Tutorial script for XFEAt program

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Contents

Abstract

XFEAt program is a coupling scheme which uses the extended finite element method and molecular dynamics to simulate metalic structurs. The structure is going to have atomistic interactions due to the applied forces that caused by inserting a dislocation in it. Finally, by observing the dislocation movement under certain applied shear strain, the Peierls stress would be found. In this Toturial we will try to creat a sample model of BCC iron with a screw dislocation in it by using the XFEAt program to show how it works.

1 Set_Up_Structure

Overview

In this folder the initial structure of our model will be created and a srew dislocation will be initialize into it. The created strucuture needs to be relaxed. So, in the next step we will relax it. From the beginnig of creating the model and inserting the dislocation inside it, after applying changes for dimension sizes of the atomisitic part(MD part) and Finite element part(FEM part) of the model, whole procedures will be done automatically by "Aniso_Relax.sh" shell file inside "1_Anisotropic_Tensor" folder. Therefore, in the following sections, the task of each folder and the details of their procedure(how to compile and run the codes) are presented in order to give you a glance of the work and its complexity.
The folders that belong to this part of program are shown in Fig. 1.1.

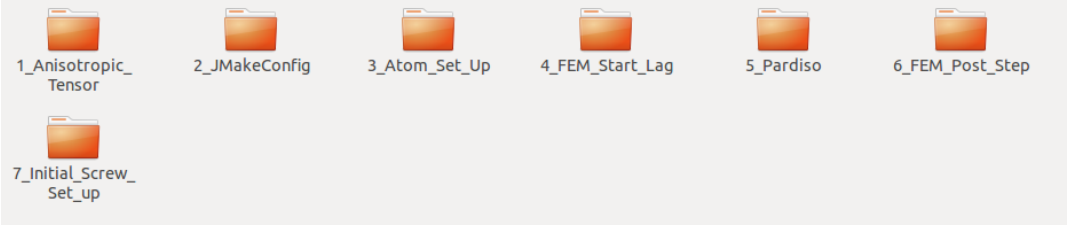
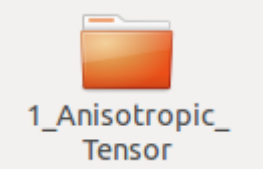


Figure 1.1: Folders that will be used to create the structure of the model and inserting the dislocation inside it(without relaxation).

1.1 1_Anisotropic_Tensor



1.1.1 Overview

In this folder, the elasticity file of your model will be created according to the elastic modulus and orientation of your model.

1.1.2 Procedure:

Write the elasticity orientation text file manually according to your material's property. The input file should look like the sample below(Fig. 1.2) by using any simple text editor. In the first line, there are bulk modulus of the material with the order of C11, C22 and C44 in unit of MPa. Next, according to your model dimension

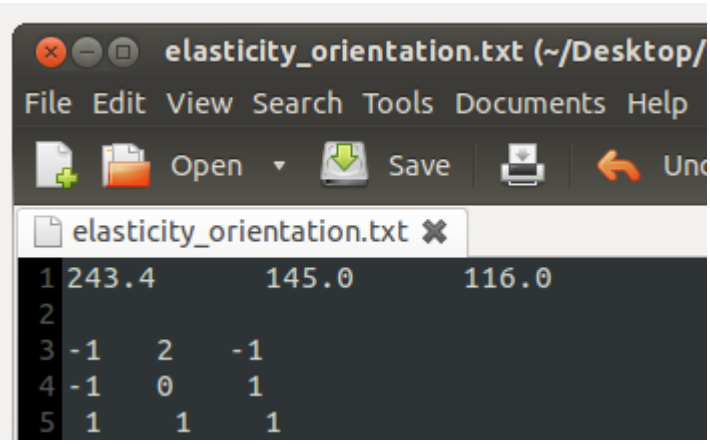


Figure 1.2: A sample for elasticity_orientation.txt file in Iron

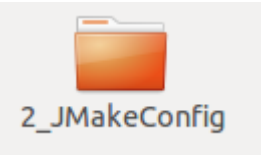
(sizes of MD and FEM parts), make the following changes:
- Go to "2_JMakeConfig" folder and open "paramBCC_Screw.param" file. Change the dimension of the model as you want in front of box_x, box_y and box_z. Save your changes and close it.
- Come back to "3_Atom_Set_Up" folder and open "Atom_Set_Up.cpp" code and change the size of FEM part of your model as you wish in "fem_size" variable. Save your changes and close it.

Make sure that there is a file with the name “crystal.conf” in the “2_JMakeConfig” folder.

Then, go back to “1_Anisotropic_Tensor” folder and compile and run the shell file called “Aniso_Relax.sh” by using the following commands:
- chmod u+x Aniso_Relax.sh
- ./Aniso_Relax.sh

Now you will get an output file called “elasticity.txt” which contains required data that will be used later as input of upcoming steps. Also, the whole process of upcoming steps until the end of “7_Initial_Screw_Set_up” folder will be done automatically by this shell file.

1.2 2_Jmake_Config



1.2.1 Overview

In this folder we should define the dimension of the MD part of our model and will create it with defining our model properties. If it is the first time that you are going to create the model on your computer, you should first create an empty folder with the name "bin" in your home directory and then read the “how to start runing IMD in new system.txt” file to make executable files for IMD. The procedure that is written below is just to let you know how the codes in this folder would work.

1.2.2 Procedure:

1. Apply size values of the model in "paramBCC_Screw.param" file by changing and save it.
2. Run the java by using command inside "compile_command.txt" file.
3. There will be an output named "unrelaxed_perfect_crystal.imd". It is copied into "Fe_MD" folder.
4. The IMD code inside "Fe_MD" folder using the command line in "readme_insertedge.txt" file is compiled.
5. The output file named "relaxed_perfect_crystal.imd.00000.ss" is renamed into "relaxed_perfect_crystal.imd" and copied it into "3_Atom_Set_Up" folder.

The resulted imd file will look like as below(Fig. 1.3) by using Atom viwer software.

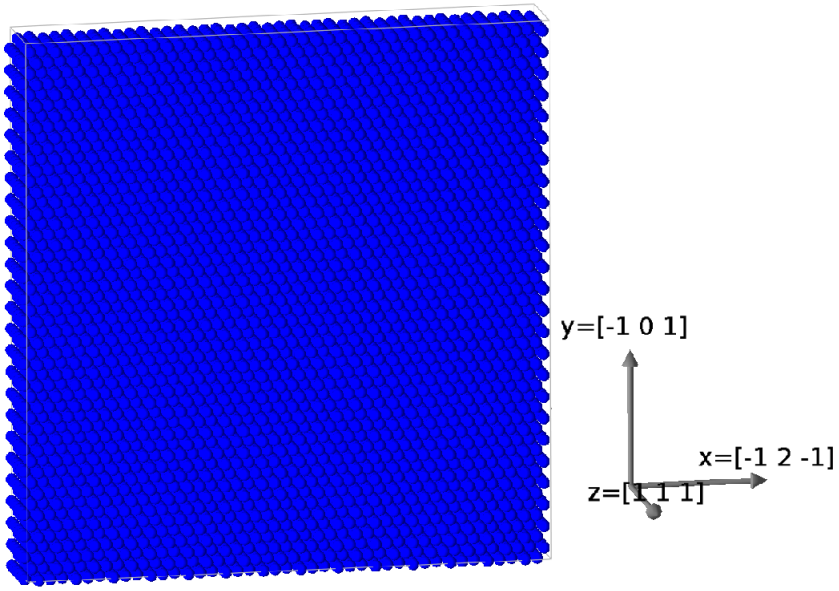
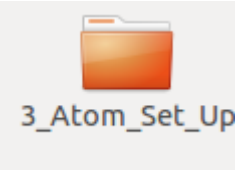


Figure 1.3: no type defined imd model

1.3 3_Atom_Set_Up



1.3.1 Overview

In this folder, the types of atoms in the MD model will be defined. By this, we will define how the atoms are going to transfer the displacements caused by the dislocation movements from MD part to FEM part and vice versa. But, finding the best dimensions for the zones that described is critical. It will affect the efficiency of the model and the required time of calculations. By experience, we found that the size of pad atoms could not be reduced more than 11Å. Also, the FEM part of the model will be created in this folder and all of the details about meshing of the FEM part will be presented in separated files which we will explain them in the following:

1. shift.txt
   For models that have shifts in their nodal connnections in FEM part, this file includes the value of the shifts that are applied to the atomistic coordinate such that they match the FEM nodes.
2. nodes.txt
   Coordinations of each node in finite element part of the model.
3. elements.txt
   Numbering of nodes for each element that are connected together.
4. inner_coordinate_of_fem_domain.txt
   Coordinates of the nodes nodes at surface of the innerbox (showed in Fig. 1.4) in FEM part of the model.
5. outer_coordinate_of_fem_domain.txt
   Coordination of the nodes on the outer boundary surface of the FEM part of the model(See Fig. 1.5).
6. fem_inputfile.txt
   This file includes information about the FEM part of the model. In the first line there are 6 numbers that indicate the variables below in the code and their meaning are explained below:
   - Njoint: The number of nodes in the FEM model
   - NEL: Number of elements in the FEM model .
   - NCON: Total number of constraints in innerbox surface and outer boundary surface.

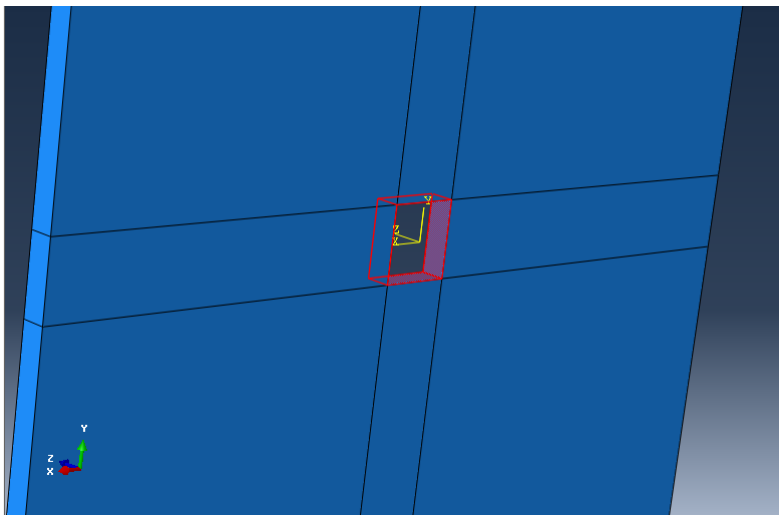


Figure 1.4: Visualization of the innerbox in FEM part of the model

- NCF: Total number of concentrated forces applied on the model which is always zero in this step.
- NENFD: Total number of nodes in outer boundary surface.
- NLAG: Total number of Lagrange constraints which means the number of nodes in the front or back surface of the FEM model that are paired together.
After the first line there are information related to the numbers that mentioned above. The order of these data are:
- Coordinations of the nodes
- Node constraints in inner box
- Node constraints in outer boundary

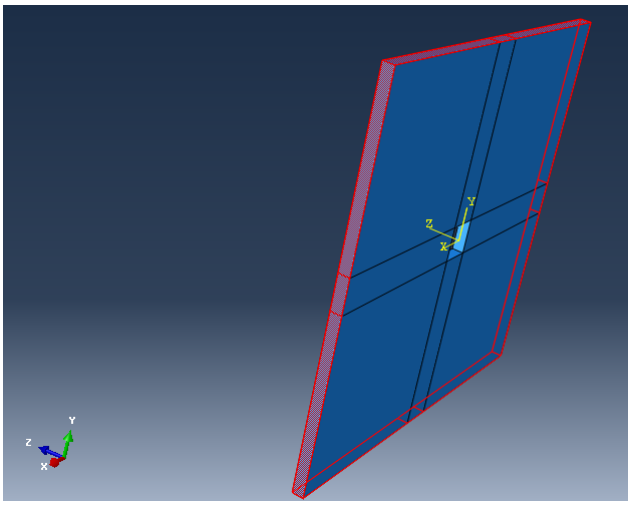


Figure 1.5: Visualization of the outer boundary surface in FEM part of the model

7. fem_inputfile_with_node_element_information.txt
   This file have two parts of the same informations in the “fem_inputfile.txt” file:
   - Njoint: The number of nodes in the FEM model
   - NEL: Number of elements in the FEM model.

8. fem_outer_boundary_condition.txt
   In this file there are 4 columns that represents in each line the number of the node, displacement boundary condition in x axis, condition in y axis, condition in z axis, respectively.

9. fem_nodal_pairs_coordinates_along_dislocation_line.txt
   As it is clear from the name of the file, it includes the list of numbers for pairs of FEM element nodes for both faces(front and back)(See) along the dislocation line.

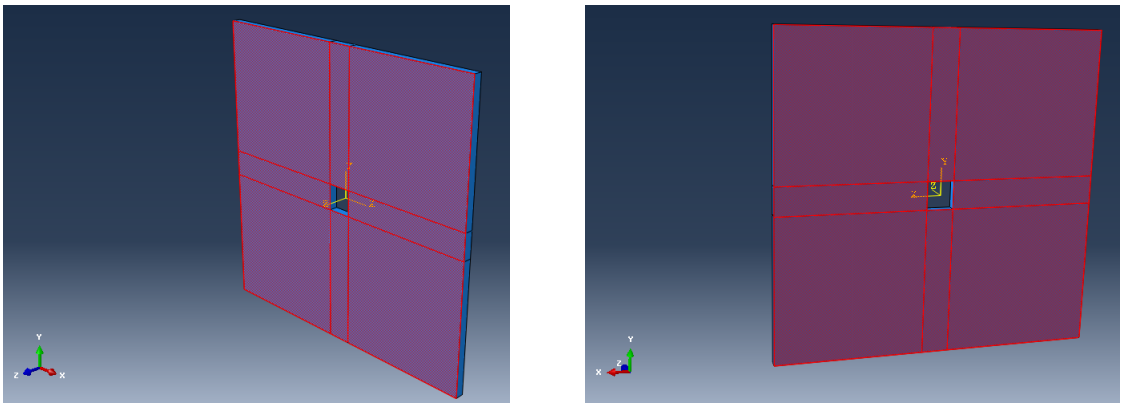


Figure 1.6: Visualization of the front(left) and back(right) surfaces in FEM part of the model

1.3.2 Procedure

The “Aniso_Relax.sh” shell file that you run in “1_Anisotropic_Tensor” folder will create an isotropic model.

Check the result file named "*relaxed_perfect_crystal_with_atom_type.imd*" by using Ovito software.(you can download it from this link for free:http://www.ovito.org/index.php/download2). Also there will be a “Box.txt” file which contains some informations about the dimensions of the FEM part.

To check that our MD part of the model is created as we would like to be, open "relaxed_perfect_crystal_with_atom_type.imd" file inside Ovito software using following instructions:

i) File –> import data(in Linux version)/Load local file(in windows version) -> choose file type ".imd" -> open the file.

ii) Go to right column of the program and change the "add modification" scroll bar into "slice"

iii) Under slice bar there should be no change in the shape of the core structure(blue square) as you change the value of the “distance” into 0 , 2.5(2b) , 5(4b), 7.5(6b), 10(8b) and 12.5(10b). Change the values of other options to zero except “Normal Z” and “Slice width” which should be change into 1 (See Fig. 1.7).

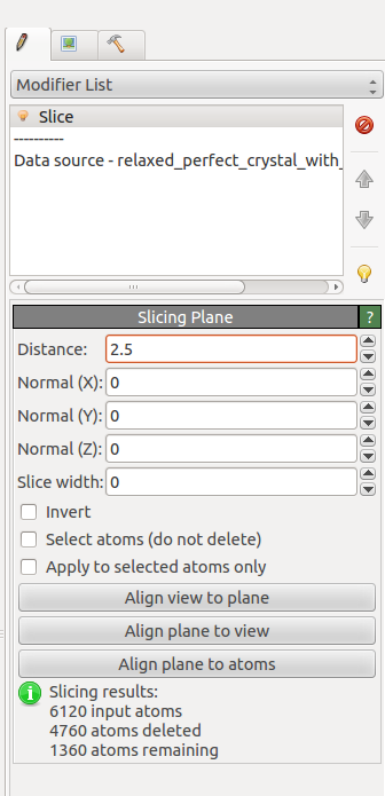


Figure 1.7: An example setting for showing a 2b layer of the model in Ovito software

iv) Now look at the "shift.txt", if the numbers were not close to zero, it means that we have shifts in the model. This should be applied in "Initial_Screw_Set_Up.cpp" step so that atoms and fem nodes at the transition zone coincide. This would be done automatically, no worries!!.

Also, we can check the types of zones which are defined by this folder with help of *AtomViewer* Software as shown in Fig. 1.9.

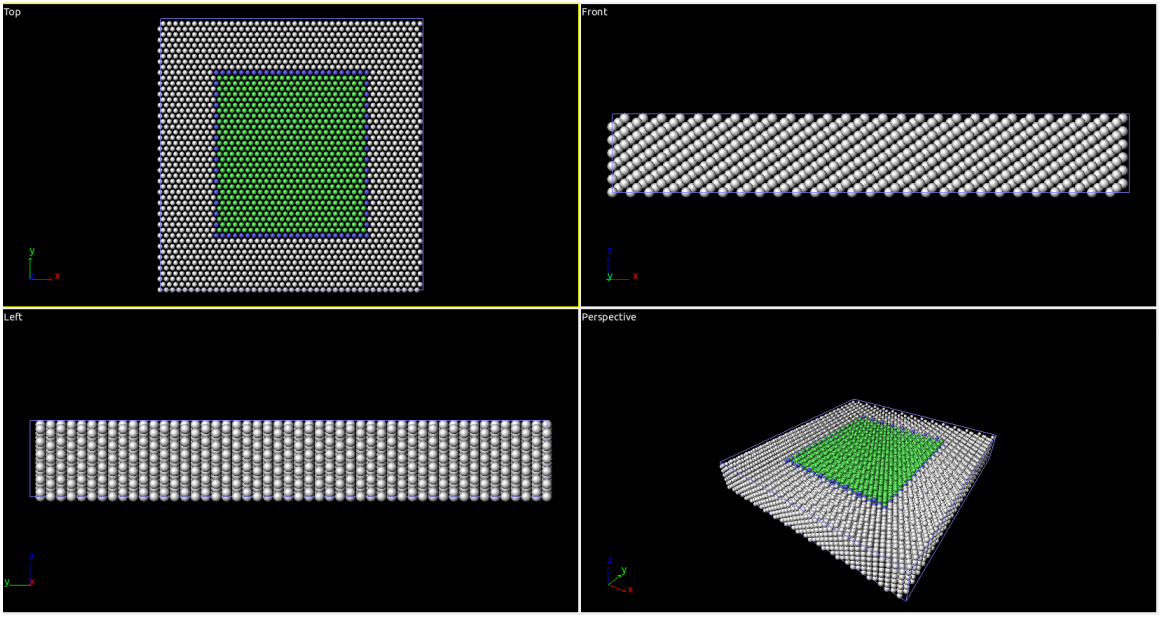


Figure 1.8: Ovito views of the sample model

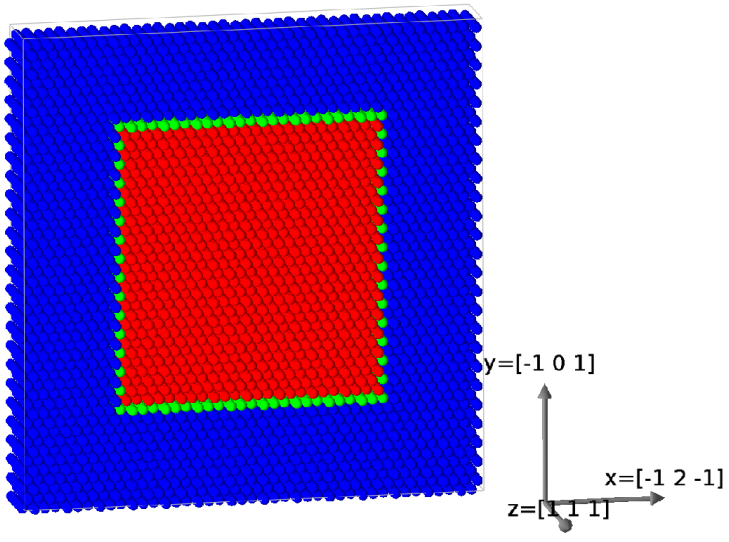
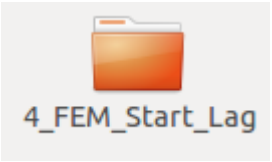


Figure 1.9: Sample model after defining the types

1.4 FEM_Start_Lag



1.4.1 Overview

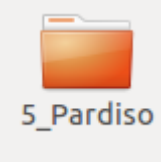
In this folder we apply the Lagrangian relaxation optimization method in order to optimize our FEM model to produce periodic boundary conditions. The procedure will be done using the “Aniso_Relax.sh”shell file in the “1_Anisotropic_Tensor” folder.

1.4.2 Procedure:

The files below:

1. “burgers_vector.txt” from “3_Atom_Set_Up” folder.
2. “fem_nodal_pairs_along_dislocation_line.txt” from “3_Atom_Set_Up” folder.
3. and “fem_inputfile_with_outer_boundary_condition.txt” & “fem_nodal_ displacement_of_inner_domain.txt” from “3_Atom_Set_Up” folder are copied here.
4. After compiling the code by using compile command which mentioned in “compile_command” file, you will get 5 outputs (“Iglob.txt”,”Aglob.txt”,”Jglob.txt”, ”Fglob.txt”, “input_pardiso.txt”).
   These files will be copy into Pardiso folder.

1.5 Pardiso



1.5.1 Overview

PARDISO is an easy to use linear equation solver for solving large sparse symmetric and unsymmetric linear systems of equations. For more information about this software, visit http://www.pardiso-project.org and there you can get a one-year free academic licence as student. The procedure below will be done by the "Aniso_Relax.sh" shell file in the "1_Anisotropic_Tensor" folder.

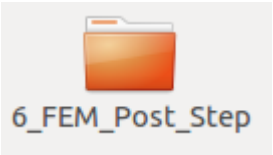
1.5.2 Procedure

a) For the first time, you should install the Pardiso solver by following the instructions in a text file named "for fist time user how to install pardiso" inside the "Pardiso"folder. But, when you want to compile the program, you should be careful about changing the user ID that belongs to your system. The place of user ID is assigned as [XXXX] inside the file.

b) The compile command for Pardiso can be found inside "newuser_compile_ command.txt" file.

d) After compiling, you should run it by typing "*./myprogram* " in terminal. Then you will get "Dglob.txt" file as output which is copied into "6_FEM_Post_Step" folder.

1.6 FEM_Post_Step



1.6.1 Overview

In this folder we will get a list of global nodal displacement in the FEM part of the model. In this step the process of automatic proceeding from "1_Anisotropic_Tensor" folder will continue until end of copying required files into the "8_Relaxation_coupling" folder (which is going to relax our coupled model(MD and FEM)).

1.6.2 Procedure

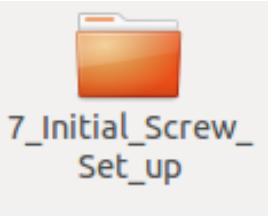
The procedure will be done using the "Aniso_Relax.sh" shell file in the "1_Anisotropic_Tensor" folder. In this folder, beside the "Dglob.txt" file, the following files are also copied from prevoius steps
1- "fem_inputfile_with_outer_boundary_condition.txt" & "fem_nodal_displacement_of_inner_domain.txt" from "3_Atom_Set_Up" folder

2- "burgers_vector.txt" from "4_FEM_Start_Lag" folder

3- "elasticity.txt" from "1_Anisotropic_Tensor" folder

After compiling and running it, you will get "fem_global_nodal_displacement.txt" and tecplot files that can be used to visualize the FEM output.

1.7 Initial_Screw_Set_Up



1.7.1 Overview

In this folder the dislocation will be inserted into the MD part of the model. The procedure below will be done by the ”Aniso_Relax.sh” shell file in the “1_Anisotropic_Tensor” folder.

1.7.2 Procedure

The files below are copied from previous steps into this folder by “Aniso_Relax.sh” file:

a) "inner_coordinate_of_fem_domain .txt" from “3_Atom_Set_Up” folder

b) "fem_inputfile_with_node_element_information.txt" file from “3_Atom_Set_Up” folder

c) "relaxed_perfect_crystal_with_atom_type.imd" from "3_Atom_Set_Up" folder

d) "fem_global_nodal_displacement.txt" from "6_FEM_Post_Step" folder

e) “shift.txt” from “3_Atom_Set_Up” folder

f) “burgers_vector.txt” from “4_FEM_Start_Lag” folder

Compile and run the “Initial_Screw_Set_up.cpp” using:

1. g++ Initial_Screw_Set_up.cpp
2. ./a.out

Then you will get the following outputs:

1. “atomistic_dislocation_with_fem_solution.imd” which has the dislocation in the atomistic structure)
2. “element_with_atom_ids.txt” which has first the number of the element and then the IDs of the atoms that are inside the element in each line.
3. atom_coordinates.txt

4. “type2_atoms_in_transition_zone.imd” which includes only the type2 atoms that are paired to each other in transition zone of the FEM part of the model.
5. “node_atom_pairs_ids.txt” which has the IDs of the paired nodes and atoms of the front and back surfaces of the FEM part of the model.

2 Relaxing the coupled model

2.1 8_Relaxation_Coupling

2.1.1 Overview

In this part, the coupled model will be relaxed. Whole procedure of preparing data files for this step is done by the “Aniso_Relax.sh” file. So, the following section is just to let you know what would be done in this part.

2.1.2 Procedure

In this folder there will be some subfolders and

- Important note!
  In this folder, just compile the codes in subfolders, do not run them!!

1. In “FEM_Pre_Step” folder , Copy
   - **i)** "fem_outer_boundary_condition.txt" and “fem_input.txt” file (from “3_Atom_Set_Up” folder)
   - **ii)** “fem_nodal_displacement_of_inner_domain.txt” (from "6_FEM_Post_Step" folder)
   - **iii)** “burgers_vector.txt” (from “4_FEM_Start_Lag” folder)
   - **iv)** “elasticity.txt” (from ../1_Anisotropic_Tensor) and the code is compiled(using ”g++ FEM_PRE_STEP.cpp” command)
2. Make sure that the “Iglob.txt” & “Aglob.txt” & “Jglob.txt” and “input_pardiso.txt” files are copied from "5_Paradiso" folder. Be careful that the code should be same as the one in previous Pardiso folder. The code is compiled using the command in “compile_command.txt” file.

3. In “FEM_Post_Step” the "fem_outer_boundary_condition.txt" and “fem_input.txt” files are copied from “3_Atom_Set_Up” folder and compiled.
4. In “Fe_MD” folder, the "atomistic_dislocation_with_fem_solution.imd" file is copied from "7_Initial_Screw_Set_Up" folder and another copy of it is rename as "atomistic_dislocation_with_fem_solution_0.imd" for having a backup file in the case that any failure in the simulation happened.
5. In “Nodal_Calc” copy (All from "7_Initial_Screw_Set_Up" folder):

   i) "node_atom_pairs_ids.txt"

   ii) "relaxed_perfect_crystal_with_atom_type.imd"

   iii) "inner_coordinate_of_fem_domain.txt". Compile it.
6. In “Iterative_Step” Copy (All from "7_Initial_Screw_Set_Up" folder):

   i) element_with_atom_ids.txt

   ii) atom_coordinates.txt

   iii) relaxed_perfect_crystal_with_atom_type.imd

   iv) inner_coordinate_of_fem_domain.txt

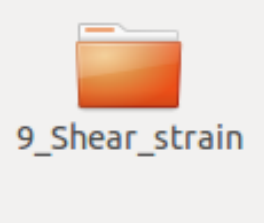
   v) burgers_vector.txt

   vi) fem_inputfile_with_node_element_information.txt and compile it using “g++ Iterative_Step.cpp” command and come back to "8_Relaxation_Coupling" folder.
7. Finally run the "text-plot.sh" file by typing "./text-plot.sh" in the terminal while being inside "8_Relaxation_Coupling" folder(Initially, for the first time in each computer system, use this code “*chmod u+x text-plot.sh*” then run it).

Now after the structure is relaxed, in the next section, we will apply shear strains into the structure to find the value as Peierls stress which is required to move the dislocation.

3 Apllying Shear stress to find the Peierls stress

3.1 9_Shear_Strain



3.1.1 Overview

In this part, we will apply shear strains to the model and will check whether the dislocation will move or not. So, if the dislocation moves at defined stress, that value of stress will be considered as the right Peierl's stress value for our material(which in this sample model, the material is iron and its Peierl's stress is 1205 MPa).

3.1.2 Procedure

In this folder we have two folders generally,"Applying_shear_stress" and "Shear_stress". First, by use of the code "Shear_Stress.cpp" inside "Applying_shear_stress" folder, an output will be generated that called "schmid_shear_stress.txt" and this output will be used in "Shear_stress" folder. Explicitly:

Create a folder named with the shear number that is going to be applied on your model(for example 1.2GPa) and copy all subfolders inside the "Shear_stress" folder into it.

Go to "Shear_Stress.cpp" code inside "Applying_shear_stress" folder and change the value of "tau_23" variable as the value of applying shear load(for our example: 1.2 GPa). Compile and run it using these command:
- g++ Shear_Stress.cpp
- ./a.out
Then you will get the "schmid_shear_stress.txt" as the output.

Copy it into the subfolders “FEM_Post_Step” and “FEM_Pre_Step” folders inside the labeled folder with the shear value.

Finally, run "text-plot.sh" file with these commands:

- chmod u+x text-plot.sh

- ./text-plot.sh

When this part finished, you can monitor the “atomistic_dislocation_with_fem_solution_*.ss” file inside “Archive” folder in “9_Shear_Strain” folder using the “AtomViewer” program to check whether the dislocation moved or not. For that:

1. Go to “AtomViewer” folder and double click on the “AtomViewer.sh” when the dialoge box opened choose “Run” option. Then. the program will open.
2. Go to “File” and choose “Open IMD file” then select the “Files of type” as “All files” and choose the “atomistic_dislocation_with_fem_solution_*.ss” file that you want to see.
3. By opening “atomistic_dislocation_with_fem_solution_1.ss” file which is the relaxed structure and then “atomistic_dislocation_with_fem_solution_[last iteration].ss” file which is the final position of the dislocation after applying the shear stress and comparing them, you can see whether the dislocation moved or not.

Acknowledgments

I wish to have my special thanks to Dr. Karthikeyan Chockalingam for his kind help in writing and correction of this toturial and Dr. Carlos Teijeiro Barjas for his huge help in modifying and making the codes more user friendly.