Technical Notes

August 2, 2012

1 Dislocation representation

The evolving dislocation configuration consists of a non-empty list of dislocation loops. Each loop is stored as a circular doubly-linked list of *segment-node* elements. A *segment-node* element represents both a node and the outgoing linear segment adjacent to that node. Each *segment-node* element has pointers to the successive and the preceding element, forming the linked list. A *segment-node* element i stores the position $\mathbf{x}_i$ of the node and the line vector $\mathbf{l}_i$ of the outgoing segment (pointing to the successive node). Every node is connected to exactly one incoming and one outgoing segment (closed linear chain).

As a special requirement (performance consideration), a dislocation loop must consist of at least two nodes/segments. That means, the initial straight dislocation segment is divided into two segments (even though one would suffice).

Nodal positions and line vectors are both stored as coordinate triplets (u, v, w), where u and v are integers, and w is a continuous coordinate along the screw direction (in units of b). This internal coordinate system is spanned by the three unit vectors

$$\mathbf{e}_u = \frac{1}{2}[\bar{1}1\bar{1}] \qquad \mathbf{e}_v = \frac{1}{2}[11\bar{1}] \qquad \mathbf{e}_w = \frac{1}{2}[111]$$

An internal vector (u, v, w) can be converted to the spatial representation (x, y, z) by multiplying it with the transformation matrix

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = a \begin{pmatrix} \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix},$$

where a is the bcc lattice parameter. The spatial coordinate system is spanned by the Cartesian unit vectors

$$\mathbf{e}_x = \frac{1}{\sqrt{6}}[\bar{1}2\bar{1}] \qquad \mathbf{e}_y = \frac{1}{\sqrt{2}}[10\bar{1}] \qquad \mathbf{e}_z = \frac{1}{\sqrt{3}}[111]$$

The Burgers vector $\mathbf{b}$ of all dislocations is $(0, 0, 1)$ in internal coordinates, and $(0, 0, b)$ in spatial coordinates.

The periodicity length $L \in \mathbb{N}$ of the system along the screw direction is specified as an integer multiple of the Burgers vector b. Nodal positions do not have to lie inside the primary image of the system. That is, whenever a node moves, it is not wrapped back into the simulation cell when it crosses the periodic boundaries. Each dislocation segment stores a line vector $\mathbf{l}_i$, which connects the two successive nodes i and $(i+1)$ of the loop. $\mathbf{l}_i$ represents the physical extension of the segment (in the internal coordinate system). Since the two nodes of the segment can be located in two different images of the system, $\mathbf{l}_i$ is only equal to the difference of the two nodal positions plus an integer multiple of the periodicity length:

$$\mathbf{l}_i = \mathbf{x}_{i+1} - \mathbf{x}_i + (0, 0, nL)$$

The net dislocation content within the simulation is conserved at all times, i.e.

$$\sum_i \mathbf{l}_i = (0, 0, L).$$

The sum of segment vectors in a single dislocation loop $\mathcal{L}$ adheres to

$$\sum_{i \in \mathcal{L}} \mathbf{l}_i = (0, 0, n_{\mathcal{L}} L),$$

with an integer $n_{\mathcal{L}}$. If $n_{\mathcal{L}} = 0$, then the dislocation is a finite (debris) loop. If $n_{\mathcal{L}} = 1$, then the dislocation is the infinite (periodic) screw dislocation. The system should contain exactly one dislocation with $n_{\mathcal{L}} = 1$ at all times, and may contain zero or more debris loops with $n_{\mathcal{L}} = 0$. To measure the velocity of the dislocation, the center of mass of only the infinite dislocation is computed.

2 Monte Carlo algorithm

One iteration of the Monte Carlo algorithm consist of the following steps:

1. Compute current velocities $\dot{w}_i$ of dislocation nodes:
   (a) First, compute velocities of existing kink segments (from resolved applied shear stress divided by kink drag coefficient, $\dot{w} = \frac{\dot{z}}{b} = \frac{\tau_g}{B}$).
   (b) Detect adjacent pairs of kinks with negative relative velocity, $\dot{w}_i - \dot{w}_{i+1} < 0$ (locked cross-kinks); reset velocity of both kinks to zero to prevent the occurrence of reverse screw segments.
   (c) Transfer kink velocities to adjacent dislocation nodes. Nodes adjacent to two kink segments with different velocity are split into two nodes (connected by a zero-length screw segment).
2. Compute minimum free migration time t^{mig} of dislocation nodes (along screw direction). t^{mig} is minimized over all nodes, with the per-node time t_i^{mig} given by the smaller of

(a) The shortest collision time with another node j on the same atomic row ($u_i = u_j$, $v_i = v_j$): $t_i^{\mathrm{col}} = \min_j \left(\frac{w_j - w_i}{\dot{w}_i - \dot{w}_j} \right)$

(b) The time needed to reach the prescribed maximum travel distance: $t_i^{\max} = \frac{\Delta w^{\max}}{|\dot{w}_i|}$

3. Generate list of kMC kink-pair nucleation events and compute their rates.

   (a) A single event is specified by

   - The screw segment
   - The (starting) position of the kink pair along the screw segment (in units of b)
   - The width of the kink pair (in units of b)
   - The kink direction (index into global list of possible direction vectors)
   - The nucleation rate (calculated from the above)

   (b) For each existing screw segment, generate n_{nuc} nucleation events.

   i. To generate one event, randomly sample kink directions, kink-pair widths, and kink-pair positions along screw segment.

   ii. Compute activation energy ΔF_{kp}.

   iii. Compute nucleation rate $j_{\mathrm{kp}} = \nu \exp\left(-\frac{\Delta F_{\mathrm{kp}}}{kT} \right)$, with a normalized attempt frequency $\nu = \nu_0 \frac{l}{n_{\mathrm{nuc}}}$. Here, l denotes the screw segment's length.

4. Generate nucleation time from exponential distribution defined by the total nucleation rate: $t^{\mathrm{nuc}} = j_{\mathrm{tot}} \exp\left(-j_{\mathrm{tot}} x\right)$, with $j_{\mathrm{tot}} = \sum j_{\mathrm{kp}}$ and a random number $x \in [0, 1]$.

5. If $t^{\mathrm{mig}} \leq t^{\mathrm{nuc}}$, then all kinks/nodes move with their current velocity for a time t^{mig}. The simulation time is incremented $t \leftarrow t + t^{\mathrm{mig}}$.

6. If $t^{\mathrm{mig}} > t^{\mathrm{nuc}}$, then all kinks/nodes move for a time t^{nuc}, and a nucleation event is selected and executed from the catalog using the kMC algorithm. The simulation time is incremented $t \leftarrow t + \frac{1}{j_{\mathrm{tot}}}$.

7. The dislocation configuration is updated/purged:

   (a) Find kink nodes that are located on top of another (screw) segment. Insert another 2-node into the screw segment here to subdivide it.

   (b) Remove degenerate screw segments with zero length.

   (c) Detect 4-nodes, i.e. two 2-nodes at the same location. Use minimum curvature criterion to decide whether the four arms of the 4-node should be flipped. The flipping operation either generates a new dislocation loop or coalesces two loops into one.

(d) Again search for degenerate scew segments and delete them.

(e) Remove redundent nodes on screw segments, i.e. coalesce two adjacent screw segments into one.

(f) Delete degenerate dislocation loops that consist of only two (kink) segments (i.e., which are not an infinite straight dislocation).