Theory Modelling and Simulation of Microstructures (TMS)

Assignment 1
(SS2019)

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Task 1:

Function **"get_internal_stress(x_coords,shear_modulus,poisons_ration,burgers_vector)"** takes in positions of all dislocations as 1D array, shear modulus of material, poisson's ratio of material and Burgers vector and gives the resultant shear stress experienced by each individual dislocation.

In above python function a one dimensional dislocation interaction is considered.

Following is the equation used for shear stress field calculation around dislocation.

$$\tau^{int} = D\frac{1}{x_0 - x} \qquad \textbf{(1.1)}$$

$$D = \frac{Gb}{2\pi(1-\nu)} \qquad \textbf{(1.2)}$$

τ^{int} – Internal Shear stress field
G- Bulk modulus
b- Burgers vector
ν- Poisson's ratio
x_0-Position of dislocation
x- Position of neighboring dislocation

A linear elastic material behavior is considered in present simulation. The internal stress around a dislocation is a linear sum of stress field due to all other dislocations.
About task1 algorithm:
The x_coords is a 1D numpy array which takes positions of all dislocations. In the algorithm a swap technique is used, such that position of dislocation whose stress field has to be calculated is placed in first position of the x_coords array. Below is the example of how the loop works.

Input- [position1, position2, position3, position4, …..]
Iteration1 over loop with [position1, position2, position3, position4, …..]
Iteration2 over loop with [position2, position1, position3, position4, …..]
Iteration3 over loop with [position3, position1, position2, position4, …..]
:
:
The stress field around dislocation will be calculated by summation of above stress equation (1.1) over all other dislocations.
The output is a 1D numpy array with internal shear stress field of respective dislocations as its elements.

Task2:

Choice of time step:
Choosing a proper time step is the key for getting a solution with minimal approximation.
In the present task the difference between final positions obtained with different time steps are checked.
Because the positions are defined in micro length scale a difference of $0.001e^{-6}$ m is used as a criterion for minimal approximation solution.

Time step size (ns)	Dislocation final positions (μm)			
	Dislocation 1	Dislocation 2	Dislocation 3	Dislocation 4
1	-0.1811	0.1735	0.5085	0.8790
0.5	-0.1688	0.1748	0.5012	0.8726
0.1	-0.1614	0.1757	0.4969	0.8687
0.05	-0.1606	0.1758	0.4964	0.8683

Table 2.1

From table 2.1 we can observe that the difference in dislocation final positions of all the 4 dislocations with 0.1 ns and 0.05 ns is according with the criterion choosen for time step selection.
So a time step of around **0.1ns** ($10e^{-11}$)sec is obtained from above method.

Task3:

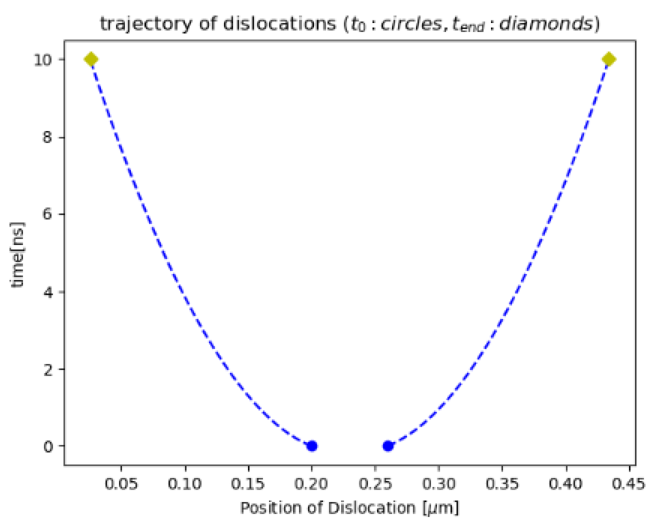


Fig. 3.1

$vel = \frac{b}{B}\tau^{int}$ **(3.1)** vel-velocity of dislocation.
B – Drag coefficient.

$X^{new} = X^{old} + (vel \times \Delta t)$ **(3.2)** X^{new} - updated position of dislocation.
X^{old} - original position of dislocation.

The trajectory of two disloactions as shown in Fig 3.1 is always symmetrical because, the stress field around two dislocations is equal in magnitude and opposite in sign and Velocity used to calculate updated position of dislocation is directly proportional to stress field.

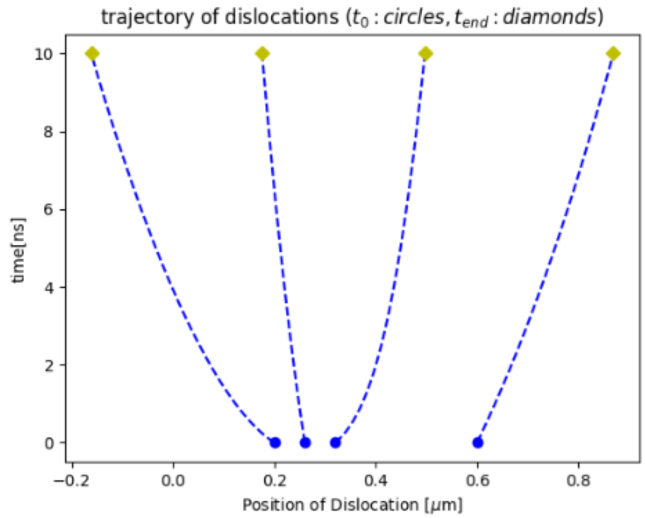


Fig. 3.2

Dislocations tends to minimize stress field around them so, the distance between the 4 dislocations will keep on increasing as in Fig 3.2

Task 4:

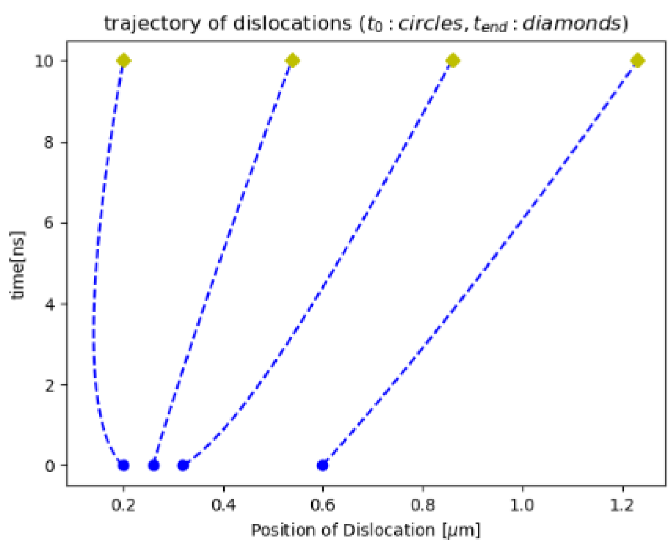


Fig. 4.1

$$v_i = \frac{b}{\mathrm{B}}(\tau^{ext} + \tau_i^{int}) \qquad \textbf{(4.1)} \qquad \qquad \tau^{ext}\text{-External stress}$$

If an external stress is added, velocity of individual dislocation can be found from equation 4.1

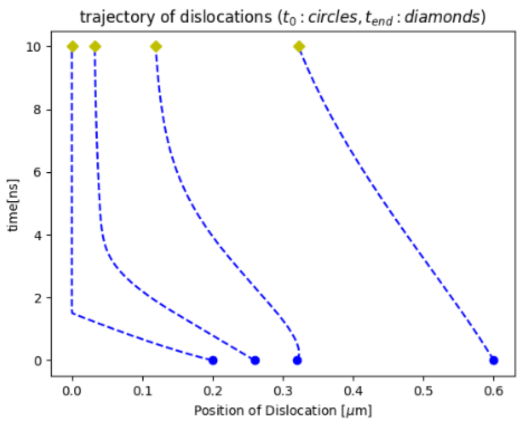
An external stress of approximately **14.15 MPa** is to be added such that at the end of simulation left most dislocation is approximately at its initial position. This behavior is shown in Fig. 4.1

Task5:

Task5a:

An impenetrable boundary condition is incorporated at location 0 µm.

Fig. 5.1a shows trajectory of dislocation over a time of 10ns and Fig. 5.2a shows trajectory of dislocation over a time of 30ns



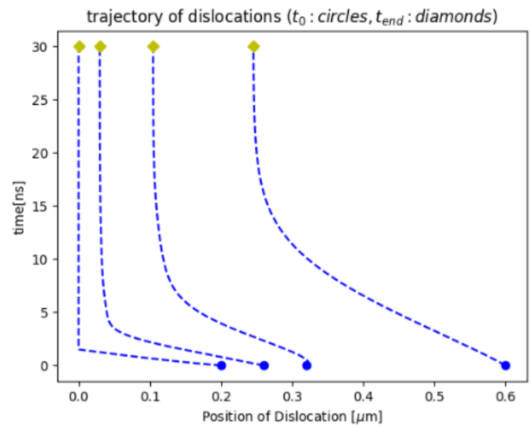


Fig. 5.1a **Fig. 5.2a**

From above two graphs we can observe that the position of dislocations will not change as the simulation time is increased. This shows the piling up behavior of dislocations at the impenetrable boundary like grain boundaries.

Task5b:

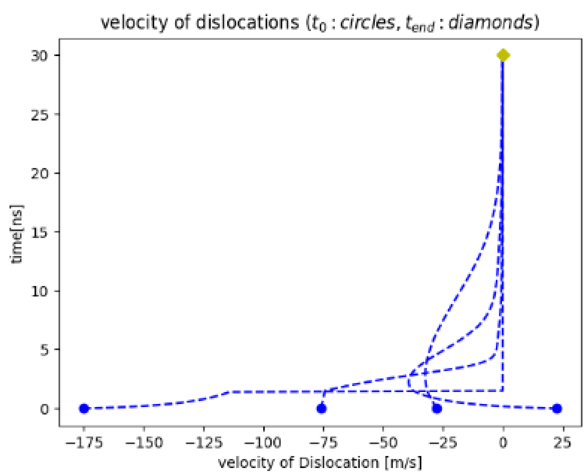


Fig. 5.1b

Task5c:

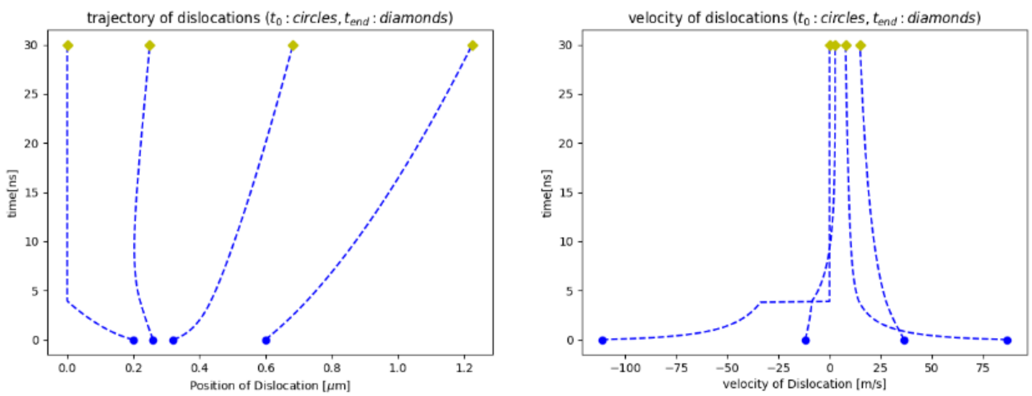


Fig 5.1c

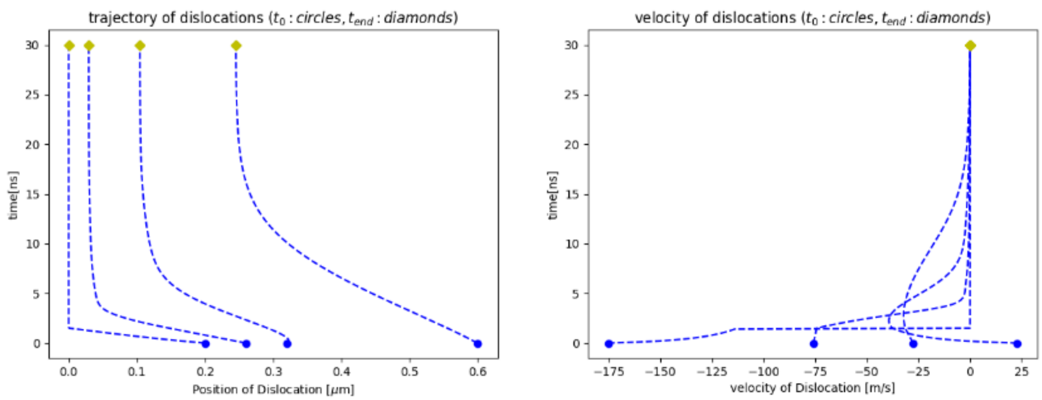


Fig 5.2c

Fig 5.1c shows trajectory and velocity of dislocations with no applied external shear stress.

Fig 5.2c shows trajectory and velocity of dislocations with an applied external shear stress of -25 MPa.

Dislocations tend to move away to minimize stress field around them as discussed in Task3 which is again shown in Fig 5.1c **with no external shear stress** applied. Velocity of each dislocatons is decreasing with time.

Whereas, in the case of externally applied shear stress of -25Mpa we can observe the pile-up behavior of dislocations at impenetrable boundary and velocity of dislocations approach zero. This behavior is observed because from equation 4.1 when the internal stress around dislocation reaches 25 Mpa velocity of dislocation will become 0 m/s. [$(\tau^{ext} + \tau_i^{int})$=0]