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Implementation of Shifted Periodic Boundary Conditions in the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) Software

by N Scott Weingarten and James P Larentzos

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REPORT DOCUMENTATION PAGE				*Form Approved* *OMB No. 0704-0188*
<td colspan="5">Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.   **PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.**</td>
1. REPORT DATE *(DD-MM-YYYY)* Aug 2015	**2. REPORT TYPE** Final		**3. DATES COVERED (From - To)** NA	
4. TITLE AND SUBTITLE Implementation of Shifted Periodic Boundary Conditions in the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) Software			**5a. CONTRACT NUMBER**	
			5b. GRANT NUMBER	
			5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) N Scott Weingarten and James P Larentzos			**5d. PROJECT NUMBER**	
			5e. TASK NUMBER	
			5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) US Army Research Laboratory ATTN: RDRL-WML-B Aberdeen Proving Ground, MD 21005			**8. PERFORMING ORGANIZATION REPORT NUMBER** ARL-TN-0687	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			**10. SPONSOR/MONITOR'S ACRONYM(S)**	
			11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
<td colspan="5">**12. DISTRIBUTION/AVAILABILITY STATEMENT**   Approved for public release; distribution unlimited.</td>
<td colspan="5">**13. SUPPLEMENTARY NOTES**</td>
<td colspan="5">**14. ABSTRACT**   To observe screw dislocation motion on an infinite glide plane in atomistic simulations, shifted periodic boundary conditions (sPBC) must be utilized. We have implemented this capability in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software application code for use in classical molecular dynamics (MD) simulations. This report presents the justification for utilizing sPBC, followed by a description of the implementation methodology. Dislocation velocities as a function of applied stress are obtained for screw dislocations in aluminum (Al) at a temperature of 300 K, and compared to prior results to verify our implementation.</td>
<td colspan="5">**15. SUBJECT TERMS**   molecular dynamics, aluminum, dislocations</td>
16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT** UU	**18. NUMBER OF PAGES** 26	**19a. NAME OF RESPONSIBLE PERSON** N Scott Weingarten
a. REPORT Unclassified	**b. ABSTRACT** Unclassified	**c. THIS PAGE** Unclassified			**19b. TELEPHONE NUMBER (Include area code)** (410) 306-0718

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1.   Introduction

Dislocations play an important role in the response of crystalline materials during deformation. Multiple mechanisms, including dislocation nucleation, the motion of individual dislocations, or the collective motion of dislocation networks, can be involved during plastic deformation.[1] Mesoscale models, such as dislocation dynamics (DD), have been developed to obtain a better understanding of these mechanisms.[2]

One key aspect of DD models is the mobility laws dictating the behavior of individual dislocations,[3] which determine how the force on a dislocation translates into motion. This is achieved by defining the velocity as a function of applied stress and temperature, while taking into account the Burgers vector, orientation, and slip system of the dislocation. However, this information is not accessible from experiment, hence molecular dynamics (MD) simulations are typically used to determine mobility functions.[4]

The MD simulation methodology involves introducing an individual dislocation to a single crystal system, and applying an external shear stress.[5] The dislocation will glide in response to the applied stress, and the velocity can be calculated. For any material system, edge and screw dislocations can occur on multiple slips systems, and for completeness, mobility laws must be determined for all possible dislocations in the material. The focus of this work is calculating accurate mobility laws for both edge and screw dislocations, which require different types of periodic boundaries.

Simulations of edge dislocation glide make use of periodic boundary conditions (PBC) in the glide plane, which mimics a series of equally spaced infinitely long dislocations.[5] The implementation of PBC can be viewed as surrounding the simulation cell with replicates of the system. Simulations of a crystal typically require that the dimensions of the simulation cell are multiples of some periodic distance of the lattice (i.e., the unit cell). This is shown for a 2-D system in Fig. 1a, where the central box represents the simulation cell. The surrounding boxes, colored in a lighter shade, are replicates of the simulation cell. Lattice planes are depicted in blue, and while the lattice planes are not parallel to the boundaries, the dimensions of the system are such that the planes are consistent across the boundaries. In a simulation, PBC would result in atoms near a boundary interacting with atoms on the other side of the system as if they were nearby, and atoms leaving the simulation cell would reappear on the opposite side. This is a commonly used technique that allows for the simulation of an infinite bulk system.
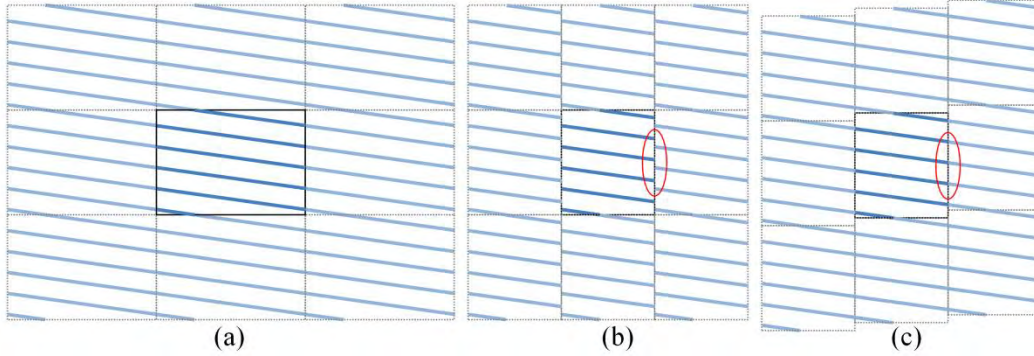
Fig. 1 **a) A depiction of PBC: a central simulation cell surrounded by replicates, with blue lines representing lattice planes. b) Same system, with the simulation cell having a shorter horizontal dimension. c) Implementation of shifted periodic boundary conditions (sPBC) results in alignment of lattice planes.**

However, if the cell dimensions are not chosen carefully the lattice planes are not consistent across the boundaries. Such a situation is depicted in Fig. 1b, which is the same crystal system as Fig. 1a with the simulation cell having a shorter horizontal length. Inside the red circle, it is seen that the lattice planes do not align across the vertical boundaries. Note that the vertical dimension of the simulation cell has not been changed and the lattice planes are consistent across the horizontal boundaries. A possible remedy for the situation in Fig. 1b is to use shifted periodic boundary conditions (sPBC), which can be seen in Fig. 1c. The replicates to the right (left) of the simulation cell are shifted upwards (downwards) a small distance in order to align the lattice planes. During the course of a simulation, atoms interacting across the boundary must include this shift when calculating forces. In addition, when atoms cross the boundary, their vertical position is adjusted appropriately before reappearing on the other side. We would like to stress that sPBC would not be the typical means of addressing the problem in Fig. 1b, which would be more intuitively solved by using a simulation cell dimension that is periodic for the crystal structure and orientation, as seen in Fig. 1a.

While PBC can be used with edge dislocation glide, accurate screw dislocation mobility laws require the use of sPBC, since PBC are insufficient to model an infinite glide plane.[6] Figure 2a shows an illustration of a screw. The threads are tilted in opposing directions on opposite sides of the screw, and displaced by a small distance represented by the dashed lines. Introducing an individual screw dislocation into a single crystal atomistic system results in a similar orientation of the lattice planes, which are depicted in Fig. 2b. In that figure, the dashed gray line represents the dislocation line, akin to the screw in Fig. 2a. The slip system of this dislocation is defined by b, the Burgers vector (which aligns with the y-axis for this screw dislocation), and the glide plane (of which the normal points in the z-

direction). The red and blue solid lines represent the orientation of lattice planes at the x-boundary. It is clear from Fig. 2b that the red and blue lines are tilted in opposite directions. Finally, Fig. 2c shows the same system as Fig. 2b, now viewed along the x-axis and projected onto the yz-plane. In addition to the same red and blue lines depicting the lattice planes, there are dashed lines representing the average y-positions of those planes. These dashed lines are separated by a distance equal to one-half the magnitude of the Burgers vector ($b/2$) of the screw dislocation.
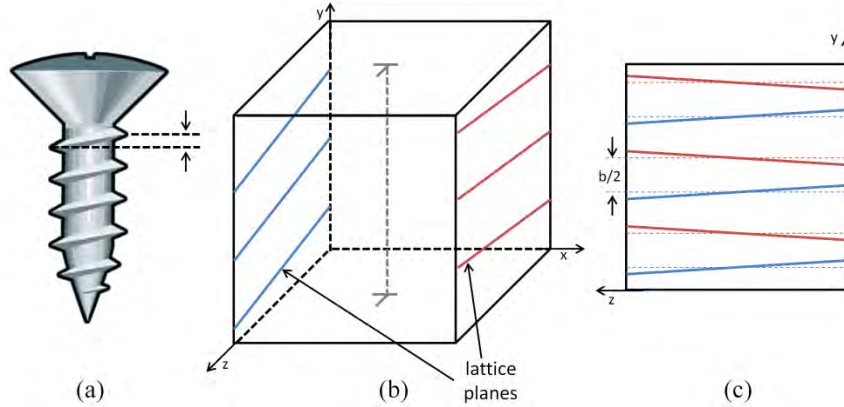

Fig. 2   a) A screw. b) A crystal system containing a single screw dislocation (gray dashed line), with the orientation of the lattice planes at the x-boundaries indicated by red and blue lines. c) The same crystal system, viewed along the x-axis, with dashed red and blue lines indicating the average y-position of the lattice planes.

In response to an external shear stress applied to the system, the dislocation in Fig. 2b is able to glide in the x-direction along an xy-plane. However, normal PBC will not allow for an infinite glide plane because the lattice planes are not consistent across the x-boundary, as seen in Fig. 2b and 2c. This is true for two reasons: they are tilted in opposite directions, and they are displaced by a distance of $b/2$. Inconsistent lattice planes exist across the z-boundary as well (not shown in the figure), but the systems in our simulations have free surfaces separated by a vacuum in that direction. The tilt of the lattice planes decreases with increasing system size (very large x-dimension), and flatness can be enforced with minimal effect on dislocation motion far away from the dislocation. But this does not account for the displacement of the lattice planes across the boundary, hence the need for sPBC in modeling screw dislocation glide on an infinite plane.

In the next section of this report, we describe the implementation of PBC in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS),[7] and the changes made to the code to implement sPBC. This is followed by a description of MD simulations of screw dislocation mobility in aluminum (Al), which we have performed as verification.

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2. Implementation of Shifted Periodic Boundary Conditions in the LAMMPS Framework

The LAMMPS software package (http://lammps.sandia.gov) is one of the premier MD codes for computational chemistry and materials science applications. LAMMPS is an open-source, highly scalable domain-decomposition-based software application developed by the US Department of Energy (DOE) at Sandia National Laboratories that is written with C++ object oriented programming. The modular nature of LAMMPS enables users to easily implement additional physics into the software. Extensive information on the structure and class hierarchy of the software is provided in the LAMMPS Developer Guide.[8] Specifically, the parallel implementation of the sPBC required modification of the *Domain* class and the *AtomVec* child classes. The relevant source code modifications are described in the following section and are current with the 9 December 2014 stable release version of LAMMPS.

2.1 Modification of the Domain Class

The *Domain* class stores the simulation box geometry and applies PBC to the particles local to a given processor. Within the native LAMMPS source code, boundary conditions are specified through the **boundary** command in the input file, followed by keyword characters to specify whether the boundaries are periodic (**p**), fixed (**f**), shrink-wrapped (**s**), or shrink-wrapped with a minimum value (**m**). The modified source code includes an additional keyword character, denoted by the **w** character, to specify the periodic direction to which the shifted boundary conditions are applied. Two additional arguments representing the shift distances are also expected. For example, shifted boundary conditions in the x-direction with a shift distance in the y-direction of 0.2 and a shift distance in the z-direction of 0.1 are specified with the following command:

```
boundary      w p p 0.2 0.1
```

The modified user manual documentation for the boundary command is provided in the appendix. Currently, the modified source code restricts the user to design the orthogonal simulation cells so that the shifted boundary conditions are in the *x*-direction (as specified in the above example). Hence, the **w** character can only appear as the first argument in the **boundary** command.

An illustration comparing PBC images and sPBC images is shown in Fig. 3, where the central simulation cell is depicted with a solid boundary. A positive shift in the y-direction is imposed when the particle crosses the yz-plane of the domain in the $+x$-direction and a negative shift is imposed when the particle crosses the yz-plane in the $-x$-direction.
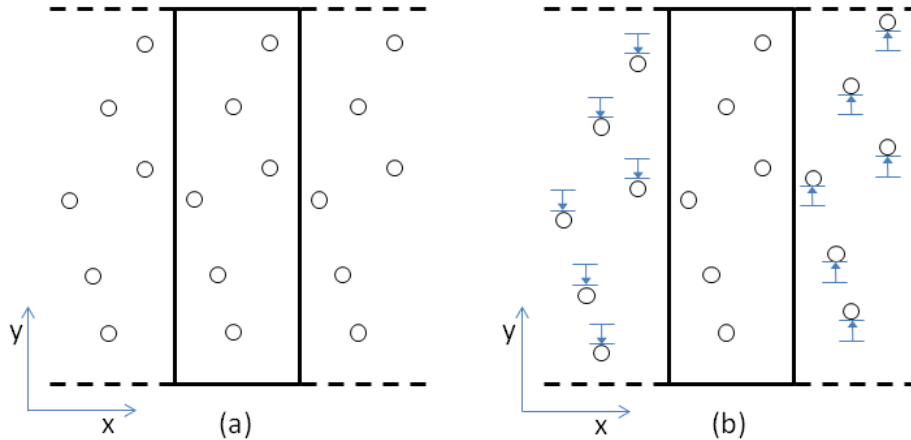

Fig. 3   A 2-D representation of the periodic images of a central cell for: a) traditional PBC and b) sPBC. The arrows are shown to indicate the amount in the y-direction that the particle has shifted relative to the central simulation cell (solid boundary).

2.2 Modification of the AtomVec Atom Style Classes

The *AtomVec* child classes store the atomic attributes (atomic positions, forces, velocities, charges, etc.). The choice of atom style depends on the type of simulation to be conducted in order to efficiently manage the amount of data that is communicated between processors. Within the *AtomVec* child classes, the forward communication buffering methods have been modified to apply sPBC to the periodic images. Forward communication refers to the flow of communication going from the locally ''owned'' particles on one processor to the corresponding ''ghost'' particles that reside on different processors within a domain-decomposition framework. The methods that are responsible for packaging the coordinates prior to the forward communication are the following: `pack_comm`, `pack_comm_vel`, `pack_border`, and `pack_border_vel`. Periodic image flags specify the location of the neighboring subdomain to which the particle coordinates will be communicated. Based on the location of the periodic image, the particle coordinates are shifted accordingly and packaged into the buffer prior to communication.

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3.   Verification of the Implementation

To verify that the sPBC have been correctly implemented, a faced-centered cubic (FCC) crystal was generated to examine the single point energy of the system as the shift distance is increased. These calculations were performed on a single processor. The shift is in the *y*-direction and the distance was varied from 0.0 Å to *a* in intervals of 0.5 Å, where *a* is the value of the lattice constant (*a* = 4.0 Å for this example). Although it may be unphysical to have such large shifts, this particular example tests whether the algorithm has been correctly implemented. At shift distances of 0.0 Å and 4.0 Å, the periodic images align as if no shift were specified; thus, the energies are equivalent, as seen in Fig. 4. The energy decreases as the shift distance is increased until a minimum is observed at half the lattice constant (2.0 Å), followed by a symmetric energy increase as the shift distance approaches *a*. This is the expected result given the periodic nature of the system and demonstrates that the periodic shift has been correctly implemented.
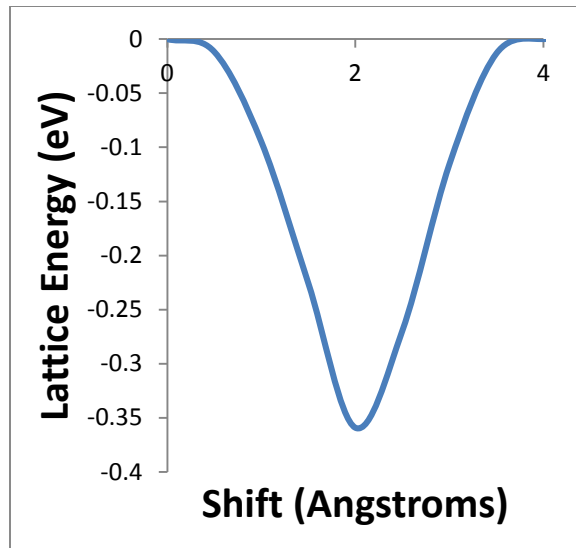

Fig. 4   **A plot showing the periodic nature of the relative lattice energy as the shift distance is varied. When the shift distance is a multiple of the lattice constant, the relative energy is zero.**

The FCC crystal analysis was successfully repeated using multiple processors, indicating that the particle information is correctly communicated to neighboring processors. It is noted that the current implementation requires that the number of processors requested in the shift direction be set to 1 when the magnitude of the shift distance for that direction is greater than zero. The number of processors in

each dimension of the 3-D grid overlaying the simulation domain can be controlled through the LAMMPS `processors` command. For example, the following command is used to specify 1 processor for the *y*-direction:

```
processors   * 1 *.
```

In this case, LAMMPS determines the ideal number of processors in the *x*- and *z*-directions since they are specified by the wild card character (*).

4.   Screw Dislocation Motion in Al

Shifted periodic boundary conditions (sPBCs) have been used in a number of previous MD studies considering screw dislocation mobility.[6,9,10] For verification, we have performed MD simulations of screw dislocation glide in Al, for comparison to work done by Olmsted et al.[10] Simulations are performed at a constant temperature and volume (NVT), using our modified version of LAMMPS. The Ercolessi and Adams embedded atom method (EAM) potential is used,[11] which was fitted to numerous material properties of Al. The timestep is 1 fs, with a thermostating rate of 0.5 ps. A full neighbor list with a cutoff of 6.063 Å was constructed every time step. The system is oriented so that the $[1\,1\,\overline{2}]$, $[1\,\overline{1}\,0]$, and $[1\,1\,1]$ crystal directions align with the *x*, *y*, and *z*-axes, respectively. Two system sizes were used: the crystal dimensions of the first are 119.05 Å × 28.64 Å × 84.18 Å, resulting in 17,280 atoms; the larger second system has 69,120 atoms, with dimensions of 238.11 Å × 28.64 Å × 168.36 Å. A screw dislocation is introduced near the center of the single crystal systems via the displacement field

$$y = b\tan^{-1}\left(\frac{z}{x}\right) \tag{1}$$

so that the Burgers vector is in the *y*-direction, and the glide plane is normal to the *z*-direction. This results in glide along the $(1\,1\,1)\left[1\,1\,\overline{2}\right]$ slip system.

Shear stress is applied to the system in the direction of the Burgers vector, resulting in dislocation motion in the *x*-direction. This is achieved by adding a positive force to atoms at the top surface, and a negative force to those at the bottom.[5] Traditional PBC are used in the *y*-direction, which is the line direction for the dislocation, while sPBC are used in the *x*-direction. The *z*-surfaces are free to accommodate the motion of atoms in opposite directions as a result of the applied force, hence a 40 Å vacuum region is introduced in this direction. The *x*-position of the dislocation is determined by averaging the location of all atoms associated with the dislocation core, defined by the centrosymmetry parameter, from which the dislocation velocity can be calculated.

Three different values of applied stress are considered, all at a temperature of 300 K: 60 MPa, 450 MPa, and 1200 MPa. The table shows the data from our simulations for both system sizes, as well as those from the previous study, which was similar in size to our 17,280 atom system. Agreement is perfect, except for our small system with an applied stress of 60 MPa, for which we did not observe dislocation glide. This is surprising considering the similarities in simulation size between the previous study and our small system. However, the x-dimension of the simulation cell (which is the direction of dislocation glide) listed in the work by Olmsted et al.[10] is not a length compatible with the periodicity of the crystal structure. If that is indeed the length they used, then the shifted periodic boundary is actually a planar defect (i.e., a stacking fault), which would interact with the dislocation and influence its glide motion. The y-dimension in the work by Olmsted et al.[10] has the correct dimensions for repeatability, and the z-dimension has free surfaces, so compatibility across the boundary is not an issue. The data in the table corresponds to the correct crystal dimensions without a stacking fault, resulting in a system of slightly different size from the previous paper.

Table   Dislocation velocities in Al as a function of applied stress at a temperature of 300 K, compared to a previous MD study

Applied Stress (MPa)	Previous[a]	Velocity (nm/ps) 17,280 atoms	69,120 atoms
60 MPa	0.8	0.0	0.80
450 MPa	1.9	1.93	1.92
1200 MPa	2.6	2.65	2.64

[a] Refer to reference 10.

Dislocation glide for the larger system with an applied stress of 1,200 MPa is shown in Fig. 5, which uses the OVITO visualization software.[12] Atoms are colored based on the value of their centrosymmetry parameter as calculated by LAMMPS during the course of the simulation. Note that atoms on the free surface (top and bottom) are correctly colored orange-red, while atoms in the interior appear blue despite the use of shifted boundaries in the x-direction. This indicates the correct implementation of sPBC in LAMMPS. The atoms associated with the dislocation core appear as light blue-green atoms near the center. Over the course of 4.0 ps, the dislocation travels approximately 110 Å in the positive x-direction.
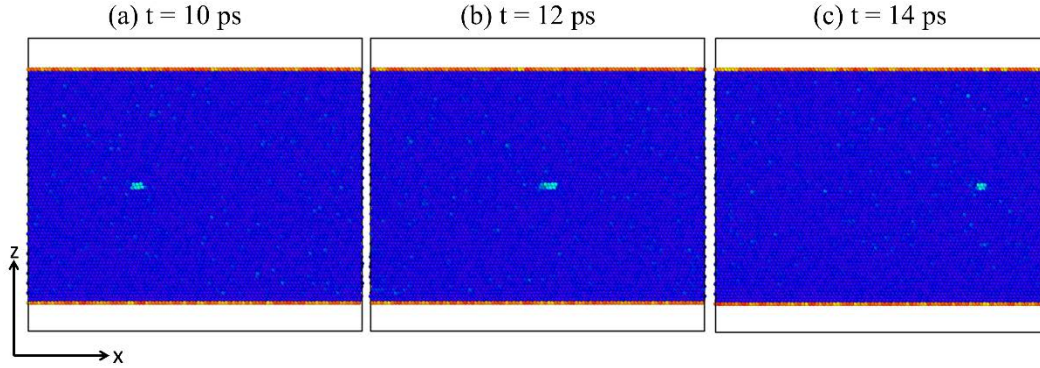
Fig. 5 **The position of the dislocation in Al at 1200 MPa for the larger system at 3 different times (as indicated) during the course of the simulation. Atoms are colored based on their centrosymmetry parameter.**

A more robust calculation of the velocity for this system is shown in Fig. 6, where the dislocation position is plotted as a function of time over a longer interval. The applied stress and the slope of best-fit lines to the data are also shown in the figure (same data that appears in the Table). Clearly, the velocity is constant for all three values of applied stress, and the values are in perfect agreement with Olmsted et al.[10] The *x*-dimension of the simulation cell is 23.8 nm, hence the dislocation has passed through the shifted boundary multiple times during the course of each of the simulations represented in Fig. 6. The dislocation core structure changes as the dislocation passes through the boundary since tilted lattice planes can not be accommodated with sPBC. However, this has no effect on the average velocity of the dislocation over long time periods.
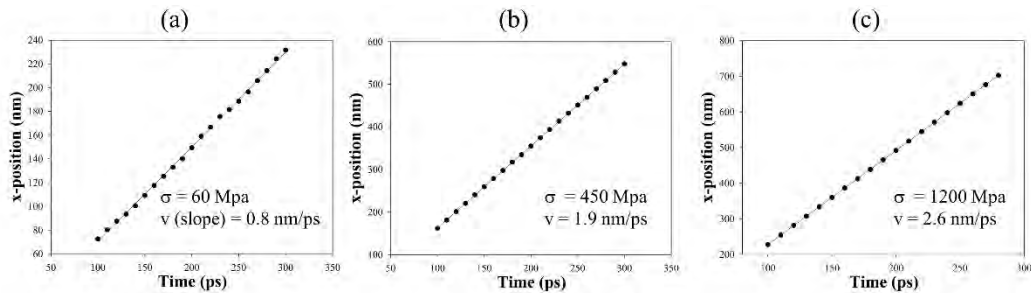

Fig. 6 **Dislocation position in Al as a function of time for the larger system for applied stresses of a) 60 MPa, b) 450 MPa, and c) 1,200 MPa. The slopes of the best fit lines are also shown.**

5. Conclusions

We have implemented sPBC in the LAMMPS software package to perform simulations of screw dislocation glide on an infinite plane. The implementation presented in this report is general with respect to the interatomic potentials

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available, and therefore to the types of materials that can be studied. The capability has only been implemented for one shift boundary (y- and/or z-shift across the x-boundary). This is not a hindrance to the development of mobility laws since slip systems are considered individually in separate simulations, and the proper orientation of the system can be preconfigured. As verification, we have performed simulations of screw dislocation glide in Al. The dislocation velocities as a function of applied stress at T = 300 K are in perfect agreement with prior results.[10] These types of simulations enable the development of mobility laws for use in DD models.

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Appendix. The LAMMPS User Manual Documentation for the Boundary Command

This appendix appears in its original form, without editorial change.

13

boundary command

Syntax:

```
boundary x y z yshift zshift
```

- x,y,z = *p* or *s* or *f* or *m* or *w*, one or two letters
- *p* is periodic
- *f* is non-periodic and fixed
- *s* is non-periodic and shrink-wrapped
- *m* is non-periodic and shrink-wrapped with a minimum value
- *w* is periodic shifted boundary condition
- *yshift* is the shift distance in y and is only necessary when shifted boundary conditions are specified for x
- *zshift* is the shift distance in z and is only necessary when shifted boundary conditions are specified for x

Examples:

boundary p p f
boundary p fs p
boundary s f fm
boundary w p p 0.2 0.1

Description:

Set the style of boundaries for the global simulation box in each dimension. A single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face. The initial size of the simulation box is set by the read_data, read_restart, or create_box commands.

The style *p* means the box is periodic, so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end. A periodic dimension can change in size due to constant pressure boundary conditions or box deformation (see the fix npt and fix deform commands). The *p* style must be applied to both faces of a dimension.

The styles *f*, *s*, and *m* mean the box is non-periodic, so that particles do not interact across the boundary and do not move from one side of the box to the other. For style *f*, the position of the face is fixed. If an atom moves outside the face it may be lost. For style *s*, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. For style *m*, shrink-wrapping occurs, but is bounded by the value specified in

the data or restart file or set by the create_box command. For example, if the upper z face has a value of 50.0 in the data file, the face will always be positioned at 50.0 or above, even if the maximum z-extent of all the atoms becomes less than 50.0.

The style *w* means the box is periodic, so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end, but will be shifted a distance of *yshift* along the shifted y-axis and *zshift* along the z-axis. The current implementation enforces x to be the shifted boundary. As a particle enters/exits the yz face, the shift is applied in the y- and z-directions. The *w* style must be applied to both faces of a dimension.

For triclinic (non-orthogonal) simulation boxes, if the 2nd dimension of a tilt factor (e.g. y for xy) is periodic, then the periodicity is enforced with the tilt factor offset. If the 1st dimension is shrink-wrapped, then the shrink wrapping is applied to the tilted box face, to encompass the atoms. E.g. for a positive xy tilt, the xlo and xhi faces of the box are planes tilting in the +y direction as y increases. These tilted planes are shrink-wrapped around the atoms to determine the x extent of the box.

See Section_howto of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command or read_restart command. See the change_box command for how to change the simulation box boundaries after it has been defined.

For 2d simulations, the z dimension must be periodic.

For the shifted boundary conditions, the simulations are restricted to orthogonal cells. In addition, only shifted boundary conditions for x are supported. When the *yshift* or *zshift* is > 0.0, the number of processors requested in the respective direction must be set to 1 with the processors command.

This command must be used in conjunction with the newton off command to enforce construction of a full neighbor list.

Related commands:

See the thermo_modify command for a discussion of lost atoms.

Default:

```
boundary p p p
```

List of Abbreviations, Acronyms, and Symbols

Al   aluminum

DD   dislocation dynamics

DOE   US Department of Energy

EAM   embedded atom method

FCC   faced-centered cubic

LAMMPS   Large-scale Atomic/Molecular Massively Parallel Simulator

MD   molecular dynamics

PBC   periodic boundary conditions

sPBC   shifted periodic boundary conditions