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A triangulation-based method to identify dislocations in atomistic models

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ABSTRACT

A simple, efficient, and fully automated computer algorithm is described that identifies dislocations in atomistic crystal models and determines their Burgers vectors. To achieve this, the algorithm maps the edges of a Delaunay tessellation to corresponding vectors in an ideal crystal. Dislocations are identified by detecting incompatibilities in this discrete elastic mapping using triangular Burgers circuits. While the presented method is limited to single crystals, it stands out due to its simplicity, straightforward implementation, and computational efficiency. It can provide a bridge from atomistic descriptions of crystals to mesoscale models based on discrete dislocation lines.

1. Introduction

Atomistic computer simulation methods such as molecular statics and molecular dynamics (MD) enable a detailed investigation of complex dislocation processes in crystals. Typically, atom filtering techniques (Stukowski, 2012) are used to make crystal defects in such simulations visible (see Fig. 4a for an example). These structural analysis techniques merely detect the disturbed arrangement of crystal atoms inside a dislocation's core. In general, however, this is insufficient to reliably discriminate dislocations from other defect types. Furthermore, critical information such as a dislocation's Burgers vector is not directly available from a visual analysis of atomistic simulation data, making the investigation of dislocation reactions laborious and error-prone.

Thus, there is a significant demand for more powerful analysis tools, which has led to the development of several computational techniques in recent years that can automatically detect and identify dislocation lines (Begau et al., 2011, 2012; Elsey and Wirth, 2014; Hartley and Mishin, 2005; Hua and Hartmaier, 2010; Stukowski and Albe, 2010a, 2010b; Stukowski et al., 2012; Wang et al., 2013). Current approaches can be divided into two categories: one family of methods (Stukowski et al., 2012; Wang et al., 2013) makes use of the Burgers circuit procedure, while the other (Begau et al., 2012; Elsey and Wirth, 2014; Hartley and Mishin, 2005) is based on the Nye tensor concept. In general, the existing methods greatly differ not only in their capabilities but also in their complexity of implementation, which is usually considerable. In the present study an exceptionally simple method is developed, which is easy to implement and yet sufficiently capable to be useful in many application scenarios.

The algorithm presented in this paper can detect full and partial lattice dislocations in atomistic descriptions of BCC, FCC, and HCP single crystals and determine their Burgers vectors. The output generated by the algorithm is a non-atomistic

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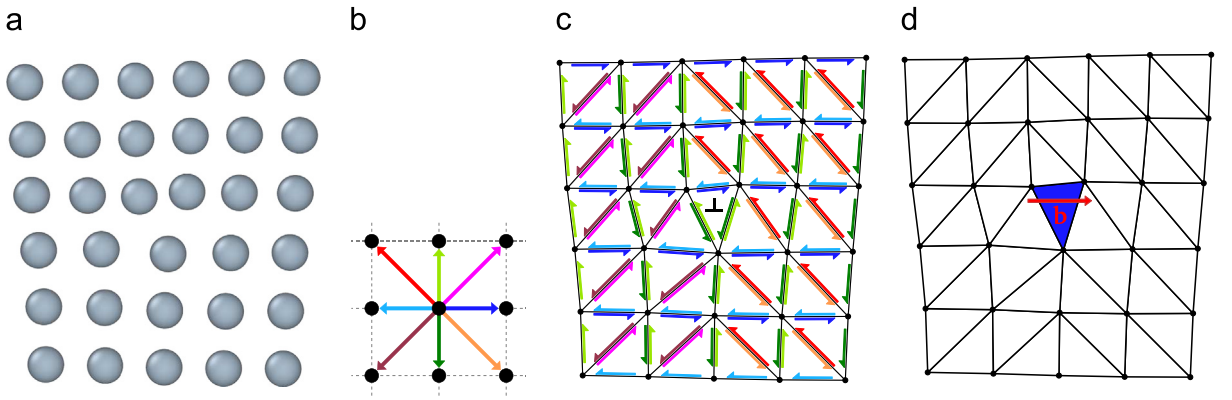

Fig. 1. (a) Example of a 2d crystal containing a dislocation to be identified. (b) Set of ideal crystal vectors, $\mathcal{L}$, for the square lattice. (c) Delaunay triangulation of the crystal; edge colors indicate the assigned ideal crystal vectors. (d) The triangular element containing the dislocation exhibits a closure failure and is marked by the dislocation identification algorithm. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

representation of dislocation segments that is suitable for topological analyses of dislocation networks and fulfills the Burgers vector conservation law. The described method thus connects fully atomistic models of crystals to mesoscale models based on discrete dislocations.

2. Algorithm description

The algorithm's input comprises the atomic coordinates $\{\boldsymbol{x}_i\}$ of the dislocated crystal (Fig. 1a) and a set $\mathcal{L}=\{\boldsymbol{L}_i\}$ of ideal crystal vectors, which needs to be specified. In case of the two-dimensional square lattice, which is used here for an introductory example, this set includes eight vectors as shown in Fig. 1b, each represented by a different color. The basic algorithm consists of three steps:

1. Construct the Delaunay triangulation for the point set $\{\boldsymbol{x}_i\}$.
2. For every edge $a \rightarrow b$ of the triangulation, connecting two atoms separated by the spatial vector $\boldsymbol{x}_{ab}=\boldsymbol{x}_b-\boldsymbol{x}_a$, assign the best-matching ideal vector from the set $\mathcal{L}$, $\boldsymbol{L}_{ab}=\min \arg_{\boldsymbol{L}_i \in \mathcal{L}} |\boldsymbol{x}_{ab}-\boldsymbol{L}_i|$, to the edge (Fig. 1c). The edge's opposite direction, $b \rightarrow a$, is associated with the reverse vector, $\boldsymbol{L}_{ba}=-\boldsymbol{L}_{ab}$.
3. For every triangle abc of the tessellation, compute its Burgers vector

$$\boldsymbol{b}_{abc}=\boldsymbol{L}_{ab}+\boldsymbol{L}_{bc}+\boldsymbol{L}_{ca} \tag{1}$$

by summing the ideal lattice vectors assigned to its three edges (in clockwise direction). Triangles with a non-zero Burgers vector contain a dislocation and are marked accordingly as shown in Fig. 1d.

3. Three-dimensional crystals

In three dimensions, the Delaunay tessellation consists of tetrahedral cells, each being bordered by four triangular facets (Fig. 2a). In the three-dimensional version of the algorithm, the Burgers vector is computed for every triangular facet according to Eq. (1), and, if $\boldsymbol{b} \neq \boldsymbol{0}$, the facet is said to be intersected by a dislocation. The same is true for the two tetrahedral cells adjacent to such a dislocated facet. Fig. 2c illustrates how dislocation lines in a three-dimensional crystal are revealed by the algorithm. The imaginary dislocation line pierces through a sequence of triangular facets, each exhibiting the same non-zero Burgers vector.

A dislocation line entering a tetrahedron through one facet has to exit it through another (Fig. 2a). A tetrahedral cell can therefore have 0, 2, 3, or 4 facets with a non-zero Burgers vector. Tetrahedra with exactly two dislocated facets form a linear chain along the dislocation line. Tetrahedra with more than two dislocated facets contain a dislocation junction. In agreement with Frank's rule, the Burgers vectors computed for the four oriented facets of every cell always add up to zero. That is for a tetrahedron $abcd$:

$$\begin{aligned}\boldsymbol{b}_{abc}+\boldsymbol{b}_{cbd}+\boldsymbol{b}_{acd}+\boldsymbol{b}_{adb} &= (\boldsymbol{L}_{ab}+\boldsymbol{L}_{bc}+\boldsymbol{L}_{ca})+(\boldsymbol{L}_{cb}+\boldsymbol{L}_{bd}+\boldsymbol{L}_{dc})+(\boldsymbol{L}_{ac}+\boldsymbol{L}_{cd}+\boldsymbol{L}_{da})+(\boldsymbol{L}_{ad}+\boldsymbol{L}_{db}+\boldsymbol{L}_{ba}) \\ &= (\boldsymbol{L}_{ab}+\boldsymbol{L}_{ba})+(\boldsymbol{L}_{bc}+\boldsymbol{L}_{cb})+(\boldsymbol{L}_{ca}+\boldsymbol{L}_{ac})+(\boldsymbol{L}_{bd}+\boldsymbol{L}_{db})+(\boldsymbol{L}_{dc}+\boldsymbol{L}_{cd})+(\boldsymbol{L}_{da}+\boldsymbol{L}_{ad})=\boldsymbol{0}\end{aligned} \tag{2}$$

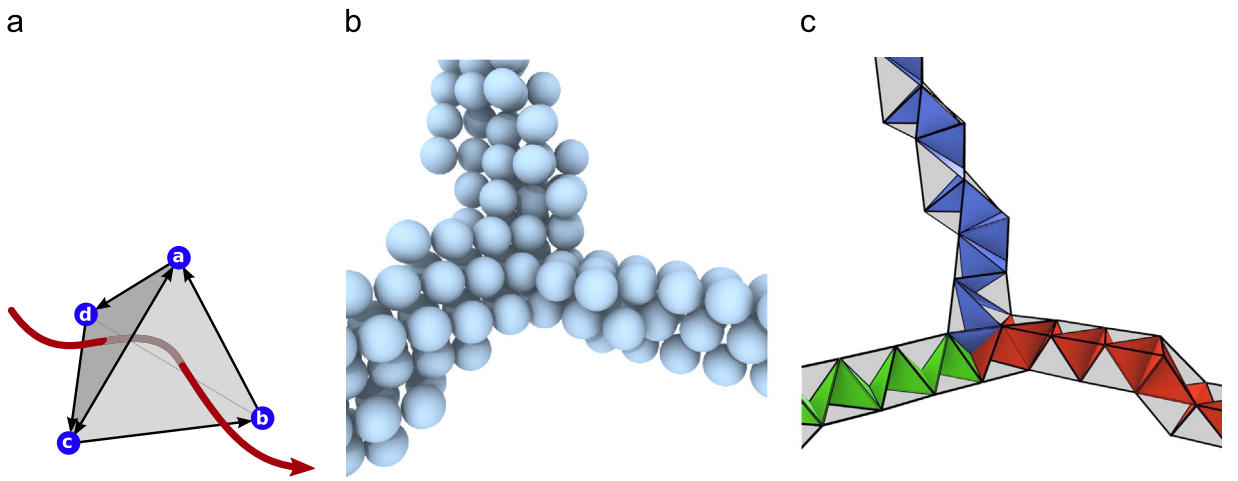

Fig. 2. (a) Schematic depiction of a tetrahedral cell intersected by a dislocation line. (b) A junction of three dislocations in BCC iron. Core atoms have been made visible using the common neighbor analysis filtering method. (c) The corresponding output of the described algorithm. Triangle facets that are intersected by a dislocation were marked with different colors to indicate their Burgers vector. The tetrahedron having three differently colored facets contains the junction. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

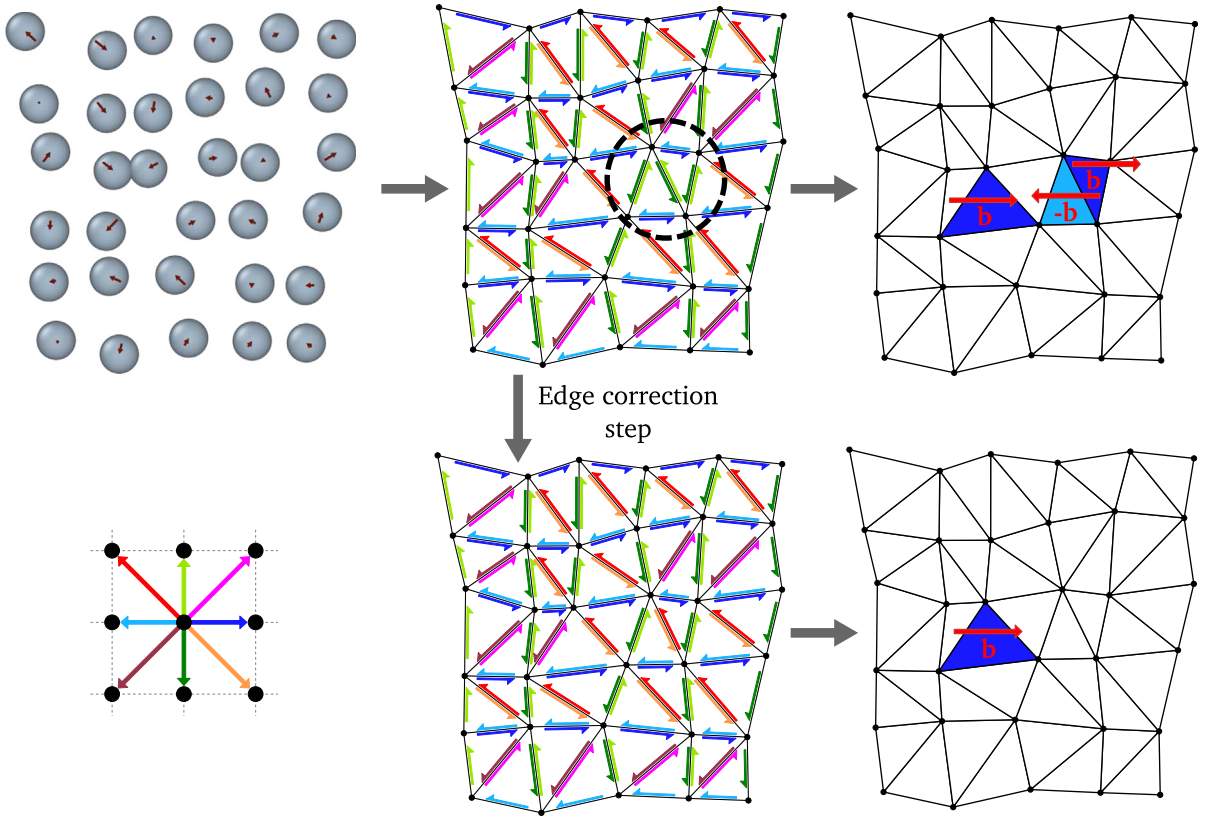

Fig. 3. Analysis of a dislocated crystal with perturbed atomic positions. The basic algorithm reports a spurious dislocation dipole (first row). The edge correction procedure described in the text suppresses the dipole (second row).

4. Improving the robustness

The atomic positions in a crystal can be randomly perturbed due to, for instance, thermal displacements in a molecular dynamics simulation. Depending on the strength of such local fluctuations, the assignment of ideal lattice vectors to edges of the tessellation may be prone to errors. To demonstrate the effect of noise on the identification of dislocations, we again make use of a two-dimensional example. Fig. 3 shows the dislocated crystal considered earlier, whose atoms have now been

randomly displaced from their equilibrium positions. The algorithm reports three triangles with a non-zero Burgers vector although the crystal contains only a single dislocation. The assignment of ideal lattice vectors to tessellation edges no longer works reliably, because the edges are heavily distorted. In this example, one of the edges was assigned a "wrong" ideal vector, giving rise to a closure failure in the two adjacent triangles. The algorithm consequently reports a spurious dislocation dipole in addition to the third dislocated element, which contains the actual dislocation.

To suppress such artifacts, we introduce an additional algorithm step that corrects the assignment of ideal vectors in most cases. The initial guess of the ideal vector, made in algorithm step 2, is reconsidered as follows: given an edge $a \rightarrow b$, with an assigned ideal vector $\boldsymbol{L}_{ab}$, every vertex c of the tessellation that is adjacent to both a and b is traversed. An alternative lattice vector $\boldsymbol{L}_{ab}^{(c)} = \boldsymbol{L}_{ac} + \boldsymbol{L}_{cb}$ is computed from the two edges leading from a via c to b. The ideal vector that occurs most frequently is finally assigned to the edge $a \rightarrow b$, possibly replacing its original vector to eliminate a spurious dipole. Note that the original vector $\boldsymbol{L}_{ab}$ is included in this voting procedure. The described correction scheme is repeatedly applied to the entire tessellation until no more edges get updated. Then the last step of the algorithm is invoked to identify dislocated cells. The second row of Fig. 3 shows that the spurious dipole is eliminated by this procedure, whose aim is to eliminate local closure failures. Note that the dislocation is localized in a different triangle compared to the first example, Fig. 1d, due to the applied noise, which renders the dislocation's position (but not its Burgers vector) uncertain to some degree.

The described correction procedure has a second favorable effect and solves a problem which has not been discussed yet and is even more critical: The cores of realistic dislocations have, depending on the material, a certain extent. That means the disregistry associated with a dislocation is not concentrated in a mathematical line but continuously spread over a certain radius, which can exceed the typical size of a Delaunay cell. Since the triangular Burgers circuits employed by the algorithm are very small, and consist of only three atoms, they may not fully enclose the extended dislocation core. As a result, the basic algorithm would report several partial dislocations instead of one full dislocation, i.e., several adjacent triangles with a non-zero fractional Burgers vector are detected. The described edge correction procedure, however, rectifies as many dislocated triangles as possible to suppress a local closure failure. This effectively concentrates the dislocation (specifically the curl of the lattice distortion field) into a single triangular cell at the center of the core. This is why we can obtain the full Burgers vector of a spread dislocation without the need to construct a larger circuit.

5. Practical considerations

We have successfully tested the described dislocation identification algorithm with typical molecular dynamics simulations of BCC and FCC crystals. In the former case, the set of ideal vectors $\mathcal{L}$ comprises the $\frac{1}{2}\langle 111\rangle$ family of nearest-neighbor vectors. In addition, combinations of these lattice vectors up to the fourth neighbor shell are included to cover Delaunay edges that connect non-nearest neighbor atoms.

In FCC crystals, partial dislocations are very common, and their identification requires partial lattice vectors. Therefore, in addition to the $\frac{1}{2}\langle 110\rangle$ family of nearest-neighbor vectors, the $\frac{1}{6}\langle 112\rangle$ family of partial vectors is included in the set $\mathcal{L}$. This enables the algorithm to identify Shockley, Frank, stair-rod and other partial dislocations whose Burgers vector is a combination of these basis vectors. Fig. 4 demonstrates the application of the algorithm to an MD simulation of an aluminum crystal under plastic deformation. Note that even twinning dislocations can be identified in FCC crystals without further effort, because ideal vectors in the twinned region can be expressed with the same basis vector set used for the matrix crystal.

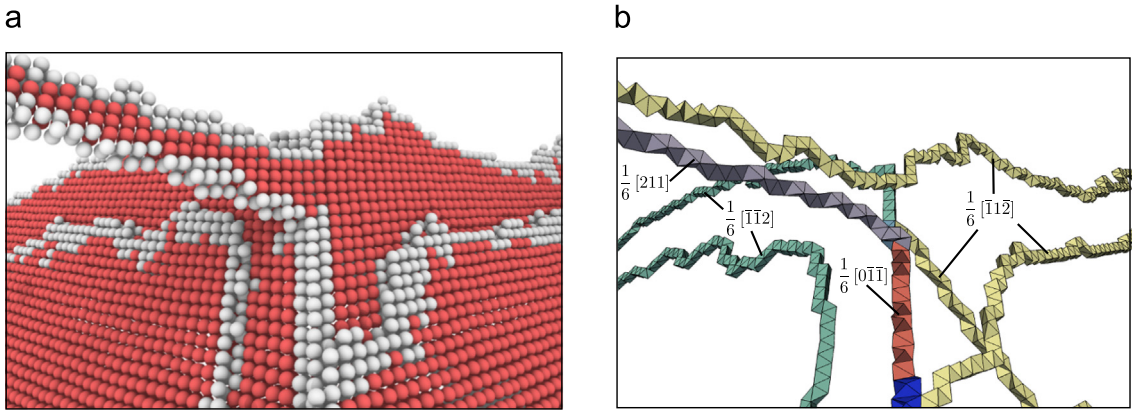

Fig. 4. (a) Conventional atomistic visualization of an MD simulation of single-crystalline Al under compression, which undergoes plastic deformation by dislocation slip and twinning. Dislocation core atoms (white) and stacking fault and coherent twin boundary atoms (red) are shown. (b) Output of the dislocation identification algorithm. Dislocated tetrahedral cells have been colored according to their Burgers vector. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

The Delaunay tessellation always covers the entire convex hull of a point set. Thus, very long elements may occur at the surfaces of a crystal of arbitrary shape. The assignment of ideal vectors to the edges of such elongated elements is problematic, because they connect very distant atoms. Being located near or outside the surface, however, they cannot be part of a dislocation; so we simply discard such elements based on a maximum edge-length criterion and, in addition, an alpha shape criterion (Edelsbrunner and Mücke, 1994).

6. Comparison with other approaches

Hartley and Mishin (2005) described a computational method to calculate the Nye (1953) tensor from a set of atomic positions and to determine the Burgers vector of a simulated dislocation. Begau et al. (2012) were able to develop a practical and fully automated dislocation identification method based on this approach. The Nye tensor concept and the Burgers circuit method, of which the latter provides the conceptual basis for the present work, are directly related as discussed by Hartley and Mishin (2005) and summarized here: a closed Burgers circuit, C', in the dislocated crystal consists of line elements $\mathrm{d}\boldsymbol{x}'$ such that

$$0 = \sum_{C'} \mathrm{d}\boldsymbol{x}'. \tag{3}$$

(The line elements $\mathrm{d}\boldsymbol{x}'$ are in the present work identified with the spatial edge vectors, $\boldsymbol{x}_{ab}$, connecting pairs of atoms in the Delaunay tessellation.) Transforming the vectors $\mathrm{d}\boldsymbol{x}'$ into their images, $\mathrm{d}\boldsymbol{x}$, in the perfect crystal lattice (which, in this work, are referred to as $\boldsymbol{L}_{ab}$) and summing them algebraically along the associated path, C, give the true Burgers vector of the enclosed dislocation:

$$\boldsymbol{b} = -\sum_{C} \mathrm{d}\boldsymbol{x}. \tag{4}$$

This forms the basis of Eq. (1), which we use to compute $\boldsymbol{b}$ for triangular circuits on the Delaunay tessellation consisting of exactly three edges. The physical vectors, $\mathrm{d}\boldsymbol{x}'$, and the ideal vectors, $\mathrm{d}\boldsymbol{x}$, are related by the lattice correspondence tensor $\boldsymbol{G}$:

$$\mathrm{d}\boldsymbol{x} = \mathrm{d}\boldsymbol{x}' \cdot \boldsymbol{G}. \tag{5}$$

$\boldsymbol{G}$ is the transpose of the inverse elastic deformation gradient. As shown by Hartley and Mishin (2005), an atomistic version of the $\boldsymbol{G}$ tensor can be computed from the nearest-neighbor bonds of an atom and a corresponding set of ideal lattice vectors using a least-squares fit. By replacing the sum in Eq. (4) with an integral, and inserting Eq. (5), we have

$$\boldsymbol{b} = -\int_{C'} \mathrm{d}\boldsymbol{x}' \cdot \boldsymbol{G}. \tag{6}$$

Applying Stoke's theorem gives

$$\boldsymbol{b} = -\int_{A} (\nabla \times \boldsymbol{G}) \cdot \boldsymbol{n}\, \mathrm{d}s, \tag{7}$$

where $\boldsymbol{n}$ is a unit vector normal to the area element $\mathrm{d}s$, and integration is over the surface A, which is delimited by the circuit C'. The integrand's first term is known as the Nye tensor:

$$\boldsymbol{\alpha} = -(\nabla \times \boldsymbol{G}). \tag{8}$$

Given that $\boldsymbol{G}$ has been computed at each atomic site, the curl operator in Eq. (8) can be evaluated numerically using a finite differences approximation (Hartley and Mishin, 2005) to obtain the Nye tensor at an atomic site. Begau et al. (2012) next establish a continuous Nye tensor field via interpolation and, finally, compute the Burgers vector of a dislocation according to Eq. (7) using numerical integration over a certain area around the atom. Note that this computation is performed on individual atoms, and $\boldsymbol{b}$ is non-zero only for those atoms in the system that are part of a dislocation.

In view of the fact that this Nye-based procedure involves several approximations (least-square fit, finite differences, numeric integration), it becomes clear that the resultant Burgers vector is only an approximation of the true Burgers vector. This means the most likely true Burgers vector has to be guessed from a predefined set of possible vectors. As a result, the Burgers vector conservation at dislocation nodes is not formally guaranteed. The triangulation-based approach presented in this paper, in contrast, directly yields true Burgers vectors without resorting to any numerical approximations.

It is worthy to note that the triangulation-based framework presented here also allows us to directly compute the elastic deformation gradient field, $\boldsymbol{F}^{\mathrm{e}}$, and the lattice correspondence tensor field, $\boldsymbol{G} = (\boldsymbol{F}^{\mathrm{e}})^{-\mathrm{T}}$, at the smallest length scale (Stukowski and Arsenlis, 2012). Considering a tetrahedral Delaunay cell, we can take a non-coplanar triplet of its edges, $\{\boldsymbol{x}_\alpha, \boldsymbol{x}_\beta, \boldsymbol{x}_\gamma\}$, and their corresponding ideal lattice vectors, $\{\boldsymbol{L}_\alpha, \boldsymbol{L}_\beta, \boldsymbol{L}_\gamma\}$, to compute the matrix products

$$\boldsymbol{F}^{\mathrm{e}} = [\boldsymbol{x}_\alpha\ \boldsymbol{x}_\beta\ \boldsymbol{x}_\gamma] \cdot [\boldsymbol{L}_\alpha\ \boldsymbol{L}_\beta\ \boldsymbol{L}_\gamma]^{-1} \tag{9}$$

$$\boldsymbol{G} = [\boldsymbol{x}_\alpha\ \boldsymbol{x}_\beta\ \boldsymbol{x}_\gamma]^{-\mathrm{T}} \cdot [\boldsymbol{L}_\alpha\ \boldsymbol{L}_\beta\ \boldsymbol{L}_\gamma]^{\mathrm{T}}. \tag{10}$$

Note that a cell intersected by a dislocation exhibits a multivalued elastic deformation gradient. That means $\boldsymbol{F}^{\mathrm{e}}$ and $\boldsymbol{G}$ depend on which three of the six edges of the tetrahedron we pick for their calculation.

The method described in this paper is derived from the *Dislocation Extraction Algorithm* (DXA) (Stukowski et al., 2012; Stukowski and Albe, 2010b), which is not only a more general technique, but also a more complex technique to extract dislocation lines from atomistic simulations. The DXA and the present approach have in common that they are both based on the Delaunay tessellation and a mapping of its edges to a reference crystal lattice. In the DXA, however, the assignment of ideal lattice vectors to Delaunay edges follows a more sophisticated procedure. By first identifying the local crystal structure formed by atoms, the method can be applied to crystals with unknown lattice orientation or polycrystalline microstructures. In addition, the DXA employs moving Burgers circuits of variable length on the network of Delaunay edges to generate a linear representation of dislocation segments. Such a discrete line model of a dislocation network enables a quantitative measurement of the dislocation density, which is impossible in the original atomistic model. The DXA is, however, a very complex algorithm, which consists of a rather long sequence of processing steps. One of the aims of the present work was therefore to develop a highly simplified algorithm, which can be implemented with only minimal effort and is on par with alternative solutions.

7. Summary

In this contribution we have shown how a space-filling tetrahedral tessellation can be used to identify dislocations in atomistic crystals. The described method provides a useful analysis tool for atomistic computer simulations, where it can help to determine Burgers vectors of individual dislocation segments and to discriminate dislocations from other defects in a fully automated way. The algorithm can be applied to FCC, HCP, and BCC single crystals and is noise tolerant, making it suitable for finite temperature simulations.

A reference implementation of the algorithm is available from the author. It comprises only about 100 lines of C++ code and uses the Computational Geometry Algorithms Library (Boissonnat et al., 2002) to generate the Delaunay tessellation.

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