep, within the elastic continuum. *Each node is characterised by a specific ID, mesh tetrahedra and nodal velocity.*

b) Dislocation segments (2D)

Segments are mathematical splines that connect adjacent dislocation nodes in a dislocation loop. The curvature of the spline corresponds with the localised Peach-Koehler force-field at the specific timestep. As such, the discretised positions of dislocation segments are not stored between timesteps as in the case of dislocation nodes. *Segments are defined by the Burgers vector, glide plane normal vector, Peach-Koehler forces and external stress tensor.*

c) Dislocation network (3D)

The network is a container of all the dislocation segments in a 3D ensemble of dislocation loops and dislocation sources. *The network defines the self-interactions of dislocation segments within a single loop and interactions between different dislocations, and asserts the consistency of elastic criteria, such as the Burgers vectors and node-balance.*

d) Finite element mesh (optional – required for certain boundary conditions)

A mesh is not necessary, however must be used to model finite volumes and surface effects. Surface forces are implemented by creating artificial image forces, according to the original description provided by Van der Giessen et al [31]. *The mesh is defined by mesh tetrahedra defined by four positional points (nodes) and four triangular faces. Each mesh tetrahedra, face and node is assigned a unique ID number.*

Computational procedure for modelling polycrystal sub-regions in DD

The distinctive element of the present approach for modelling DD is the concept of 'region IDs', which can be assigned to all mesh tetrahedra within a user-specified geometry. Hence, all the mesh tetrahedra within the mesh region geometry (crystal) share the same region ID. The mesh is faceted with faces defined by any three of the four mesh nodes in each of the mesh tetrahedra. Each facet must always share the region IDs of the two adjoining tetrahedra or be a surface with only one region ID, and hence mesh facets must either have one or two region IDs. For the present case with a bi-crystal containing only one GB, this is sufficient to describe the interface. However, the method is also capable of modelling GB junctions of three or more crystals by identifying points lying on a mesh-line adjoining tetrahedra with more than two region IDs.

The mesh is independent of the dynamic behavior of the simulations, and hence within the current framework the region ID is an immutable component of the initial-state crystal geometry. While this inhibits the implementation of GB migration within the current framework, it is valuable to assure efficiency and avoid arbitrary distortion of the interfacial mesh. Hence, this original approach to defining the GB structure provides a robust, efficient and 'generic' basis for modelling polycrystals of complexity within a DD simulation.

To establish a polycrystal mesh, a template MATLAB script was developed [36] which could be modified to define the size of the mesh, interface orientation, and crystal region IDs for either a rectangular prism or a cylinder bi-crystal geometry. The mesh itself was generated with tetgen, using a Delauney tetrahedralization constrained by maximum tetrahedron volume to control the coarseness of the mesh [37]. All the mesh tetrahedra within the one of the sub-domains defined by the matlab script are assigned the same integer (region ID), that is unique to the crystal. It was necessary to ensure that dislocation nodes that intersect the mesh faces shared by two region IDs are coincidental with the GB interface. This was achieved by identifying any tetrahedra nodes that were within a nominal floating point distance tolerance interface plane, and modifying the positions of two adjacent mesh nodes so that the mesh faces were correctly aligned. Hence, the mesh-elements of the GB were defined so that any nodes incidental with a face sharing two region IDs would align correctly with both the GB plane and the internal crystallographic lattice.

Utilizing a dislocation array based on atomistic calculations to model GB structure

GBs may be described as a crystallographic structure of repeated atomistic structural units containing intrinsic GB dislocations (GBDs). However, characterization of the GBDs in high-angle GBs (misorientation > 15°) has been difficult to achieve due to the overlapped nature of the dislocation cores within the plane [20, 38]. Low-angle GBs are more readily modelled, due to the greater spacing between GBDs and subsequently greater ease for classifying the distinct atomistic dislocation cores [15, 39]. Three pure-tilt grain boundaries were simulated in full-atomistic from, using bi-crystals obtained with LAMMPs molecular dynamics simulations [40]. The GBD structure of the fully atomistic GB plane were analyzed using Stukowski's dislocation extraction algorithm [41]. The results are shown in Figure 1. The dislocation line-direction is parallel to the tilt axis, which is the same [0 0 1] direction for all three GB structures (as shown in Figure 1.A).

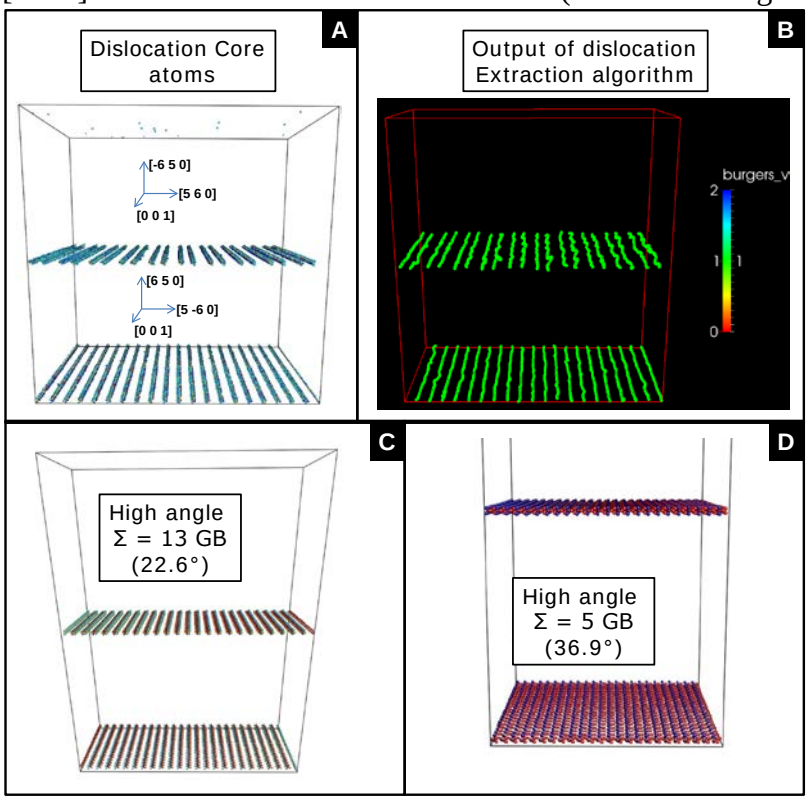

Figure 1: Structure of high and low angle GBs described in two formats. Atomistic structural GB units [20]: A) low angle (8.1°); C) high angle (22.6°); D) high angle (36.9). AND B) low angle GB - array of GBDs

Figure 1.b shows that the dislocation extraction algorithm effectively identifies intrinsic dislocations spaced at intervals equivalent to the atomistic structural GB units, only for the low angle GB case. However, the direct comparison of the atomistic structures of the different GBs provides an invaluable insight for modelling with some of the high angle GBs. This is because the spacing of atomistic structural units can be evaluated despite being unable to extract the dislocation content. For the current crystallographic misorientation, the inter-GBD spacing is 15.7 Å, (i.e., 6b, where b is the Burgers vector). The GBDs can be considered 'perfect' edge dislocations with full Burgers vectors aligned in the direction of the GB normal (the [6 5 0] or the [-6 5 0] directions). This is consistent with the symmetric pure-tilt 'parallel-edge wall' GBs described in ref. [42]. It is noteworthy that the 'nose-to-tail' spacing of the 'C' atomistic structural units (which are also described in detail in ref. [21]) is 6.1 Å for the Σ=13 case. Furthermore, for the case of the Σ=5 GB, which has a higher misorientation angle, the nose-to-tail spacing is 0.0 Å (i.e., there is no inter-GBD gap) between qualitatively identical 'C' atomistic structural units. This suggests that high angle GBs can be modelled in a similar manner as low-angle GBs, however with a reducing spacing between GBDs. The validity of this claim is the subject of future studies.

For the present study, the structure was based on the low-angle atomistic case to provide a first-case benchmark for comparison. As shown in Figure 2, intrinsic GBDs were assigned in DD simulations of a bi-crystal containing a planar GB with a normal vector in the vertical direction, with an equivalent spacing and Burgers vector character as obtained from atomistic analysis.

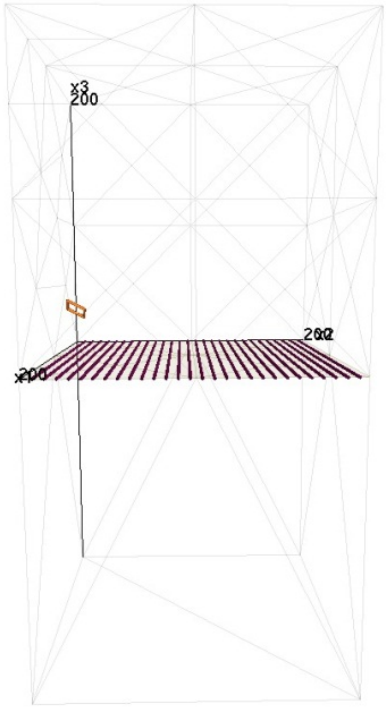

Figure 2: DD simulation of bi-crystal containing interfacial GBDs with identical spacing as an 8.2° GB

The description of GBs as dislocation arrays in DD is ideal for modelling dislocation interactions such as annihilation, junction formation (i.e., absorption and recombination of lattice dislocations); and nucleation that results in slip transmission. The details of modelling dislocation – GB interactions are primarily accommodated by well-established junction formation procedures within the conventional DD framework [13]. However, the computational procedure to obtain 100% confidence that the dislocations would not arbitrarily cross the interface involves extensive modifications to the simulation code. It, it was also necessary to establish a new simulation procedure to enable dislocation nucleation and, hence, slip transmission.

Algorithms to simulate dislocation intersection and absorption into the GB plane

The procedure to inhibit the arbitrary crossing of dislocations across the GB interface involves a necessarily complex and intensive procedure. It was necessary to ensure that a robust system of checks was utilized for all dislocation nodes, including pre-existing mobile nodes, nodes from network re-distribution (annihilation and generation of new nodes) and 'special nodes' in dislocation junctions external surface ledges.

To enforce that dislocations do not artificially cross the GB interface, an algorithm was developed to check the region ID of the mesh position that the node is projected to move towards along its current trajectory at each timestep. When the projected position would lie within a mesh tetrahedron that is assigned a different region ID than the current position's region ID, a complex procedure was triggered to implement dislocation-GB intersection. It is noteworthy that a system of projected positional checking was already a necessary component of fixed-boundary simulation with finite volume. However, the currently described procedure for GB intersection is more complex due to the formation of GBD junctions and ongoing mesh re-distribution of internal (not boundary) segments.

To model intersection with the GB, it was necessary to first identify the interfacial mesh facet shared by tetrahedrons with two different region IDs along the trajectory of the dislocation node. This is achieved by looping over the faces of all tetrahedra in the trajectory between the initial nodal point to the final position. Once the tetrahedron on the path within the original region ID is found that contains this interfacial facet, the dislocation node is then placed at the point along the original dislocation trajectory that intersects this mesh-face.

Once a dislocation node is positioned at the point of intersection on a facet connecting two region IDs, the node is designated as a GB node by assigning a fixed unit vector that defines the GB normal direction (V_{normal}). V_{normal} is thereafter used to eliminate the component of the nodal velocity projected in the direction normal to the GB plane, so that the motion of GB nodes is accurately constrained within the GB plane. In addition to being constrained to glide within the GB plane, GB nodes are also constrained to the original glide plane or by the constraints of a dislocation junction with any intersecting GBDs.

Slip transmission and dislocation nucleation from GBs

Atomistic studies have demonstrated that dislocations rarely penetrate GBs directly at the original point of intersection, but rather that the localized stress concentration activates dislocation 'nucleation' from an adjacent GB lattice site on a new slip system. In the present framework, 'nucleation' involves a recombination reaction between the interfacial GBDs and the trapped lattice dislocation lying on the interfacial 'displacement complete shift' lattice.

Nucleation is only initiated after a check of the resolved Peach-Koehler forces of all segments containing two dislocation nodes within the GB interface is identified to exceed a threshold value. This involves looping over all aforementioned segments, checking the available slip systems of the secondary region ID and computing the forces for all of the 12 FCC slip directions.

When nucleation is triggered, 'slip transmission' is implemented by generating a new dislocation loop comprised of 3 nodes lying in the second crystal and 2 nodes on the GB interface. The GB nodes are placed equidistantly from the midpoint of the lattice dislocation segment lying within the GB, however rotated appropriately so that the dislocation loop is normal to the new glide plane. Subsequently, recombination occurs between the lattice dislocation and the nucleated segment in the GB plane. This segment remains constrained inside the GB normal plane, however the newly

nucleated lattice dislocation nodes in the second crystal are free to move along the new slip system. Unfortunately, because the threshold nucleation stress and/or Peach-Koehler force is strongly dependent on the localized GB structure and/or presence of defects such as GB ledges, there is uncertainty about the most-appropriate nucleation thresholds [25]. Probabilistic modelling may provide an ideal work-around for this limitation in the future, however will need to be tailored to the specific misorientation angle (particularly for high-angle vs low-angle GBs). To avoid unnecessary complexity for low-stress interactions without dislocation pile-ups, nucleation and transmission may be enabled or disabled very easily by modifying one line of code.

Stability testing and robustness of mesh-region barrier

The most-critical requirement of the current computational approach is the assertion that no elements within the dislocation network will ever arbitrarily cross the interface between different mesh regions. If this were to occur at any point in the simulation procedure, the mesh region ID check would fail to correctly identify an intersection event at the subsequent node – motion step. After extensive stability testing, a few challenges were identified and subsequently were resolved to obtain a robust framework which ensures that the GB is never 'arbitrarily penetrated'.

The first challenge observed for artificial interface-crossing, involved an inherent numerical (rounding) error that occurred after dislocation nodes were made to intersect the GB plane. In this case, nodes moving within the GB plane sometimes were incorrectly identified with only one region ID due to truncation and rounding errors, so the node was no longer on a shared mesh face (GB). No solution was identified to completely eliminate this effect, however fortunately this issue has been overcome entirely by asserting that nodes intersecting the GB are constrained to the plane defined by the GB normal vector, without requiring a check for the mesh region ID.

The second issue identified provided a more fundamental challenge for the modelling, caused when lattice dislocations formed a junction that intersected with the GB plane. In this case, in order to assert crystallographic consistency it was necessary that dislocation nodes be placed at the exact point intersecting the glide planes of the lattice dislocations and the GB plane. This was further complicated, when junctions also were formed with GBDs, requiring a point of intersection between four independent planes (mathematically improbable). This meant that in certain cases there was no existing direct solution which effectively merged the dislocation segments into a junction at a point which was also coincidental with the GB plane. The conventional junction-formation protocol assertions would result in a junction that artificially crossed into the second crystal. A temporary fix has been implemented, which disables dislocation junction formation if the projected intersection position that is coincidental with the three (or more) constraining planes does not remain in the original region ID. It is a future aim to establish a new approach to more rigorously model junction formation at the GB by performing sequential junction formation and re-alignment. Due to the crystallographic constraints, it is likely that this will involve a complex procedure of annihilation, nucleation and recombination to maintain the conservation of Burgers vector and glide-plane constraints that are an intrinsic property of dislocation dynamics [43].

Careful checking and testing with a variety of stress conditions, dislocation densities and geometries of the fixed micro-pillar boundaries has demonstrated that the present version of the code is empirically an 'inherently stable' simulation framework. This has very positive implications for 3D DD modelling in the future with dislocation pile-up formations in polycrystals and for modelling the accumulation of very high internal dislocation densities. Examples are provided in Figure 3.A and in Figure 3.B. to demonstrate the efficacy of the presently described method to model arbitrarily complex systems and dislocation pile-ups. It is also noteworthy that this method is also

exceptionally well-suited for simulating defects or precipitate hardened alloys that involve impenetrable inclusions.

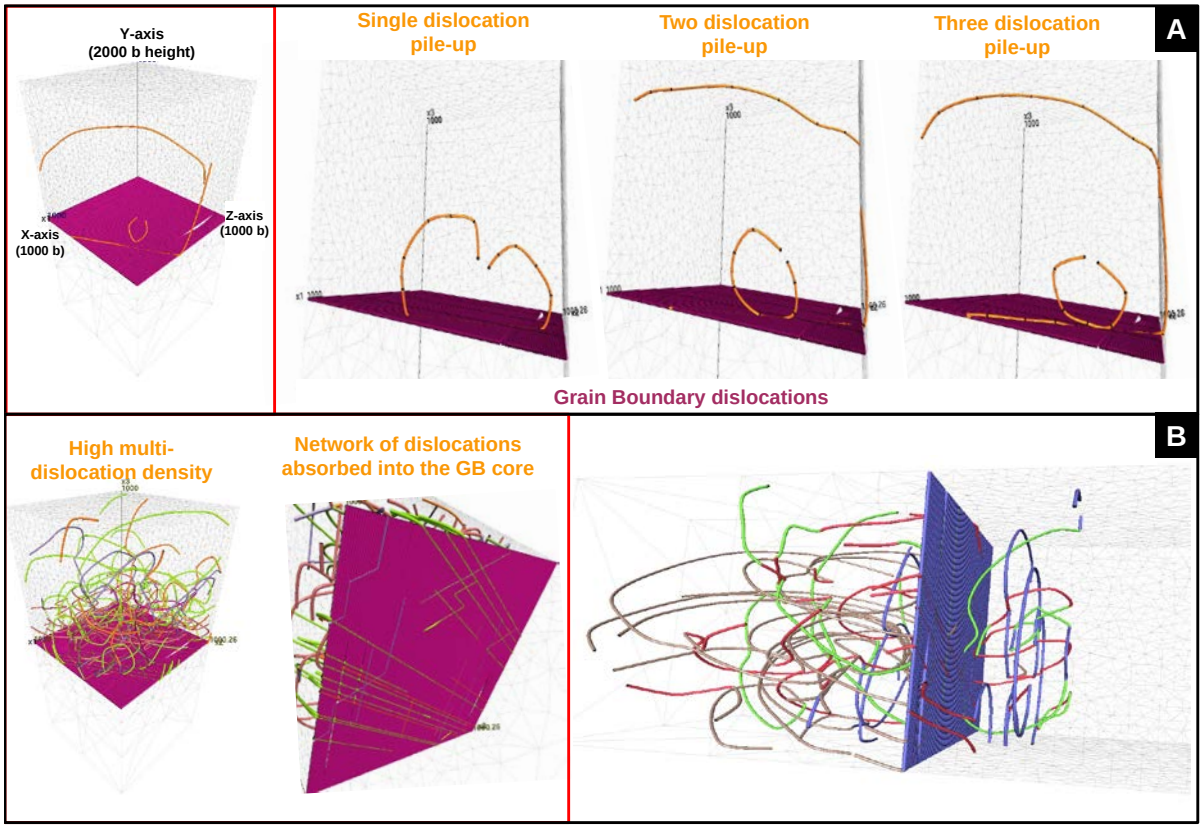

Figure 3: Robust modelling of 'impenetrable' mesh-region interface, up to very high dislocation densities: a) Examples of dislocation pile-up formations at the GB under a singular slip system; b) Examples of multi-junction formation and high dislocation density accumulated at the GB interface.

Dislocation nucleation and slip transmission through the GB

One of the novel elements of the present framework is the capability to model inter-granular plastic deformation, which occurs by slip transmission into the secondary crystal. This has been achieved at both a rudimentary level in terms of a singular set of crystal slip systems, and has also been recently applied to model nucleation along a user-specified selection of secondary crystal slip systems. The definition of crystal-specific slip systems remains in a state of development; however the present study demonstrates that the framework has the capacity in the future. An example of nucleation from a dislocation pile-up located at the GB is demonstrated in Figure 4.

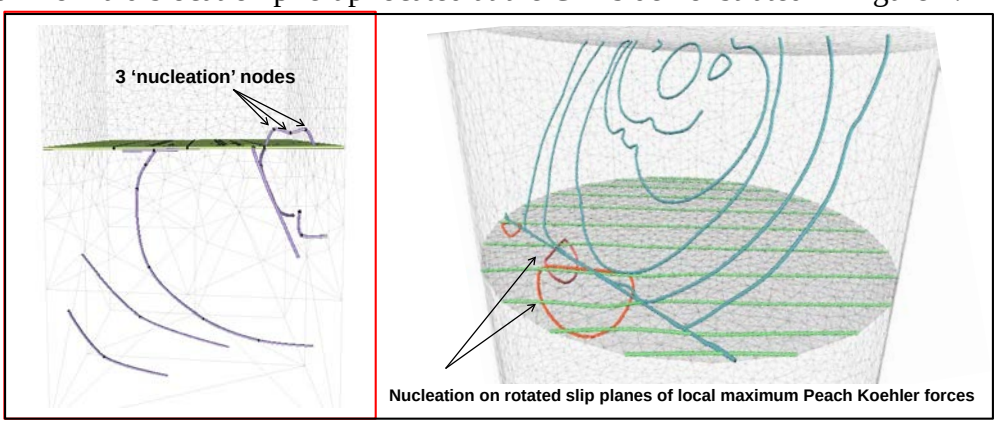

Figure 4: Demonstration of dislocation nucleation. A) Example of nucleation procedure by generating three 'nucleation nodes' from high-density GBDs; B) nucleation on rotated slip systems with low GBD density

Conclusions

This paper has described the implementation of a novel approach to achieve mesoscale dislocation dynamics simulations in polycrystalline materials. The method utilizes a modified mesh, in order to assign a unique 'region ID' to dislocations contained within different crystals. A series of algorithms have been developed to provide a modelling framework that ensures that dislocations do not arbitrarily cross the mesh region-interface. The code also asserts that dislocations which would otherwise cross the grain boundary (GB) interface will instead will exactly intersect the GB plane. An additional modification that remains in a development stage enables slip transmission by initiating dislocation nucleation from the GB into the secondary crystal, which is initiated when the maximum local Peach-Koehler force exceeds the threshold value.

Molecular dynamics simulations coupled with a post-processing method to extract the dislocation content were used to determine the atomistic structure of a low angle GB, and explicitly convert this into a dislocation format (i.e., a planar array of GBDs). On the basis of the atomistic analysis of this interface, replica GB structures were modelled with the modified DD, using the MoDEL library. It has been demonstrated that the code is inherently stable, and will not allow for slip transmission across the mesh-region interfaces unless dislocation nucleation is triggered. This has been used to demonstrate stress concentration within a dislocation pile-up, dislocation absorption into the GB core and the accumulation of high local dislocation density adjacent to the GB. In addition, the complex algorithms used to model slip transmission via the nucleation of dislocations along secondary crystallographic slip systems has been demonstrated to be an effective approach. The future opportunities to discretely evaluate the junction formation; annihilation; recombination and nucleation dislocation reactions between lattice dislocations and GBs can be used to provide significant insights into the defect mechanics of trans-granular plastic deformation.

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