B.Tech Project (MTN - 400B)

“A Meta Study of the KMC Algorithm for simulating Cottrell Atmospheres around a moving Dislocation”

Under the Guidance of

Dr. Arka Lahiri

Metallurgical and Materials Engineering

Submitted By:

Abhay Mudgal (17118001)

Sourabh Magadum (17118070)

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1. Introduction

The movement of dislocations dictates the deformative behavior of a material which has been extensively studied by Material Scientists for the practical applications of the materials. The interaction of dislocations with crystal defects play a key role in defining the deformation of a crystal. For example, the addition of little quantities of C to Fe produces steel which has significantly better physical properties compared to pure iron. The main component of the interaction is the interaction between the stress fields that these defects generate. Analysis of related phenomena suggests that at lower driving forces the dislocations are pinned by solute atoms but at higher driving forces the motion is unimpeded by the solute atoms. The phenomenon at higher temperatures is dictated by the solute-dislocation interaction that depends on the dislocation velocity which in turn depends on the distribution of solute in the matrix.

Kinetic Monte Carlo Methods have been extensively used to simulate the behavior of dislocations in various settings and a similar KMC model is used to study the behavior of dislocations in the presence of Cottrell atmospheres. The Monte Carlo model allows for stochastic solute diffusion, the formation of a solute cloud around the dislocation core and the motion of the Cottrell Atmosphere. The model considers the solute atoms to be misfitting spheres in an infinite isotropic linear elastic medium. The statistical mechanics of the solute distribution follows Fermi Dirac statistics and the solute concentration at a point does not exceed unity or that no two solute atoms may occupy one site due to quantum probabilities.

The solute atoms are free to diffuse along the two dimensional solvent medium and at low driving forces form a protective barrier around the dislocation core inhibiting motion. In this study, the diffusing solute atoms interact with the edge dislocation gliding in either a positive or negative x-direction in two spatial dimensions. The Monte Carlo model is to show the behavior of solute atoms at high driving forces and the supposed retardation of the motion of the dislocation due to the interactions with the solute atoms.

2. Kinetic Monte Carlo Simulations

Macroscopic properties are the measurable properties of the system at the bulk level, e.g., the measured temperature, pressure and volume of the system. Following the principles of Statistical Mechanics, these macroscopic properties of the system can be generated as a summation of the microscopic properties. Any system undergoing a process goes through an infinite number of

microstates. A Monte Carlo or the Molecular Dynamics simulation tries to replicate the same trajectory of the system by simulating a few of these microstates at discrete time intervals.

Several rules are defined to limit the scope of a simulation to generate plausible replicable models. The Monte Carlo simulation does not take into account the order in which the microstates are accessed, it only considers the list of microstates accessed and the frequency with which they were accessed. Another key feature of a Montecarlo Simulation is the dependence of the features being determined on the location. In MC simulations, the macroscopic property is only a function of the location or potential energy of the system and the kinetic energy is considered to be constant.

A Monte Carlo simulation can be understood by the following example. Let us consider a system that has a single vacancy and two different kinds of solute atoms. Solvent atoms are called atoms of type 1. Type 2 and 3 correspond to the two different kinds of solutes in the system. There are three kinds of bonds in the system: (1)-(1), (1)-(2), (1)-(3). The relative bond energies are assumed to be, $E12 < E11 < E13$. As the vacancy moves around with time, different bonds are broken and vacancy takes different locations and generates different microstates.

Monte Carlo algorithm can be understood through the problem of finding the macroscopic potential energy of this system. Thus we can calculate the macroscopic property such as Macroscopic potential energy (Umacro), by calculating the ensemble average of U over the discrete microstates. And each microstate is noted with a different jump of the vacancy that leads to the breaking and forming of different kinds of bonds that result in the net change in energy. It is important to mention that in this problem we are ignoring the atomic vibrations and considering only the atomic jumps. Hence, we do not have to average over the potential energy fluctuations that happen due to atomic vibrations. The atoms near the vacancy will jump in the vacancy leading to a change in energy of the system and thus creating a new microstate. As the vacancy moves around with time, it generates different microstates.

Monte Carlo simulation consists of three steps:

1. Sampling
2. Evaluation
3. Decision

Steps 1, 2 and 3 define an iteration of the Monte-Carlo algorithm which is called a “trial”.

Sampling: The first step in the Monte-Carlo simulation is to randomly choose the neighbour which makes an attempt to jump into the vacancy. Whether the jump will be successful or not will be determined in the subsequent steps.

Evaluation: This step evaluates how favourable is the jump made in the first step. The jump is favourable if the potential energy of the system reduces after making the jump. This is evaluated by calculating the relative probabilities of the initial and the final microstate. From Statistical Mechanics,

$$P_{ms1}/ P_{ms2} = \exp((U_{ms2} - U_{ms1})/ kT) = P_{jump} \text{ --- (equation 1)}$$

where,

P_{ms1} = Probability that the system is in microstate 1

P_{ms2} = Probability that the system is in microstate 2

This formula is used to compare relative probabilities of different microstates, which is used to evaluate the probability of the jump. As jumps of atoms are random/stochastic in nature, energetically unfavourable jumps may still take place, but with a lower probability than favourable jumps.

Decision: In this step, whether or not the random jump is made is decided. This step has 2 cases.

Case 1: If the P_{jump} (calculated in the 2nd step) >= 1. In this case the jump is allowed.

Case 2: If Pjump<1.

- In this case a random number R is generated between 0 and 1.
- If the random number R <= P_{jump}, the random jump is accepted
- If R > Pjump , the random jump is rejected.

The trail is repeated until the desired result is achieved.

3. Simulation Method

The results presented in the report assume that there is minimal interaction between the solute atoms and that can be neglected. The only interaction that is responsible for change in energy of the system is that of the solute atom and the single dislocation. The solute atoms are strictly substitutional. Both the solute atoms and the dislocation are constrained to move on the sites of the

square lattice and each movement in a trial is of the magnitude of one burgers vector b, which is assumed to be 1 to simplify the process. Initially the dislocation is placed at the center of the two-dimensional simulation cell and the solute atoms are distributed randomly throughout the cell subject to Fermi Dirac Statistics.

The number of solute atoms N_s is obtained from the formula:

$$N_s = C_0 * H * W$$

where, C_0 is concentration of solute atoms,
H, W are the height and width of the dislocation cell.

The Energy associated with the interaction of the pressure fields of the dislocation and a solute atom is given by the:

$$E(x, y) = P(V_s - V_a)$$

where, P is the pressure field associated with the dislocation
V_s is the volume occupied by a solute atom and V_a is the volume occupied by a solvent atom.

For this simulation and the simulations in this study, the difference $V_s - V_a$ is taken to be positive.

$$P = \frac{Gb(1+\nu)}{3\pi(1-\nu)} \frac{y}{x^2 + y^2}, \qquad (1)$$

$$P = \frac{Gb(1+\nu)}{3H(1-\nu)} \sum_{n=-\infty}^{\infty} \frac{\sin 2\pi Y}{\cosh 2\pi\left(X - n\frac{W}{H}\right) - \cos 2\pi Y}, \qquad (2)$$

The equations 1, 2 define the pressure field that is present in the simulation cell. Equation 1 describes the pressure field that results from the interaction between one dislocation and one solute atom where the x, y are positions of the solute atom relative to the dislocation. Here G is the isotropic shear modulus and υ represents the poisson ratio. But as the simulation is performed with periodic boundary conditions, the effect of the images of the dislocation have to be considered to map the correct interaction of stress fields. For this purpose we use equation 2 that summarizes equation one by summing up all the effects. X = x/W and Y = y/H. However it was observed that the value of the summation primarily lies between -4<=n<=4 and for -5<=n<=5 the change in P is only 6×10^{-6} %. As such the summation range is only [-4, 4] in the simulation. The dislocation or the solute atoms in motion when they exit from the simulation cell reemerge from the other side.

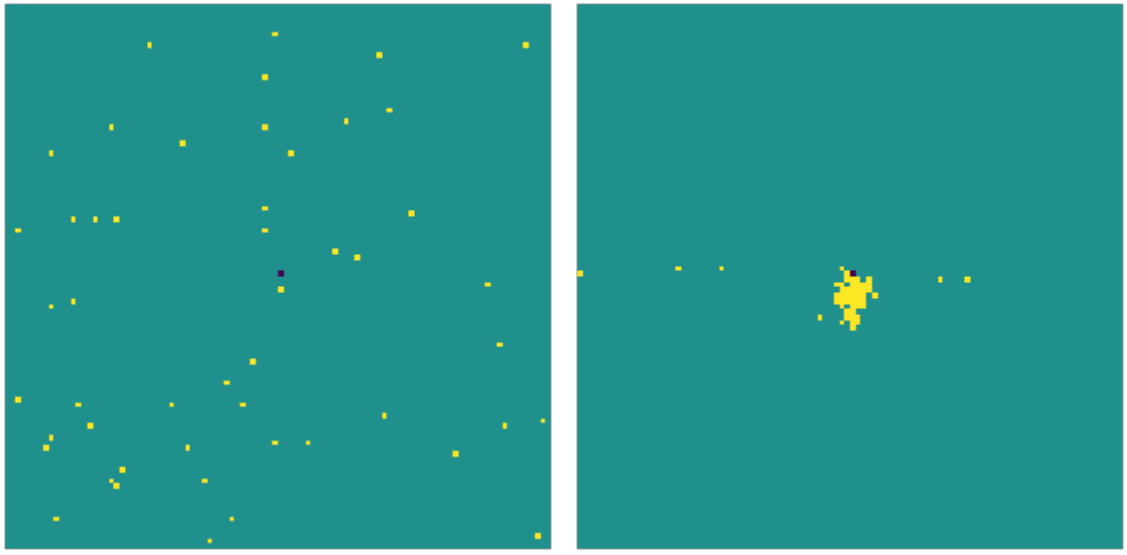
3.1 Static Dislocation Results

For the current version of the simulation, the behavior of solute atoms for a static dislocation is simulated. A solute atom is chosen at random and the four plausible jumps are iterated for this solute atom. Then the energy of the solute atom is calculated for the original position and the new position and the energy difference ΔE is calculated. A random number n is chosen in the range [0, 1). If the random number is less than the Metropolis Function given by

$$B = \min\left[1,\ \exp\left(-\frac{\Delta E}{kT}\right)\right],$$

move is accepted.

The below images describe the working of the algorithm. The parameters chosen for this simulation are at Concentration of 0.5% and the value Gb(1+ υ)(ΔV) / 3H(1-υ)kT is taken to be 200. This simplifies the calculation for energy in the simulation steps and in the metropolis function. Another plausible inference from this is that different materials whose parameters are



optimized in the above manner will show similar movement of dislocations and solute clouds.
In the images, the dimensions of the simulation cell is 100x100 and the black dot represents the dislocation while the yellow dots represent the solute atoms.

4. Dynamic Dislocation Simulation

The above results display the movement of solute atoms when the dislocation is held static in the absence of an external stress. The algorithm is modified to incorporate the movement of dislocation in the presence of an external stress. For the convenience of the calculations, the external stresses that are applied will be functions of G, the isotropic shear modulus of the material.

In real life scenarios, the dislocation and solute atoms move simultaneously but it is desirable to move one entity at a time in the simulation. The solute atoms and dislocations will have different mobilities and this difference is used to determine which entity is being moved in the dislocation. We define the term mobility ratio (M_R) to be the ratio of the mobility of the solute to that of the dislocation and use it as a variable whose value is input at the start of the simulation.

$$M_R = M_S/M_D$$

where M_S and M_D represent the frequency at which we try to move a solute atom and a dislocation. The quantity R which represents the likelihood of moving anyone of the solutes is defined as

$$R = 1 + N_S*M_R$$

1/R is the probability of moving a dislocation in a single Montecarlo Step. Selection is achieved by generating a random number in the range [0, R) and if the number is less than 1, we proceed to move the dislocation randomly in a positive and negative x direction else we proceed to select a random solute atom and proceed to move it.

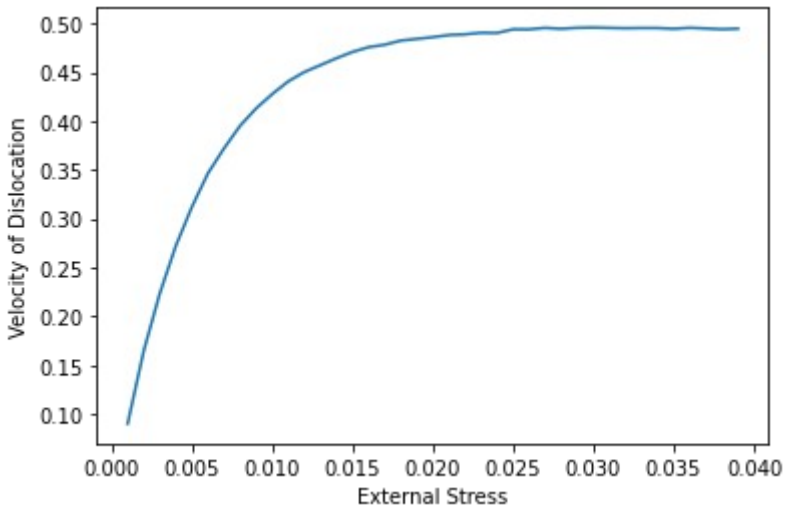
The energy for the motion of dislocation is generated due to the external stress that is applied. The total solute dislocation stress field interactions account to a very small fraction of energy and are ignored. The change in energy for the motion of a dislocation in a single step is given by

$$\Delta E = \sigma_{ext} * b^2$$

where σ is the external stress applied and b is the burgers vector.

For simplification of calculations, it is assumed that Gb^2/kT is equal to 200 for lower temperatures and 50 for higher temperatures.

The simulation with no solute atoms at lower temperatures and with varying external stress to obtain the steady state dislocation velocity in each case. The graph below demonstrates the

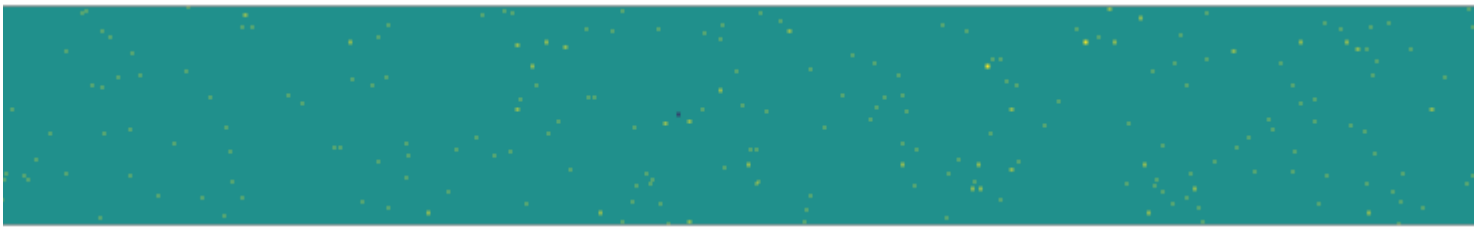


results. As the dislocation motion involves a random choice between 0 and 1, the maximum dislocation velocity that can be obtained in the direction of applied stress is 0.5.

Further the movement of dislocation is tracked via a relative velocity that is represented in terms of distance moved per montecarlo step. Variations in the behavior of the material is noted by using different external stress, the results to which are presented below.

Parameters used:

- $Gb^2/kT = 50$
- $Gb(1+ \upsilon)(\Delta V) / 3H(1-\upsilon)kT = 200$
- Concentration of Solute = $3 \text{ X } 10^{-3}$
- Mobility Ratio = 0.02
- Width = 1000
- Height = 100

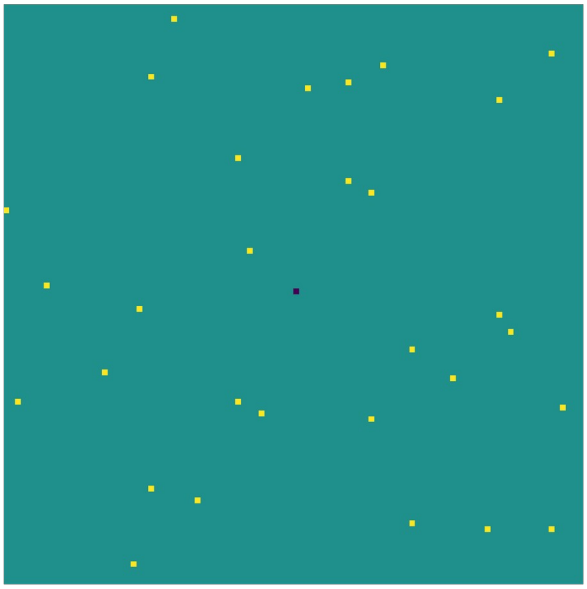


The instantaneous solute distribution and dislocation position at the beginning of the simulation using the parameters mentioned below.

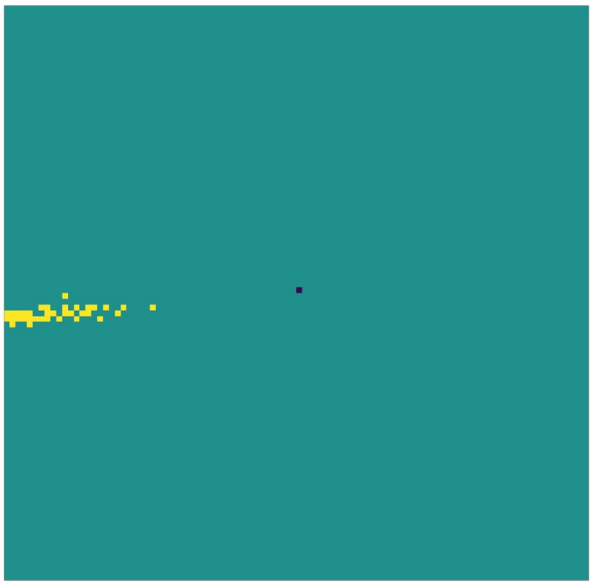
Multiple variations of the simulation are run with these parameters and varying the external stess. The simulation is run with three external stresses 0.00033G (low), 0.003G (medium) and 0.03G (high). The resutlts are presented below.

4.1 Low Stress Condition

At low external stresses the velocity of the dislocation is very slow. The average dislocation velocity per 1000 steps of the algorithm is 0.0012. The velocity of the dislocation at the same stress in a solute free matrix as observed from the dislocation movement graph is approximately 0.02. Factoring in the values that the movement of dislocation is a random uniform selection with a probability 1/R, we get the average disloctaion velocity of the without any effect from solute atoms would be 0.0033. We see a drop of approximately 64% in the velocity of the dislocation due to the formation of solute clouds.



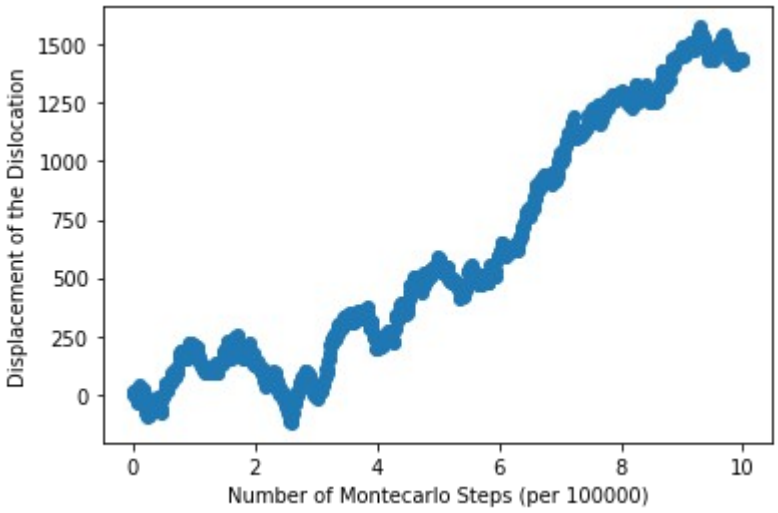
1000 steps. Δx = 1b



500000 steps. Δx = 430b

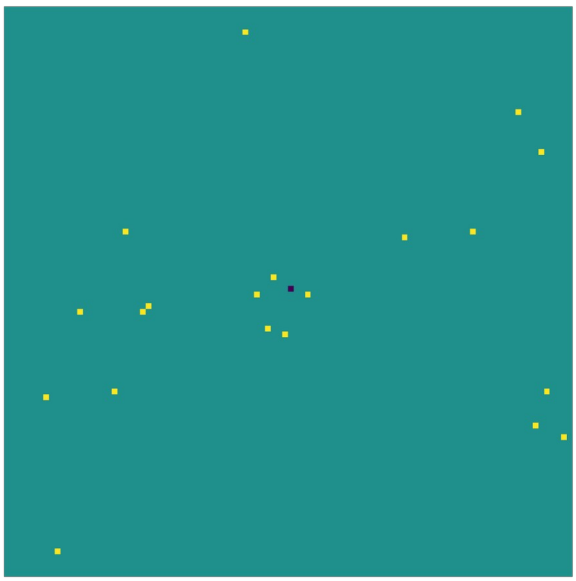
1000000 steps. Δx = 1020b

Magnified images of the simulation cell are presented at different Monte Carlo steps. The images provide the description of how solute clouds form and chase a moving dislocation. During the initial phase of the dislocation, the distribution of the solute atoms is random while during the middle phase the solute atoms tend to form a solute cloud and move towards the dislocation core. In the End phases, the solute atoms seem to have caught up to the dislocation. From the images presented above, it can be inferred that the solute cloud that forms around the dislocation chases it across the simulation cell. This coupled with the drop in displacement of the dislocation presented in the below image verifies the phenomena that solute accumulation slows dislocation motion and slower motion results in greater solute accmulation. The movement of dislocation seems random in positive and negative x directions with a small inclination to the positive x direction.

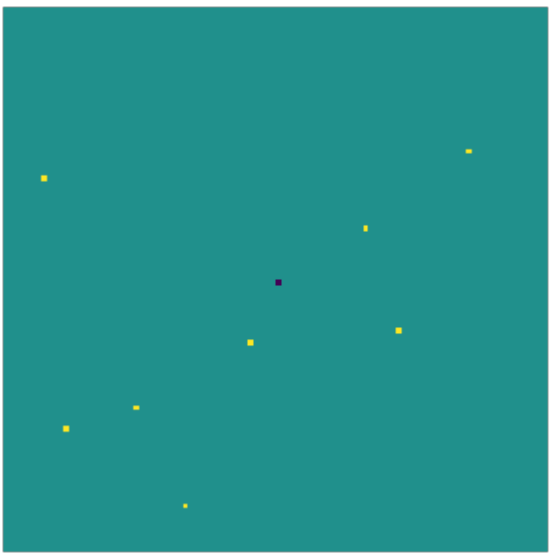


4.2 Moderate Stress Condition

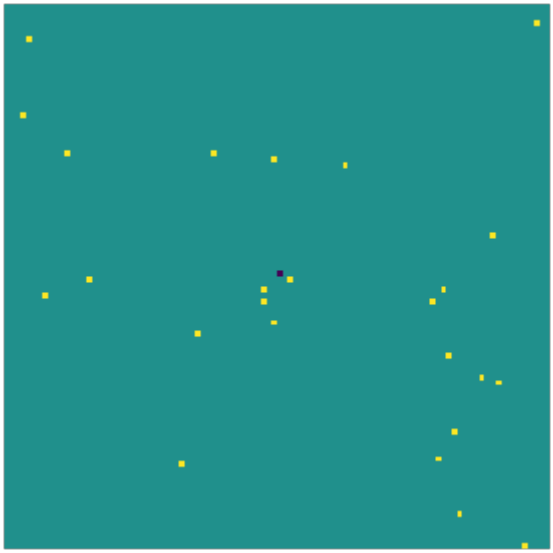
The external stress for the dislocation is increased by an order of magnitude keeping the other parameters constant. The dislocation moves at a greater velocity compared to that of the low external stress case due to the increased stress contributing to a greater change in energy. In the simulation, the dislocation moves with an average velocity of 0.0102. A drop in average velocity of the dislocation is observed. Observations of the simulation matrix at different Montecarlo steps shows that the behaviour of the cell follows a certain pattern. The dislocation fails to form a large solute cloud as in the case of lower stress situation but steadily attracts the solute atoms in its vicinity towards itself forming a somewhat distant cloud around it. Incorporating the randomness of the algorithm, the theoretical average dislocation velocity in absence of solutes would be 0.0212. The drop in dislocation velocity in the medium stress case is probably the result of the sparse solute clouds.

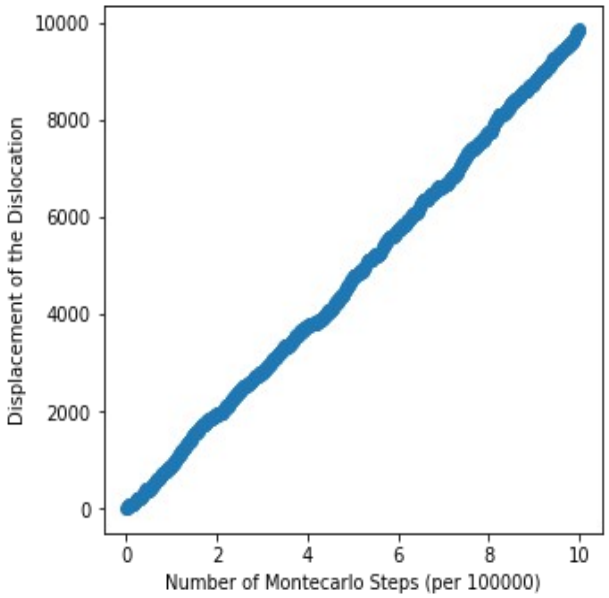


1000 Steps. Δx = 3b



500000 steps. Δx = 5566b



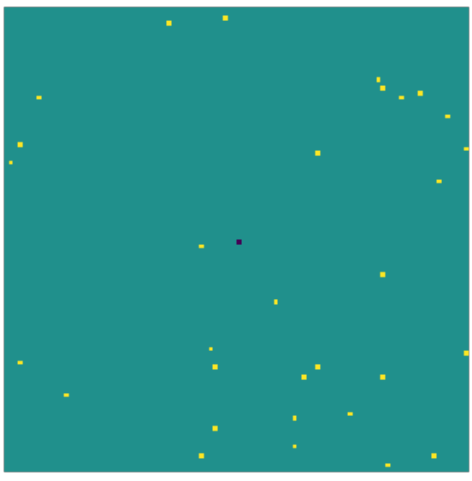


1000000 steps.Δx = 10601b

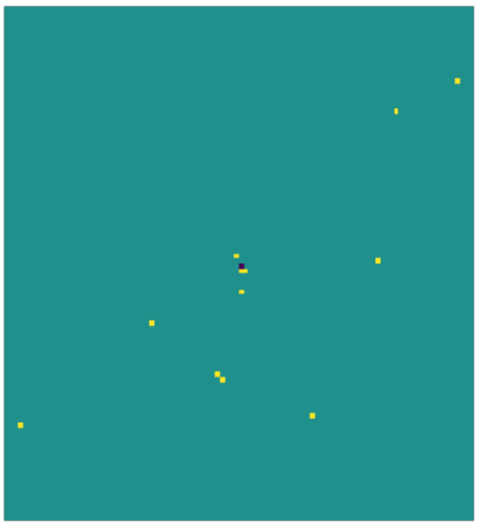
The displacement of the dislocation follows a nearly linear increase. The irregularities in the displacement increase are due to the very less negative motion that is generated from the randomness in selection and metropolis function. It is observed that the increase in stress decreases the negative motion substantially as compared to the low stress condition. The definitive difference here is that the dislocation rarely influences the solute atoms distant form it but tends to form sparse and small dislocation clouds while in the low stress case the dislocation affects most of the solute atoms and moves while dragging the solute cloud with it.

4.3 High Stress Condition

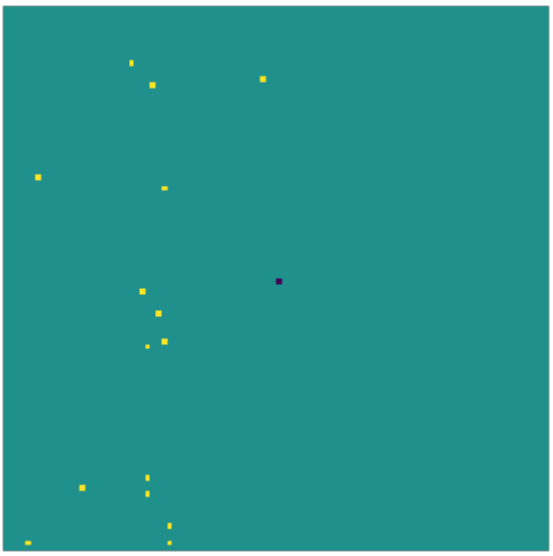
The external stress applied to the simulation matrix is increased by another order of magnitude as compared to the medium stress case. Observation of the distribution of solutes at different Montecarlo steps indicated that the solute distribution around the dislocation is very sparse and is rarely influenced by the dislocation as in the case of medium and lower stresses.



1000 steps. Δx = 52b



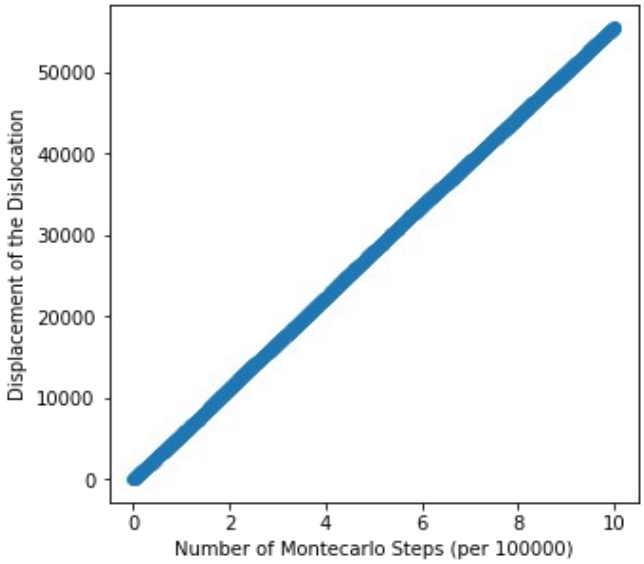
500000 steps. Δx = 28032b



1000000 steps. Δx = 55531b

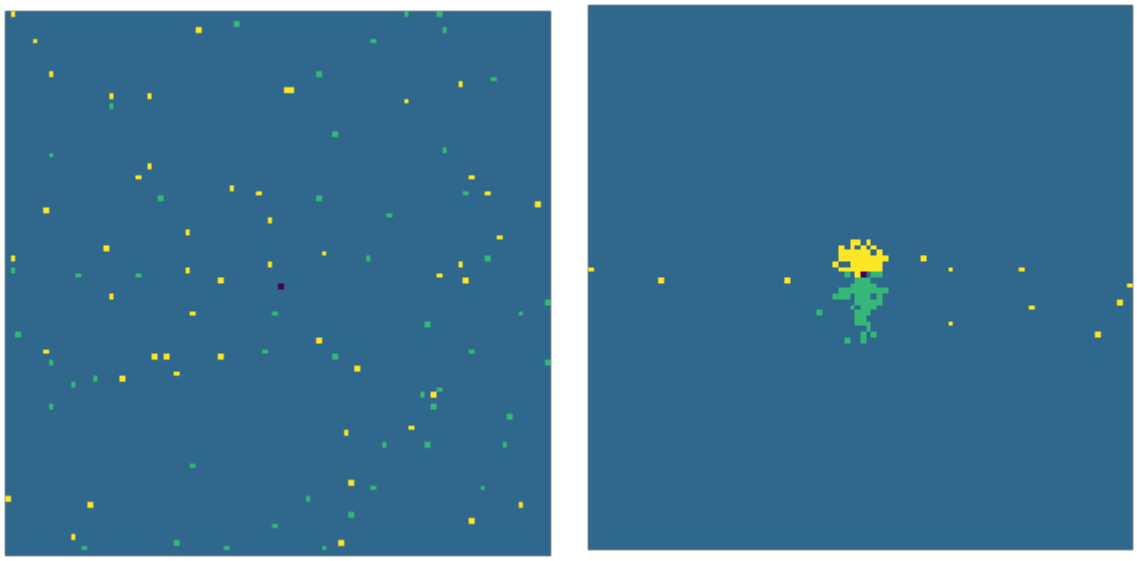
The average dislocation velocity in this case is 0.052. It is interesting to see a drop in dislocation velocity here. Despite the stresses being high enough to disregard the solute atoms nearby the dislocation core and stimulate ample motion, the dislocation velocity is only 20% of that of the theoretical case.

The value of external stress on the dislocation in this case is greater than the threshold required to overcome negative motion of the algorithm. This is observed in the below graph indicating a steady state velocity throughout the simulation.



5. Multi Component Systems

The algorithm was partly modified to incorporate multiple solute atoms in the same matrix. The parameters used in the simulation of single solute alloy were used for the simulation. The results that are presented below are obtained by using two solutes with different misfits compared to each other. The yellow solute atoms are smaller than the solvent atoms and the green atoms are bigger by the same proportion. The results obtained align themselves with the standard expected behaviour. The random selection of the solutes in each monte carlo step ensures that the probability of motion of each solute variety is the same. Due to similar proportions that energy functions are the same for both the solute atoms resulting in almost uniform motion of both types towards the dislocation throughout the simulation.



6. Future Prospects

The simulation has a lot of other prospective areas where it can be used when modified. The value of Gb^2/kT is dependent on the temperature and the misfit volume of the solute. These were held constant throughout the simulation conducted during the project but using these as the independent variables of study can lead to results that would further help in understanding of the properties of solutions and increase the ease segments of industrial processes such as testing for the life of materials. Another plausible study that can be generated from this is the comparison of the variability of the dislocation velocity and external stress for different solutions of the same base material. Results from such a study could also be used to calculate the probable critical stresses and temperatures for unpinning dislocations from solute clouds. Another independent variable for the study could be the concentration of solute atoms. However the simplicity of the algorithm limits it to non miscible species.

The multicomponent modification holds tremendous potential as a subject of study. Application of the theoretical interaction of different solute atoms in the simulation would introduce more accurate systems capable of describing the behaviour of materials.

7. References

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