Enhanced mobility of dislocation network nodes and its effect on dislocation multiplication and storage

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Abstract

Discrete Dislocation Dynamics (DDD) is a mesoscopic computational approach to predicting crystal plasticity and strength. The method’s key premise is that, to the extent each individual dislocation in the model knows how to respond to stress, crystal plasticity should emerge in all its realistic complexity by letting a statistically representative ensemble of dislocations interact and collectively evolve in response to deformation. DDD integrates much of the dislocation theory developed over nearly 90 years, and yet exactly how dislocations behave in a plastically flowing crystal had been hidden for our inability to resolve dislocation motion in full atomistic details. Fast forward to the present, large-scale Molecular Dynamics (MD) simulations are emerging as an alternative to DDD for predicting crystal plasticity. Where feasible, MD simulations are unsurpassed in providing most detailed insights into the physics of material deformation and, whereas a DDD model only knows of dislocation behaviors that its developers knew to implement, MD uncovers mechanisms not anticipated a priori. Cross-comparison between DDD and MD simulations performed under identical conditions exposes glaring discrepancies in predicted strength and microstructure evolution. Deeper inquiry pins the observed discrepancies to contrasting behaviors of network nodes – dislocation intersections. Whereas in DDD the nodes strongly restrict dislocation motion, in atomistic simulations the same nodes enable networked dislocations to move in ways previously thought impossible and not permitted in DDD. Only after base kinematic rules are extended to include previously unaccounted freedoms of dislocation motion, DDD simulations fall closely in line with the “ground truth” atomistic simulations.

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Over nearly 90 years since their initial discovery, lattice dislocations have been firmly established as the main agents of crystal plasticity. Yet quantitative prediction of macroscopic crystal plasticity directly from dislocation behavior remains an elusive grand challenge [1]. Computational method of Discrete Dislocation Dynamics (DDD) is widely viewed as a promising approach in which motion of each individual dislocation as well as interactions among dislocation lines are explicitly accounted for and thus directly define the overall crystal plasticity response [2–7]. Given the drastic reduction of degrees of freedom embodied in dislocation lines, the method promises to reach microstructural length and time scales relevant for crystal plasticity but far inaccessible to atomistic MD simulations. This promise of DDD as a bridge between microscopic dislocation theory and macroscopic crystal plasticity meets serious computational limitations: although much less computationally demanding than MD, DDD simulations are still notoriously expensive often demanding large computing resources to evolve an ensemble of dislocations statistically representative of macroscopic crystal plasticity. Algorithmic advances coupled with impressive developments in computational capabilities are bringing about DDD simulations on ever increasing length- and time-scales [8].

Having collectively spent decades working to further computational efficiency of DDD simulations within the ParaDiS development project [7], here we focus on a different challenge – limited or unknown physical fidelity of mechanisms of dislocation behavior presently included in DDD models. Being a mesoscopic approach, a DDD simulation only knows of mechanisms that the developer knew about and cared to include in the model formulation. Mechanisms of dislocation behavior are known to be multiple and complex and one of the known good uses of DDD is for parametric studies in which relative contribution of any one of the known mechanisms can be amplified or reduced at will. But what if one or several mechanisms of dislocation behavior are not known and thus never included in the DDD model?

Historically, dislocation theory has been concerned with the behavior of single dislocations. Examples include mech-
anisms of dislocation mobility, dislocation core structure, cross-slip, climb, etc. Until first TEM observations of dislocations in the late 50’s, understanding of dislocation behaviors was based nearly exclusively on physical intuition and deductive reasoning. Yet, despite subsequent impressive developments in material characterization, including in situ TEM, direct experimental observations are not sufficiently resolved and may not reveal sufficient details of dislocation motion needed to discover its yet unknown mechanisms. Since 60’s of the last century, atomistic simulations of individual dislocations and, subsequently, small groups of dislocations have been increasingly used as means of inquiry into dislocation behaviors augmenting experiment. Yet the key premise of DDD was and remains unchallenged: once it is learned in sufficient details how individual dislocations move in response to forces they experience and this knowledge is accurately translated into a DDD model, crystal plasticity would be accurately predicted in all of its realistic complexity [9].

The same advances in HPC that are helping DDD to meet its challenge of computability have recently enabled direct fully dynamic atomistic simulations of crystal plasticity at scales previously thought to be unachievable [10, 11]. Performed at the limits of super-computing, such MD simulations involve simultaneous motion and interactions of thousands of dislocation lines in statistically representative material volumes sufficient to directly compute plastic response of a single crystal subjected to straining at rates of the order $10^6$/s and higher.

Equally important as their scales is that such direct MD simulations are fully atomistically resolved so that every single feature in the computed stress-strain curve can be unambiguously connected to the underlying dynamic events in the life of dislocations. In tandem with the recently developed accurate and efficient methods for dislocation extraction and indexing (DXA) [12, 13], direct MD simulations now serve as an ideal in silico computational microscope. And unlike the more traditional atomistic simulations invariably probing behaviors of single dislocations or small groups of dislocations in configurations presumed relevant for crystal plasticity, in massive MD simulations one observes how dislocations collectively and naturally respond en masse to applied straining. Such simulations reveal a plethora of dynamic behaviors and mechanisms, some of which have been never envisioned or hypothesized. Large-scale MD simulations of crystal plasticity are especially informative when contrasted against DDD simulations performed under identical conditions, a practice we will refer to as cross-scale (X-scale) matching. In this paper we present one example where X-scale matching bears fruit by exposing glaring shortcomings - missing mechanisms of dislocation motion - common to most if not all DDD models presently in use. We further show that, once the new missing mechanisms are added to the base DDD model, DDD predictions fall close in line with corresponding MD simulations precisely where the two previously disagreed.

Our findings concern dislocation junctions that form when two or more dislocation lines – parents – collide and cross each other resulting in zipping a third common line, a product dislocation junction. Forming at the junction’s ends are two network 3-nodes in which two parent dislocations and the product dislocation merge together (Fig. 1). It has been invariably assumed and seemingly supported by simulations and experiment that such network 3-nodes act as pinning points hindering further motion of all three dislocations resulting in an increase in the flow stress. Furthermore, depending on applied stress, specific junction geometry and/or type, network 3-nodes were shown to make major contributions to dislocation multiplication [14, 15]. In attempting to match DDD and MD simulations of plastic flow in BCC tantalum we observed gross discrepancies in the kinetics of dislocation multiplication between these two types of simulations. Closer inspection revealed striking differences in dislocation networks: whereas DDD simulations led to gradual buildup of increasingly dense dislocation tangles resulting in seemingly permanent storage of immobile dislocations, in MD simulations no such dense tangles formed and no permanent dislocation storage was observed. Additional analyses of MD simulations revealed geometric characteristics of dislocation networks incompatible with commonly assumed motion kinematics of network 3-nodes. Based on MD observations, kinematics of nodal motion was updated to enable previously unknown modes of nodal motion which resulted in a drastically improved agreement of the kinetics of dislocation multiplication predicted in DDD and MD simulations.

The remainder of this paper is organized as follows. We begin by describing kinematic rules for 3-node motion commonly employed in DDD simulations, which we contrast with observations in large-scale MD simulations of unusual behaviors of dislocation network 3-nodes seemingly incompatible with the standard kinematic rules. We continue by describing MD simulations of smaller, elemental fragments of dislocation networks specifically devised to elucidate root causes of observed unexpected behaviors of network 3-nodes. Detailed analysis of MD simulations reveals two distinct and previously unaccounted mechanisms allotting dislocation network 3-nodes additional degrees of freedom for conservative motion. We then use our DDD implementation in ParaDiS as an illustrative example to describe how to incorporate the newly discovered motion mechanisms into DDD simulations by modifying their kinematic rules. After validating our implementation of modified kinematics in DDD simulations on elemental network fragments, we proceed to demonstrate the critical importance of the newly discovered modes of 3-node mobility for dislocation multiplication and crystal plasticity by selectively turning on or off the newly implemented mechanisms of nodal motion in full-scale DDD simulations. Finally we conclude with a discussion and summary.

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network 3-nodes

\[ \mathbf{n}_1 \times \mathbf{n}_2 = \mathbf{l}_3 \]

Figure 1: Collision and intersection of parent dislocations 1 and 2 (dashed green and blue lines) moving towards each other on their geometric glide planes with normals \( \mathbf{n}_1 \) and \( \mathbf{n}_2 \) results in merging the parents together into a product junction dislocation 3 (thick magenta line). The junction dislocation segment is bounded on its ends by two 3-nodes in which all three dislocations meet together (thick green, blue and magenta lines). To conserve net Burgers vector at each network node, the Burgers vector of the product dislocation must be equal to the sum of the Burgers vectors of two parents: \( \mathbf{b}_3 = \mathbf{b}_1 + \mathbf{b}_2 \). The product dislocation zips along line \( \mathbf{l}_3 \) common to the glide planes of two parent dislocations, \( \mathbf{l}_3 = \mathbf{n}_1 \times \mathbf{n}_2 \). Because the geometric glide plane of the product dislocation is defined by the cross-product of its Burgers vector and its line vector: \( \mathbf{n}_3 = \mathbf{b}_3 \times \mathbf{l}_3 \), the three normals \( \mathbf{n}_3, \mathbf{n}_1 \) and \( \mathbf{n}_2 \) are all co-planar. For all three dislocations to remain in their respective glide planes, the 3-node can only move along the junction line \( \mathbf{l}_3 \).

3-node motion in BCC crystals

Kinematics of conservative motion of network 3-nodes

Before we proceed to describe unexpected behaviors of dislocation network 3-nodes observed in large-scale MD simulations, it is useful to review kinematics of nodal motion as it is generally described in textbooks [16] and implemented in our ParaDiS DDD model and code [7]. We searched relevant literature and observed that, where described, other DDD models presently in use rely on similar if not identical rules. Consider the schematic in Fig. 1 where dislocation lines numbered 1, 2 and 3 merge in a 3-node with their three Burgers vectors and normal vectors of their glide planes all numbered accordingly. A dislocation with Burgers vector \( \mathbf{b} \) and line tangent vector \( \mathbf{l} \) can glide or move conservatively, i.e. not requiring any diffusional mass transport, in its geometric glide plane defined by plane normal \( \mathbf{n} = \mathbf{b} \times \mathbf{l} \). Derived by considering an infinitesimal displacement of a 3-node in which all three lines entering the node preserve their geometric glide planes, the conventional rule for conservative motion of a 3-node can be summarized as follows: the node is permitted to glide or move conservatively in the subspace complementary and orthogonal to the space spanned by the normal vectors of three glide planes. This concise rule seemingly covers all relevant cases of conservative motion. When three normals are non-coplanar, the complementary motion subspace is 0D meaning that the 3-node is not permitted to glide conservatively at all. When three normals are co-planar, the permitted complementary subspace is 1D so that the node can move along a line perpendicular to the plane spanned by the three normals. This covers the most frequently encountered situation depicted in Fig. 1 when one of three dislocations is a junction formed in a collision followed by zipping of two parent dislocations that have been gliding conservatively before and after the collision. When three normals are all colinear, the motion subspace is 2D and the 3-node can move conservatively in the common glide plane of three constituent dislocations. The latter condition covers the case of a planar junction (and planar junctions networks). The same rule applies when one or more dislocations are pure screw. Since the glide plane normal for a screw dislocation cannot be defined, the screws are excluded and only the normals of non-screw dislocations are used to compute the nodal motion sub-space. In particular, when all three dislocations are screws, the subspace spanned by three (undefined) normals is 0D meaning that the node can glide unconstrained in 3D [17]. The same concise rule defines the motion subspace for a dislocation network node of arbitrary degree \( n \geq 3 \).

X-scale observations

In recent direct large-scale MD simulations of crystal plasticity we observed flow stress, dislocation density and other characteristics of material response to attain stationary values and to stay subsequently unchanged provided straining conditions, i.e. temperature, straining rate, crystal orientation, etc., are maintained unchanged over a sufficiently long time [10, 18, 19]. However, in comparing DDD simulations performed on models parameterized specifically to reproduce as closely as possible straining conditions of direct MD simulations, we observed considerable discrepancies between MD and DDD predictions. Perhaps
the most glaring discrepancy was the inability of DDD simulations to attain a state of stationary flow of the kind observed in MD simulations [10]. One example to be discussed in more detail later is shown in Fig. 8 where dislocation density computed in a typical DDD simulation never saturates. Reflecting a well recognized connection between dislocation density and flow stress – Taylor hardening [20, 21] – flow stress in the DDD simulations continues to rise. Such “hardening forever” response is in striking variance with the MD simulations which we regard as “ground truth” in the context of X-scale matching.

Subsequent parametric studies suggested that a state of steady flow can be attained in a DDD simulation, but at the cost of raising climb mobility of dislocation segments well above physically admissible levels. However at strain rates where the ground truth MD simulations were performed, climb is exceedingly unlikely and can be ruled out on the relevant time scales of nanoseconds. Zeroing in on climb, we further observed that, for steady flow to become attainable in a DDD simulation, it was sufficient to artificially raise climb mobility for only the segments entering the network nodes while keeping climb mobility of all other segments near zero. In parallel, we visually observed spectacular differences in the dynamics of dislocation networks emerging in MD and DDD simulations. In addition to growing significantly denser, dislocation networks in DDD simulations develop persistent dislocation tangles that never dissolve and grow increasingly dense under continued straining (Fig. 2a and Movie 1). In corresponding MD simulations dislocation tangles also form but are much less dense and sooner or later dissolve and do not persist throughout the simulation (Fig. 2b and Movie 2). Taking MD simulations as the ground truth, permanent storage of dislocations in dense tangles and unceasing hardening observed in DDD simulations are both deemed spurious.

So what holds the dense tangles together leading to ostensibly permanent storage of dislocations in DDD simulations? And do the tangles indeed dissolve in MD simulations due to an inexplicably elevated climb mobility of dislocation segments entering the 3-nodes? An essential clue leading us to eventually solve the puzzle came from watching movies of dislocation network evolution extracted from MD simulations. One typical sequence is shown in Fig. 3a-d and Movie 3. In the three snapshots shown in the figure and especially in the video, one can observe 3-nodes to not only move along straight lines zipping or unzipping straight junction dislocations, as prescribed by the rule for conservative motion described earlier, but to also move along distinctly curved paths in space. Resulting from such motion, many junctions appearing in MD simulations become curved, developing bends and even sharp corners (Fig. 2d). This is in contrast to perfectly straight junctions drawn and abundant within the dense tangles observed in DDD simulations (Fig. 2c). According to the conventional kinematic rule, for the 3-nodes to move along such curved trajectories one has to permit climb or some of the three dislocations entering the 3-node should be screws. Additional careful analysis revealed that in most instances when curved junctions appear, none of the three dislocations segments were screw. Furthermore, on short - typically a few ns - time scales of our MD simulations no non-conservative motion (climb) is observed. What was observed instead was that, immediately preceding the instances when a junction bends, the 3-node attains a configuration in which the normals to the three geometric glide planes become non-coplanar. According to the kinematic rule of nodal motion implemented in our DDD simulations, such non-coplanar 3-nodes should be immobile or “sticky”. Yet in MD simulations such 3-nodes are observed to move briskly, most often sideways, nearly instantly after attaining a non-coplanar geometry.

Fig. 4 explains how a sticky 3-node can glide fully conservatively and why such 3-nodes often move sideways. It is useful to recognize that any network 3-node can be represented in three distinct but physically indistinguishable ways. As depicted in Fig. 4a, it is possible and, for our purposes, helpful to view one of three dislocations merging in a 3-node as a passive or product dislocation (junction) formed by zipping together two active or parent dislocations. There are obviously three possible ways to define a parent pair and the product and, hence, three representations of the same 3-node: 1+2=3, 1+3=2, and 2+3=1. As depicted in Fig. 4b, each of the three pairs of dislocations can zip an additional segment of the third product dislocation along the line shared by the glide planes of two parents. Any such zipping motion is fully conservative whether or not the 3-node is non-coplanar. But when the 3-node is indeed non-coplanar before zipping, the newly
Figure 4: Mechanisms of coordinated conservative motion of a 3-node. (a) Three equivalent representations of a dislocation network 3-node. (b) Mode 1 entails zipping line 3 along the intersection of glide planes 1 and 2 shown as a solid black line. Glide planes 1 and 2 are also shown semi-transparent in colors matching the active lines. In this example the 3-node is non-coplanar in its initial configuration on left and the newly zipped segment is not colinear with the previously existing junction segment. When such is the case, additional zipping creates a bend on the junction line shown on right. (c) Mode 2 entails unzipping line 3 by coordinated motion of dislocation 1 and 2. When the 3-node is non-coplanar, the unzipped segment is not colinear with the intersection of glide planes of two active dislocations. For such unzipping motion to remain conservative, two active dislocations must cross-slip leaving two corner nodes on the dashed lines passing through the original 3-node position and parallel to the Burgers vector of each line. (d) In Mode 3, lines 1 and 2 zip an additional segment of line 3 while simultaneously cross-slip and leaving corners nodes on the lines passing through the initial 3-node position and parallel to the corresponding Burgers vectors.

drawn segment is not colinear with the tangent vector of the previously existing segment of the same product dislocation. Thus, zipping past a non-coplanar 3-node geometry unavoidably creates a bend or a corner on the product line. Zipping a junction past a non-coplanar node is one of the previously unaccounted mechanisms of nodal motion we observed in our MD simulations. Non-coplanar nodes that are sticky in DDD, can also move conservatively by unzipping, Fig. 4c, which is yet another mechanism by which dislocations can develop corners. In unzipping, an inactive product dislocation is split as two active dislocations separate along the product line. When the 3-node is non-coplanar, purely conservative unzipping motion of two parent dislocations is still possible at a cost of creating two corners, one corner on each parent. At each corner, the corresponding active dislocation changes its original glide plane to a new glide plane defined by the cross-product of its Burgers vector and the tangent of the product segment being unzipped. Unzipping mechanism illustrated in Fig. 4c is just one manifestation of a previously uncounted wider class of mechanisms of nodal mobility we here term nodal cross-slip by which one or more dislocations entering a network node change their glide plane(s). Unlike conventional cross-slip that entails change in a glide plane of a screw dislocation, nodal cross-slip mechanism of the kind depicted in Figs. 4c does not require any of the three participating dislocations to be screw. A still more general mechanism of nodal cross-slip is schematically illustrated in Fig. 4d where two active dislocations zip past a 3-node while all three dislocations simultaneously change their respective glide planes. In MD simulations reported here we observed only the mechanism of nodal cross-slip shown in Figs. 4b-c. In yet another series of MD simulations to be reported elsewhere we observe and analyze the mechanism of nodal cross-slip depicted in Fig. 4d. We note that the 3-node does not have to non-coplanar to facilitate nodal cross-slip.

Bearing in mind three alternative representations of a 3-node in Fig. 4a, multiple modes of coordinated conservative motion are potentially available for each 3-node, sticky or not. These previously unaccounted mechanisms enable 3-node to move past and resolve non-coplanar node geometries. Unexpectedly, by virtue of their connectedness into a network at 3-nodes, dislocation acquire greater mobility than each one of them can afford individually.

Verification of zipping and unzipping mechanisms

To follow in detail how the mechanisms outlined above enable conservative motion of a sticky 3-node, we inserted an elemental dislocation network containing a single sticky 3-node into a periodically replicated BCC crystal. Full 3D periodic boundary conditions (3D-PBC) are convenient for our purposes as they enable relatively straightforward and accurate control of applied stress and eliminate unwanted boundary effects while preserving translational invariance. The price one pays for using 3D-PBC is that a minimum of two dislocation networks have to be inserted for the net Burgers vector of the entire ensemble to remain zero. Here we will focus our attention on only one of the two dislocation networks. The network is constructed so as to contain one non-coplanar 3-node per repeat volume: each 3-node connects two $\langle 111 \rangle$ dislocations and one $(100)$ dislocation in the geometry defined in Fig 5a. In this geometry the 3-node is non-coplanar as none of three line tangent directions is parallel to the intersection of glide planes of two other dislocations.

After inserting the networks into a periodically repeated fragment of a BCC crystal containing ~2M atoms, Fig. 5b, the configuration was annealed at 300K under zero stress using langevin thermostat and nph barostat in LAMMPS [22] and an interatomic potential for Ta [23]. CNA and DXA analyses implemented in Ovito [24] were used to make sure that no defects other than the three dislocation lines were introduced in the simulation volume. Following annealing, the crystal was subjected to uniaxial tension at rate of $2 \times 10^8$/s held constant over 200ps. Evolution of
shown in Fig. 5c, according to the conventional conservative mechanism of motion of a co-planar 3-node. On reaching its original position before annealing the 3-node again becomes momentarily non-co-planar but continues its motion by unzipping the junction dislocation along its as-inserted direction [16 7 0]. This motion proceeds by the conservative unzipping mechanism schematically depicted in Fig. 4c in which two $\frac{1}{2}$ (111) {112} are pulled into their cross-slip planes.

Neither zipping motion shown in Fig. 5c nor unzipping motion shown in Fig. 5e are permitted within the conventional rules for conservative motion of 3-nodes as described earlier.

**Implementation of enhanced 3-node mobility in DDD (ParaDiS)**

Here we augment kinematics of nodal motion in DDD to permit conservative motion of sticky 3-nodes observed in our MD simulations. Although our implementation is specific to ParaDiS, we hope the description below will suggest appropriate modifications to motion kinematics implemented in other DDD models and codes. We note that, although intended primarily to remove non-physical restrictions on the motion of non-co-planar 3-nodes, for uniformity the resulting augmented rules can be applied to all types of 3-nodes, sticky or otherwise. Indeed, all modes of conservative motion depicted in Fig. 4 are and should be made available for all 3-nodes.

Conservative zipping of a junction connected to a 3-node is always possible but, when the 3-node happens to be non-co-planar, such zipping motion changes direction of and leaves behind a corner on the junction line. The corner appears at the same point where the non-co-planar 3-node was located and delineates the newly added junction segment from the previously existing junction. Two junction segments connected at the corner find themselves in different glide planes, as if the junction dislocations cross-slipped. However, this change of the geometric glide plane is not cross-slip in itself because the junction dislocations did not change its plane while gliding but instead was passively zipped from its original glide plane into a different glide plane. As shown in Fig. 6b, unless the junction is indeed subdivided into two segments joined at a corner node, change in the junction zipping direction would necessitate a substantial non-conservative displacement of the junction segment out of its geometric glide plane. The only physical mechanism that can make a junction move in such a way is climb. Indeed, as was previously discussed, artificially elevated climb mobility improves DDD agreement with MD simulations to an extent. However real climb mobility in tantalum at 300K is so low that climb on time scales of our MD simulations (typically ~ 10 ns) simply does not happen. Rather than trying to correct one wrong (sticky 3-nodes) with another wrong (artificially enhanced climb), we add a new kinematic rule to enable conserva-
tive junction extension beyond a sticky 3-node by forming a junction corner, Fig. 6c.

Similar to zipping, unzipping of a junction past a sticky node would necessitate climb unless two active dislocations are allowed to cross-slip to glide planes defined by the cross-products of their Burgers vectors with the tangent vector of the junction. As depicted in Figs. 4c and 6d, cross-slip of two active lines entails formation of two cross-slip corner nodes – one node per active line – delineating new segments pulled into the cross-slip planes from segments moving in the original glide planes of two active dislocations. Junction unzipping beyond a sticky 3-node is purely conservative for as long as each of the two cross-slip nodes moves along the line originating at the location of the sticky 3-node before unzipping and parallel to the Burgers vector.

To implement additional rules illustrated in Figs. 6c and 6d in ParaDiS we added two additional topological operators derived from the original SplitMultiNode operator implemented in ParaDiS to handle dissociation of network nodes of degree four or higher, Ref. [7]. Split3Node generates trial split configurations for three modes of unzipping and three modes of zipping. In principle, each one of the six modes of 3-node motion can proceed in either direction along an appropriate intersection line, but usually only one of two directions is aligned with the Peach-Koehler force computed on the 3-node before splitting. After six out of 12 modes are selected, for each one of them an appropriate infinitesimal (in practice finite, but small) trial split node configuration is generated and its rate of power dissipation is computed (see [7] for details). The trial mode with the highest dissipation rate is accepted and only then the so-selected change in the 3-node is executed.

We note that, in principle, appropriate topological operators can be added to handle dissociation of sticky network nodes of degree four and higher. Our approach is to use the SplitMultiNode operator existing in ParaDiS to test for favorable dissociations of multi-nodes into 3-nodes based on the maximum power dissipation criterion. If and when dissociation of a multi-node is deemed favored, every 3-node resulting from the accepted multi-node dissociation is then tested for a favorable zipping or unzipping motion.

DDD simulations with amended kinematics of 3-node motion

We first validate our augmented 3-node mobility kinematics by performing a DDD simulation on the same elemental dislocation network previously simulated using MD, Fig. 5. To be consistent with MD simulations, the DDD simulation followed precisely the same sequence as MD – first relaxation then uniaxial straining – as was previously described. The DDD model was parameterized with material parameters computed for the same interatomic potential model of tantalum as in the corresponding MD simulation: lattice constant $a_0 = 0.33032$ nm, shear modulus $\mu = 55$ GPa and Poisson’s ratio $\nu = 0.34$.

We employed linear mobility functions both for edge and screw dislocations however drag coefficient for the screws was more than 100 times greater than that of the edges, at $5.0 \times 10^{-2}$ Pa.s and $3.8 \times 10^{-4}$ Pa.s respectively. The screw mobility function was of the pencil type [7, 25]. Two DDD simulations were performed with the same material parameters, one using the old set of kinematic rules and the other using the augmented kinematics permitting conservative motion of sticky 3-nodes. In both cases, drag coefficient for climb motion was set to a high value of $10^4$ Pa.s so that climb was effectively suppressed.

In the DDD simulation with the original kinematic rules, no motion of the sticky 3-node is observed both during relaxation and during subsequent uniaxial straining. In the latter stage, under continued straining the sticky 3-node serves as an indestructible pinning point for an incessant Frank-Reed dislocation multiplication. In the DDD simulation with the augmented kinematics, the evolution is qualitatively identical to that in MD. As shown in Fig. 7b, during the initial relaxation the junction spontaneously zips past the initial 3-node position thus forming a corner on the junction line. Upon application of tensile straining, the newly formed junction segment is seen to unzip all the way to and past the corner node, after which the 3-node stops at a position close to that attained in MD, Fig. 7c. Only then the two active lines begin to bow.

![Figure 6: Topological operations introduced to enable additional modes of 3-node motion. (a) Initial configuration of a 3-node with two active dislocations (green) in glide planes with normals $n_1$ and $n_2$ and a passive dislocation with line direction $l_j$ (magenta) not parallel to the intersection of two glide planes (dashed line defined by $n_1 \times n_2$). (b) Without adding an additional node, zipping motion of the 3-node along the dashed line changes orientation of the junction segment tilting it away from its geometric glide plane (as indicated by the black arrow), which can only take place by climb. (c) To enable mode 1 (zipping, no x-slip), the 3-node is split in three with the original node becoming a corner node and the new node moving along the dashed line. (d) In mode 2 (zipping, x-slip), the 3-node is split in three with the original 3-node moving along $l_j$ and two new corner nodes gliding along their respective Burgers vectors $b_1$ and $b_2$. Two short segments connecting the 3-node to the new corner nodes lie in glide planes with normals $n'_1 = b_1 \times l_j$ and $n'_2 = b_2 \times l_j$.](image-url)
out and to produce new dislocations, Fig. 7d. Comparing Figs. 5 and 7, a close agreement is observed overall between the MD simulation and the DDD simulation with the augmented kinematics of 3-node motion. Even if the agreement is not fully quantitative, it is qualitatively robust and holds irrespective of such details as the mobility functions.

To observe effects of augmented kinematics on macroscopic plasticity response and, in particular, on dislocation multiplication, we performed bulk DDD simulations in a material volume equal to that of a large-scale MD simulation. Just like in MD, the initial configuration consisted of 12 prismatic dislocation loops randomly seeded in the simulation volume. The crystals were then subjected to compression at the same rate of $2 \times 10^8$/s along the same [001] crystallographic axis. Evolution of stress and dislocation density predicted in MD and DDD simulations with and without augmented rules for 3-node mobility is shown in Fig. 8. Two DDD simulations predict very different behaviors: whereas the simulation with the old kinematics (old DDD) predicts unending dislocation multiplication, the simulation with the augmented kinematics (new DDD) predicts saturation of dislocations density in close agreement with the MD prediction also shown on the same plot. The flow stress attained in the new DDD simulation is lower than the flow stress observed in MD which is attributed to an over-simplified dislocation mobility function, i.e. linear pencil mobility, used in both DDD simulations. However the fact that flow stress clearly saturates in the new DDD simulation is significant and does not depend on the specific mobility function. At the same time, flow stress in the old DDD simulation is markedly higher than in MD and new DDD and, consistent with the steadily rising dislocation density, shows a tendency to continued hardening. These clear differences are attributed to continued spurious growth of dislocation tangles in the old DDD simulation, Fig. 8d, in contrast to MD and new DDD simulations in which enhanced nodal mobility resolves dislocation tangles before they grow excessively dense, Figs. 8c and 8e.

**Discussion and summary**

Significant effects of dislocation network nodes on crystal plasticity and dislocation microstructure have been recognized for a long time, however simulation results and analyses presented in the preceding sections add an unexpected new twist to the existing understanding. Not only the network nodes constrain dislocation motion by tying dislocation together, but the very same nodes furnish additional degrees of freedom for dislocation motion that individual dislocations do not possess. Paradoxically, when tied into knots, dislocation lines may well become more mobile than otherwise. Previously unaccounted for mechanisms of nodal motion observed and rationalized in this work suggest that, despite significant body of work focused on interactions among dislocations, consequences of dislocation connectedness into a network are not sufficiently understood. A pertinent example from this work is that conservative unzipping of a sticky non-coplanar 3-node unavoidably forces one or two active dislocations to cross-slip. This phenomenon of coordinated nodal cross-slip is principally different from a previously proposed enhancement of cross-slip rates at dislocation intersections [26] or an enhanced rate of cross-slip on a screw dislocation connected to a regular co-planar 3-node [27]. To our knowledge, all earlier proposals for enhanced cross-slip focused on screw dislocations, whereas nodal cross-slip can and does take place when none of the participating dislocations is of screw or near-screw character.

In DDD simulations based on commonly accepted but over-constrained kinematics of nodal motion, network 3-nodes – especially of the sticky (non-coplanar) variety – act as strong pinning points arresting dislocation motion and
promoting relentless dislocation multiplication. Inability of dislocation networks to get rid of such sticky nodes leads to formation and proliferation of dense dislocation tangles growing ever denser with continued strain. In DDD simulations continued to large strains, dense tangles persist and never dissolve resulting in ostensibly permanent dislocation storage and "strain hardening forever". When enabled in a DDD model, additional modes of conservative motion identified and classified in this work make it possible for the 3-nodes to glide aiding dislocation annihilation and dynamic dissolution of dense dislocation tangles. In full qualitative agreement with MD simulations, spurious dislocation storage and strain hardening associated with the unphysical dense tangles are thus eliminated and DDD simulations asymptotically attain a state of steady flow in which dislocation multiplication is balanced by dislocation annihilation.

3-nodes with non-coplanar normals of three glide planes are found to be an essential and pervasive component of dislocation networks observed in MD simulations of BCC tantalum. But how do such non-coplanar 3-nodes form in the first place? To see how non-coplanar 3-nodes come to existence, we followed evolution of a few fragments of dislocation networks in very high time frame resolution. In a few instances where 3-node motion was observed to deviate from the initial straight junction line, such events were preceded by cross-slip of one of two parent 1/2⟨111⟩ dislocations. As illustrated in the schematic in Fig. 9, the segment pulled into a cross-slip plane by a parent dislocation subsequently glides all the way to and impinges on the 3-node. Thus, a regular co-planar 3-node initially formed by zipping two parent dislocations together, becomes non-coplanar by virtue of one of two parent dislocations subsequently cross-slipping. Although we do not rule out that cross-slip may initiate at the 3-node itself – as was posited in [26] – in a few MD sequences that we analyzed cross-slip was taking place away from the 3-nodes. It is possible that this preference reflects the known predominance of screw dislocations in BCC crystals plastically deformed at low and intermediate temperatures. Furthermore, as a well-recognized consequence of a much lower mobility of screws relative to the edge dislocations, in our MD and DDD simulations alike we observe that, away from the network nodes, most dislocation lines are of screw or near-screw character. Owing to a compact (undissociated) structure of the screw dislocation core, cross-slip of screw dislocations in BCC crystals is not a rare event of the kind observed in FCC crystals. It remains to be seen how frequently non-coplanar nodes may form and what could be detailed mechanisms of their formation in materials with crystal structure other than BCC.

Behaviors and mechanisms discussed in this work were observed in atomistic simulations performed at very high deformation rates as was needed to reach sufficiently large plastic strains and see a complete evolution of dislocation microstructure within the short time-scales presently accessible to large-scale MD simulations. It remains to be seen how much the same mechanisms matter in crystal plasticity at lower rates including quasistatic straining conditions. But, although established here through X-scale matching of MD and DDD simulations performed on the same short time-scales, the very existence of previously unaccounted conservative mechanisms of nodal motion is firmly established. The same mechanisms must be operational on any time scales and should be enabled for DDD simulations to be predictive. The drastic improvement in the agreement between high-rate MD and DDD simulations achieved here by enabling conservative motion of sticky nodes is indicative of potentially broader importance of such mechanisms in crystal plasticity.

In summary, we report previously unknown mechanisms of enhanced mobility of dislocation network nodes. In analysing dynamic evolution of dislocation networks in large-scale MD simulations, we observe that 3-nodes with non-coplanar normals are fully mobile and are not at all sticky as has been commonly assumed and observed in DDD simulations. In their motion, 3-nodes are observed to follow curved trajectories forming bends and corners on the dislocation lines. Closer examination of the dynamics of elemental dislocation networks reveals two new mechanisms of fully conservative motion of non-coplanar 3-nodes in which one or two or even all three participating dislocations are transferred into different glide planes. Enabling the newly observed conservative mechanisms of nodal motion in DDD code ParaDis brings DDD simulations in close qualitative agreement with MD simulations performed on the same scales and under identical straining conditions. Our findings of previously unaccounted mechanisms of dislocation motion and subsequent demonstration of their essential role in crystal plasticity showcase constructiveness of X-scale matching in which fully resolved MD simulations are compared against mesoscopic DDD simulations performed in identical conditions.
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