

Centro-symmetry parameter studies of defects in deformed copper single crystal

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In
Metallurgical and Materials Engineering

By

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CERTIFICATE

This is to certify that the thesis entitled “**Centro-symmetry parameter studies of defects in deformed copper single crystal**” submitted by SibasishRath, Roll No. 111MM0107 and Joy KiranToppo, Roll No. 111MM0384 in partial fulfillment of the requirements for the award of Bachelor of Technology degree in Metallurgical and Materials Engineering at the National Institute of Technology, Rourkela (Deemed University) is an authentic work carried out by them under my supervision and guidance. To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University/Institute for the award of any Degree or Diploma.

DATE :- 6/05/2015

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ABSTRACT

Molecular Dynamics (MD) simulations of uniaxial tension at nano-scale was carried out for strain rate of 0.0001ps^{-1} and at temperatures of 10K and 50K respectively on perfect Cu single crystal and having a horizontal and vertical surface defects in order to investigate the stress-strain response. Also the mechanical properties were investigated at the above stated temperatures. It was seen that mechanical properties were significantly influenced with respect to temperature and with respect to defects. The engineering stress-strain diagram observed for all the specimens showed a zig-zag behavior after the first drop. The first drop in the stress-strain curve is due to the yielding of the material and subsequent drops could be due to formation of deformation mechanism dominated by twins. The substructural features such as twins are observed using centro symmetry parameter studies with the help of Ovito software.

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1. INTRODUCTION

Materials which have at least one dimension in the range of 1-100 nanometers, i.e. at least one nanoscaled dimension are called nanomaterials. Nanomaterials have higher surface areas as compared to their bulk counterparts. Nanoscale materials can be engineered from minerals and almost any chemical, and they differ with respect to size, shape of particle, surface coatings, composition and strength of particle bonds. Nanoparticles differ from bulk phase materials in electronic, optical, chemical, mechanical and other aspects. They exhibit fascinating and very useful properties, which can be applied for a variety of applications, both structural and non-structural[1]. Properties like color, strength, weight, electrical conductivity change at the nano-scale level. This can be utilized to make devices with very high power storage capabilities, or ultra-light materials that require less energy to operate.

Nanowires are nothing but very thin wires which have diameters in the order of 1nm. Suspension and deposition are the two processes by which nanowires can be manufactured. Nanowires have two directions which are quantum-confined but one direction available for electrical conduction which is not confined. This makes nanowires suitable to be used in applications where electrical conduction required more than tunneling transport. Nanowires are expected to exhibit significantly different optical, magnetic and electrical properties to their bulk 3-D crystalline counterparts because of their distinctive density of electronic states in the limit of small diameters. It has been found that metallic nanowires exhibit a unique mechanical behavior and properties, and show a size effect and are distinctively delicate to environmental conditions [2]. A notable variation is seen of the nanowires from their bulk phase in the properties such as strength, hardness, elastic modulus and yield strength, and found that the strain rate sensitivity was related to the grain size. There are certain properties of nanowires that are similar to their bulk counterparts while there are other properties which are different. However from applications standpoint, nanowires have an advantage as there are certain properties that they exhibit which can be independently controlled. By exploiting the aspects of the 1-D electronic density of states, certain properties exhibited by the nanowires can be enhanced too. Their various application include their use in the electronic devices, in the sensing of proteins and chemicals, use in optics, power conduction and numerous other fields [3]. Nanowires are now being applied to glass and plastics which results in improved computer displays and chips.

Computational simulation technique has been established to compute the mechanical properties of the nanowires [4]. Simulations that use realistic molecular dynamics model are proficient of demonstrating some methods to explain the essential mechanisms of nanomaterials getting deformed, formation of plastic region and breaking of nanomaterial under stress. However for this, it is essential that the nanomaterial is strained and relaxed at very displacement amplitudes and high velocities.

2. Literature Review

[5] Dan Huang, Qing Xhang, PizhongQiao: Molecular Dynamics Simulation (MD) was carried out using Modified Embedded Atom Method (MEAM). Each nanowire was made to experience a different tensile axial loading at different strain rates. In each loading case, to initiate the simulation after eliminating the unfavourable configurations, the nickel nanowire model was initially relaxed for 100 ps, by conducting 50000 iterations with a constant time step of 2 fs. After the relaxation process was executed, the uniaxial tensile loading was conducted at a uniform deformation rate along the z-axis at a temperature of 300K. During the Molecular Dynamic simulation, the Newtonian equations of motion were evaluated with a timestep of 2fs, and Velocity-Verlet algorithm was used to obtain the positions, velocities and forces between the atoms. As per the MD simulation process output, stress-strain curves were plotted and the various parameters like elastic modulus, yield strength, fracture strength are found. The nanowires under the uniaxial tensile loading followed a similar trend in the curve of stress strain as in polycrystalline metals.

The elastic modulus, yield strength and fracture strength is seen to increase with increasing strain rate. The stress-strain plots can be divided into three parts, the linear or elastic part, the plastic part and the failure region. In the initial part, the average atomic stress follows a linear relationship with strain, resembling to that of the polycrystalline metals under tensile loading. Based on the results of the simulation, a set of formulae were found to describe the strain rate sensitivity of the nanowires on the mechanical properties. The elastic modulus of the Ni nanowires along with the yield stress and fracture strength showed a linear relationship w.r.t the logarithm of the strain rate. The yielding strain of nanowires is not dependent on the strain rate and cross sectional area. A quantitative analysis of strain rate and size effects was done, and comprehensive nonlinear correction formulae were obtained to elaborate the combined strain rate and cross-sectional effect on the mechanical properties of Ni nanowire.

By using the given MD system and fitted correlation formulae, the mechanical behavior of Ni nanowires were precisely described, and the elastic modulus, yield stress and fracture strength w.r.t the loading rate and cross-sectional size were predicted. As witnessed, the mechanical properties of the metallic nanowire with respect to the loading rate are consistent with the experimental and numerical results.

[6] Ken-Huang Lin, Jia-Yun Li, Jenn-Sen Lin, Shin-Pon Ju, Jian-Ming Lu and Jin-Yuan Hsieh; In this study, the multi-shell structure of the ultrathin nanowires had been created by SABH (Simulated Annealing Basin Hopping) . In this SABH method, the conjugate gradient method was replaced by the limited memory BFGS method (LBFGS), which is be used to simulate a system containing of a large number of atoms. The simulated annealing technique was also applied with the BH method to be a SABH method, which included a wider searching domain within the potential energy surface. The loading state of the MD simulation for the tensile test to be carried out is as follows: the load was applied along the axis, the fixed layers were the top and bottom layers, and the other layers were set as thermal controlled layers.

In this undertaken work, understanding the width effect on the mechanical property and the mechanism of deformation, 3 different breadths of Tungsten nanowire with equilibrium at 300 K for 50 ps were taken. The outcomes after calculation of radius, cohesive energy, Young's modulus, yielding stress, yielding strain, and maximum strain for 3 types of nanowires were listed. The equivalent plots of stress–strain plots for the tensile process of various types of nanowires were presented. It was observed that as the wire breadth falls, there is a rise in the maximum stress and the slope of curve of stress–strain . The effect of size and temperature was

determined. In the 3 types of tungsten nanowires, it was seen that as there is increase in strain , there is gradual growth in the necking area of the structures. The maximum strain and the cohesive energy increase depend on the variation of the size of the nanowires, but the Young's modulus, yield stress, and yield strain represent results which are opposite.

[7]A.R. Setoodeh, H. Attariani, M. Khosrownejad; The mechanical properties of Ni nanowires at diverse temperatures were investigated using MD simulations. The inter-atomic interactions are characterized by the use of “embedded atom potential”. In case of uniaxial load application, the curve of stress-strain at various strain rates was plotted after the simulation. The effects of temperature and volume/surface ratio on the mechanical characteristics of Ni nanowire were demonstrated. Particularly, the modeling of the loading-unloading procedure and the effect of the unloading on the plot of stress–strain in the region of plasticity was inspected. Then, the mechanical characterisation in the compression loading was done and the machinery of deformation was explained clearly based on the current model. It is shown by the results of compression modeling that the computed tensile yield stress is higher than the obtained yield stress.

An molecular dynamic simulation was carried out to observe the mechanical behavior of Nickel nano-wires with the use of embedded-atom model potential. The effects of size, strain rate, and temperature were investigated. The yield stress is found to increase with an increase in the strain rate, though Young’s modulus did not depend on the strain rate. The current model demonstrated that by increasing the temperature of simulation, the elastic modulus and the yield stress were found to be linearly decreasing .For the size effect, it is seen that there is an increase in yield stress with a decrease in the volume/surface ratio. The plot of stress–strain for loading–unloading of simulated nanowire showed that the path does not concur with the ordinary tensile curve after the second stage of process of loading. The behavior observed is relatable to the decrease of dislocation density during the process of unloading. Then in the stage of compression loading, lesser values of Young’s modulus and yield stress were obtained as compared to the tensile test which the free surface effect can introduce.

[8] Maxim A. Makeevand Deepak Srivastava; In this paper, Tersoff many-body bond-order reactive potential was used to define the inter- atomic interactions (Si-Si, Si-C and C-C) between the atoms of model 3C-SiC (crystalline).The response of mechanical characteristics of 3C-SiC nanowires having 6 differing diameters, lying between 0.89nm to 3.56 nm were investigated through the atomistic simulations. 2 more nanowires of diameters4.61nm and 7.7 nmwere taken into consideration to ensure that the scaling relations are valid., Depending on the nanowire diameter, the quantities of atoms that are present in the simulated systems correspond to the range between 1536 and 18816. The unit cells of the nanowires were carved out from the matching structures of bulk 3C- SiC crystal, which were eventually relaxed using the molecular dynamics GTBMD scheme. The dynamic loading process was carried out in adiabatic approximation. Edge atoms, existing within several planes of atoms at both the ends, were kept fixed during the procedure of the Molecular Dynamic relaxation, applied between the subsequent steps of loading. The total quantity of fixed atoms varied from 48 to 588, depending on the radius of nano-wire. The locations of these atoms of the edges were moved at a fixed rate according to the desired strain, whereas the system, with the use of MD simulations is dynamically relaxed. Each loading and relaxation step required the heating of the system to a

temperature of 800 K for 1000 iterations and cooling gradually to a temperature less than 0.1 K for 5000 iterations. The computation of elastic strain energies w.r.t the initial state was done. The mechanical response characteristics were investigated till the threshold of the structural stability of the nano wires was reached under the given conditions of strain.

Using MD simulations, investigation of the elastic properties of 3C-SiC nanowires of different diameters and their structural changes, caused due to the external loadings was done. Under uniaxial tensile as well as compressive loading, the moduli of elasticity and the structural integrity limits were found to be autonomous of the wire diameter. However, in case of nonaxial torsional and bending strains, the elastic response and structural deformation mechanism near the elastic limit strongly depend on the diameter of the nanowire. By decreasing the nanowire diametric dimensions, we can fluctuate the mechanical properties in torsion and bending.

[9] JIJUN LAO,MEHDI NAGHDI TAM,DINESH PINISETTYand NIKHIL GUPTA; reviewed Molecular Dynamic studies to understand and investigate the effects of strain rate, temperature, and cross-sectional area on the mechanical properties of FCC (face-centred cubic) metallic nanowires. The yield stress of FCC metallic nanowires was found to be 100 times higher than that of the corresponding metals in bulk state. The fracture stress and yield strain of the metallic nanowires were also found to be significantly higher compared with those of the bulk metals. The influence of slip and twinning deformation mechanisms on the mechanical properties of FCC metallic nanowires was discussed. FCC metallic nanowires were found to exhibit novel structural reorientation, pseudoelasticity, phase transformation,elastic recovery and shape memory effect (SME) .Metallic nanowires with BCC (body-centred cubic) and hexagonal closed-packed crystal structures were compared with the FCC metallic nanowires. The phenomenon of pseudoelasticity was also observed in BCC metallic nanowires similar to that of FCC metallic nanowires.Densenano-twin arrays were found in Magnesium nanowires despite the energy of the high twin boundary.

[10] S. J. A. Koh , H. P. Lee, C. Lu and Q. H. Cheng; This study was focused on the Molecular Dynamics simulation of an infinitely long, cylindrical nanowire of Pt, with a width approximately 1.4 nm. A uniaxial tensile strain was given to the nanowire along the [001] axis. Analysis of the changes in structure of crystal during deformation was done and its mechanical properties were determined from the simulation. The Classical Molecular Dynamic simulation was used in this study, with the empirical Sutton-Chen pair function being used to define the interatomic potential between the atoms of Pt. For finite temperature control of the simulated system, the Berendsen loose-coupling thermostat was selected with a time constant of 25% of the total relaxation time for each increment in strain. Different strain rates used were 0.04% ps⁻¹, 0.4% ps⁻¹ and 4.0% ps⁻¹, at varying simulation temperatures of 50K and 300K, in order to analyze the effects of different strain rates and temperatures on the mechanical properties and deformation characteristics of the nanowire. It was seen that the response of stress-strain curve showed a clear periodic, dislocation-relaxation- recrystallization behavior at strain rate and low temperature. The beginning of amorphous crystal deformation occurred at strain rate of 0.4% ps⁻¹, and full deformation of amorphous crystal occurred at 4.0% ps⁻¹, with melting of amorphous crystal being definite at 300K. At higher strain rate and temperature, because of higher entropy of the nano-wire, periodic behavior of stress-strain curve turned less clearly defined, and phenomenon of super-plasticity was seen. This feature was significantly boosted due to the formation of a single-walled helical substructure at temperature of

300K, at which the nano-wire was deformed at a lesser value of strain rate. The Poisson's ratio did not show much change with respect to its bulk counterpart while the Young's modulus showed around 50-75% change.

[11] Subramanian K. R. S. Sankaranarayanan, Venkat R. Bhethanabotla, and Babu Joseph; MD simulation was used to study the mechanical properties of cylindrical bimetallic Pd-Pt nanowires of infinite length with a diameter of approximately 1.4 nm and two different configurations i.e. 25% and 50% Pt. The nano-wires were subjected to uniaxial tensile strain with varying strain rates of $0.05\% \text{ ps}^{-1}$, and $5.0\% \text{ ps}^{-1}$ respectively, at temperatures of 50K and 300 K, to study the effects of strain rates and temperature on the mechanical properties and the characteristics of deformation of the nano-wire. Investigation of the deformation and rupture mechanism was done. The discussion of effects of lattice mismatch on the observed deformation modes in bimetallic nano-wires was also done. The simulations indicated that Pd-Pt nano-wires of different compositions, had undergone similar deformation and rupture upon stretching uniaxially. It was found that fracture and yielding mechanisms depend on the strain rate applied and the atomic arrangement, as well as temperature. The transformation from crystalline to amorphous state took place at high strain rates of $5\% \text{ ps}^{-1}$, with amorphous melting detected at 300 K. Deformation of nanowires at higher strain rates and low temperature, where the superplasticity characteristic is greatly enhanced, developing a multi-shell helical structure as a result of it. Mechanical characteristics of the nanowires were vastly different from that of bulk phase and are governed by the strain rate applied, alloy composition, temperature and the structural reordering associated with nano-wire elongation. We find that Young's modulus of the single component as well as alloy nano-wires depend on the strain rate applied and is found to be about 70–75% of the value in bulk phase. Ductility was significantly improved because of the wires developing and reorganizing into a multi-shell helical structure which had occurred at higher values of strain rates. The Poisson's ratio of Pd-rich alloys is 60–70% of its bulk phase value, whereas that of Pt-rich alloys is not significantly changed for nanowires. The calculated alterations in mechanical properties of the nanowires are shown to have important effects on their applicability in detecting and catalysis and other areas.

[12] Wei-dong WANG, Cheng-long YI, Kang-qi FAN; A molecular dynamics study of the tensile properties of ultrathin nickel nano-wires in the 100 orientation with diameters of 3.94, 4.95 and 5.99 nm respectively was done at different temperatures and strain rates. The strain rate and temperature dependences of tensile properties were investigated. The simulation results showed that the elastic modulus and the yield strength are slowly decreasing with increasing temperature, while with the increasing strain rate, the stress-strain curves fluctuated more prominently and the ultrathin nickel nano-wires ruptured at a smaller strain value. At a temperature of 0.01 K, the yield strength of the nano-wires dropped rapidly with the increasing strain rate, and at other temperatures the strain rate had a little effect on the yield strength and elastic modulus. In the end, the influence of size on the tensile properties of ultrathin Ni nanowires were discussed.

[13] Peng Wang, Wu Chou, Anmin Nie, Yang Huang, Haimin Yao, and Hongtao Wang; An organized study of the mechanisms of deformation of molybdenum (Mo) nano-wires was conducted using MD simulations. Both wire thickness and axial orientation were found to have critical roles in determining the pathways of deformation. In case of the nano-wires with orientation $110/\{111\}$, full dislocation plasticity was seen to be activated on $\{110\}$ planes. For both $100/\{110\}$ and $100/\{100\}$ nano-wires, the major mechanism is twinning with $\{112\}$ forming the coherent twin boundaries. A continuous process of slip lead to a 41% uniform elongation and the 100 wire axis got reoriented to 110. In case of $100/\{100\}$ nanowires, the reorientation mechanism was seen to stop operating when the diameter was less than 1nm or more than 8nm ($d < 1 \text{ nm}$ or $d > 8 \text{ nm}$). The chains of atoms were preferred energetically for ultrathin nano-wires after occurrence of yielding because of the similarity of the surface to close-packed body-centred cubic (BCC) planes, whereas numerous slip systems tend to be activated for larger nanowires. Eventually, a theoretical model was proposed for explaining the primary mechanism of dependence of size on the stress required for yielding.

3. Objectives

- MD simulation of uniaxial tensile deformation was carried out on defect and defect free single crystal Cu sample
- Temperature of deformation: 10 K, 50 K
- Strain rate: 10^8 s^{-1}
- Sample size : 20 Å x 50 Å x 40 Å
- MD codes for tensile deformation are written in LAMMPS.
- The atomic position snap shots for identifying the defects such as dislocations, twins are visualized by using OVITO software

4. Procedure of Molecular Dynamics Simulation

4.1 Molecular Dynamic Simulation

Molecular simulation is a very useful tool in molecular modeling and theoretical study of metal molecules. It enables us to understand the structure and dynamics with extreme detail on scales within which motions of individual atoms can be tracked.

This computational method calculates the time dependent behavior of a molecular system. The actual motion of atoms is simulated by evolving the atomic configuration (atomic positions and velocities) with time by integrating Newton's Equation of motion

$$\text{Force} = \text{mass} \times \text{acceleration}$$

The atoms and molecules present in the system are allowed to interact for a period of time. The trajectories obtained of the interacting particles are determined by numerically solving Newton's equations of motion where forces between the particles and potential energy are calculated by molecular mechanics force fields.

4.2 Working of MD Simulation

1. Initialize the positions and velocities of the atoms
2. Calculate energy:
 $E_{\text{total}} = E_{\text{bond}} + E_{\text{torsion}} + E_{\text{bond-angle}} + E_{\text{non-bond}}$
3. Calculate the forces on the atoms
4. Move the atoms and integrate Newton's equations of motion to obtain atomic trajectory

$$\vec{F} = m\vec{a}$$

$$v_i(t + \Delta t) = v_i(t) + a_i(t) \cdot \Delta t$$

$$x(t + \Delta t) = x(t) + v_x(t)\Delta t + \frac{1}{2}a_x(t)(\Delta t)^2$$

5. Update the new positions and velocities after timestep 0.001 ps (Δt)

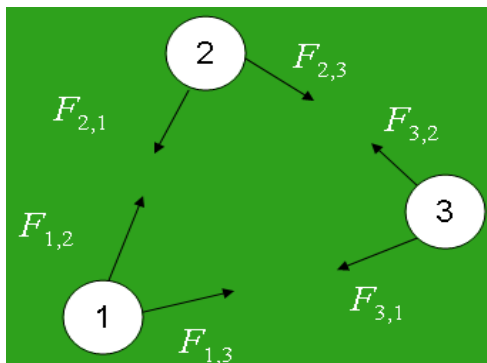


Fig 3.1 Equilibrium of forces of particles

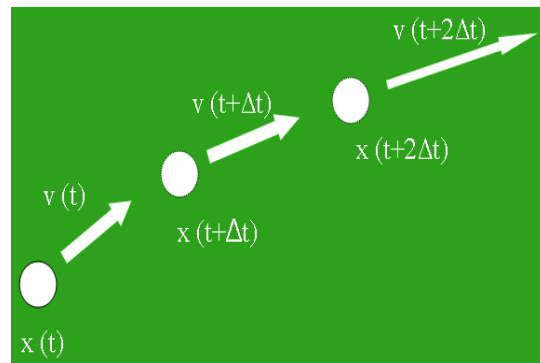


Fig 3.2 Trajectory of the particle

4.3 Ensembles:

Ensembles are collections of all the possible systems having different microscopic states but are similar in macroscopic or thermodynamic state.

Ensembles with varying characteristic are:

- Microcanonical ensemble (NVE) : The thermodynamic state is characterized by a fixed number of atoms, N , a fixed volume, V , and a fixed energy, E . This corresponds to an isolated system.
- Canonical Ensemble (NVT): This is a assortment of all the systems whose thermodynamic state is characterized by a fixed number of atoms, N , a fixed volume, V , and a fixed temperature, T .
- Isobaric-Isothermal Ensemble (NPT): This is characterized by a fixed number of atoms, N , a fixed pressure, P , and a fixed temperature, T .

Grand canonical Ensemble(VT): The thermodynamic state for this ensemble is characterized by a fixed chemical potential, a fixed volume, V , and a fixed temperature.

4.4 Software used

4.4.1 LAMMPS [14]

- LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator
- It is a molecular dynamics program
- It is free, open-source software that is distributed under the terms of the GNU General Public License
- For computational efficiency LAMMPS uses neighbor lists to keep track of particles present at nearby location. The lists are optimized for systems with particles that are repulsive at small distances. This results in the local density of particles never to become too large [5]. The code is written with the help of C++. The designing structure of the code is so flexible that it can be easily modified and extended with new applications.
- A proper combination of pre and post-processing tools are also packaged with LAMMPS, some of which can convert input and output files to/from formats used by other codes.
- LAMMPS makes use of MPI(Message Passing Interface) for parallel communication and

4.4.2 OVITO[15]

- Ovito Stands for *Open Visualization Tool*
- OVITO is a software that translates the raw atomic coordinates of a system generated from Lammmps , into a meaningful graphical representation.
- OVITO is freely available visualization and data analysis software for atomistic datasets as output by large-scale molecular dynamics/statics and Monte-Carlo simulations

4.5 Procedure

4.5.1 Input

- LAMMPS software is downloaded and installed to our personal computer or laptop, which is itself a free source and is easily available on Sandia National Laboratories website.
- For a simulation to run effectively, three basic files or components are always required. They are as follows:
 - In file (program file that is written to create models and perform simulations for desired operations)
 - Potential file (consists of data about inter atomic bond energy and force field between atoms)
 - Executable file (lmp_win_no-mpi.exe, required to run the commands in the in file). →
- After having all the above necessary files, command prompt screen is opened (dos environment).
- Then the screen will display the path address in which all the above mentioned files are present.
- Next to the path address 'lmp_win_no-mpi.exe< in file name ' is typed and enter is pressed.
- Then automatically the in file will be executed by the .exe file and if there is any error in the in file then it will be displayed in the command prompt screen and subsequent rectification can be done.

4.5.2 Output

After successful running of the in file, we will get three out-put files as follows:

- DUMP file (with an extension of .lammstrj containing the atomic co-ordinates of the final structure after simulation and also for deformation studies it contains the stress component values)
- Log file (containing thermodynamic data e.g. temperature, pressure, volume, and total energy after a particular no of steps)
- Log. lammps file
- Now, the Dump file with the extension .lammpstj is opened with the help of ovito to see the simulation process visually
- The following adjustments are done in the Ovito
 - Centro-symmetry and colour coding is selected
 - The maximum range for colour value is given as 12 and minimum ranger for colour value is given as 0.

4.6 Flow Chart for the Program proceeds

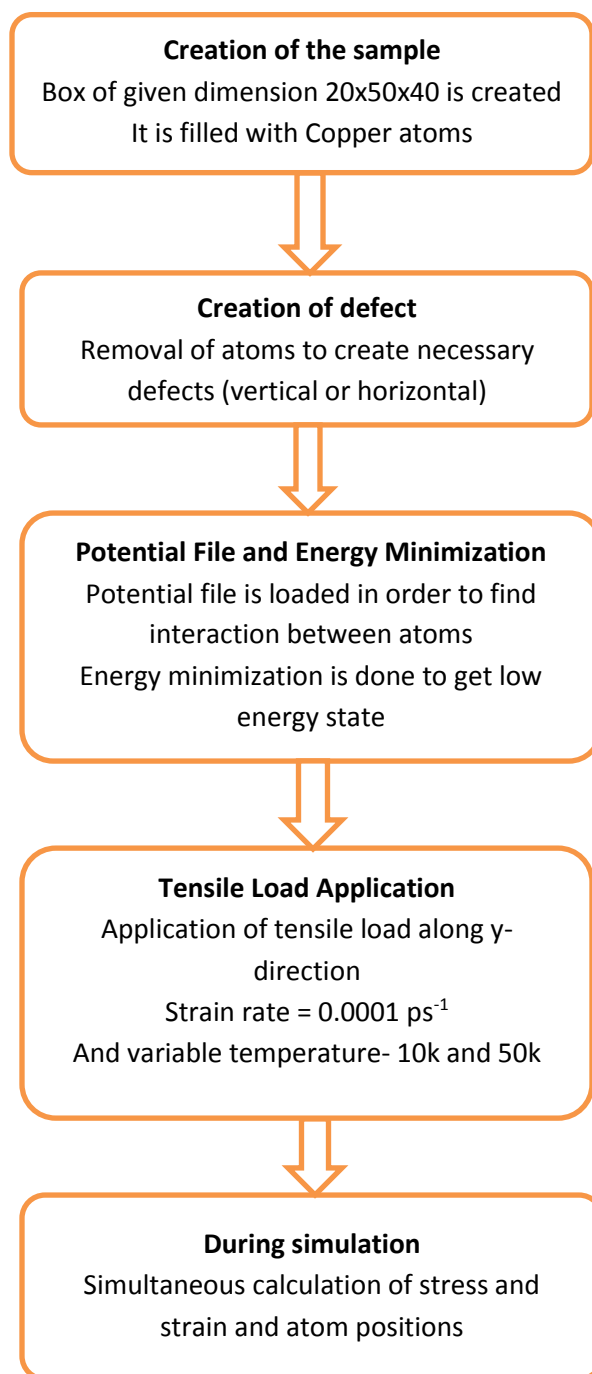


Fig 3.3

5. Work Plan

The following Table lists the sample dimensions, temperature, strain rate and type of defects used for conducting the simulation studies.

Table 5.1

Sample	Dimension	Mode of Deformation	Strain rate (in ps ⁻¹)	Temperature (in K)	Defects
Cu	20x50x40	Tensile	0.0001	10	Perfect
Cu	20x50x40	Tensile	0.0001	10	Vertical
Cu	20x50x40	Tensile	0.0001	10	Horizontal
Cu	20x50x40	Tensile	0.0001	50	Perfect
Cu	20x50x40	Tensile	0.0001	50	Vertical
Cu	20x50x40	Tensile	0.0001	50	Horizontal

5.1 Tensile tests at 50 K :

5.1.1 Program for perfect crystal

```

units      metal //determines units of all quantities used in the program
echo      both //finds fault and displays error messages
atom_style atomic
dimension 3
boundary  s p s
region    box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40
create_box 1 box

lattice    fcc 3.61 //lattice parameter for Cu crystal
region    Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms 1 region Cu units box

timestep  0.002 //sets the timestep for subsequent simulations
pair_style eam/alloy //interaction between two atoms Embedded Atomic Method,
                  calculates pair wise interaction
pair_coeff * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                  potential file

# Energy Minimization
minimize  1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state

fix 23 all nvt temp 50 50 0.01 //fixes temperature for energy minimization of atoms
run      1000

```

```

compute      csym all centro/atom fcc
compute      peratom all pe/atom

variable     tmp equal ly
variable     lo equal ${tmp}
variable     strain equal (ly-v_lo)/v_lo

variable     p1 equal "-pxx/10000"
variable     p2 equal "-pyy/10000"
variable     p3 equal "-pzz/10000"

variable     p12 equal "-pxy/10000"
variable     p23 equal "-pyz/10000"
variable     p13 equal "-pxz/10000"
variable     fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
variable     fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" ##### Von Mises Stress

variable     t equal "v_fm/v_fv"
variable     fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm)-(v_p12)^2*(v_p3-v_fm)-
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress

# principal stresses

variable     I1 equal "(v_p1+v_p2+v_p3)"
variable     I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-
(v_p23)^2-(v_p13)^2"
variable     I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-
((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
variable     A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-
(3*(v_I2)))^(3/2))))/3"

variable     s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
variable     s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
variable     s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos      10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style custom step temp vol press pekeetotal

dump         1 all custom 10000 Cu_perfect_tensile_50K.lammpstrj id type x y z //dumps a
            snapshot of atom quantities every 10000 timesteps to the specified file
dump         2 all cfg 10000 Cu_defect_tensile*.cfg id type xsyzszsc_csymc_peratom

```

```

#dump      3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
           c_1[5] c_1[6]

log        NVTlog_compress_al.data

velocity   all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

fix        2 all deform 1 y erate 0.0001 units box //application of tensile deformation
           force of 0.0001ps-1

fix        3 all print 10 "${strain} ${p2}" file
           stress_strain_data_Cu_perfect_tensile_50K//gives the stress-strain
           data

# temperature controller

fix        1 all nvt temp 50 50 0.01 //fixes the temperature (50 K)and pressure of the
           given system

fix        def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
           Cu_defect_tensile_von.txt

run        6000000 //number of iterations

```

5.1.2 Program for vertical defect

```

units      metal //determines units of all quantities used in the program
echo       both //finds fault and displays error messages
atom_style atomic
dimension  3
boundary   s p s
region     box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40
create_box 1 box

lattice    fcc 3.61 //lattice parameter for Cu crystal
region     Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms 1 region Cu units box

region     dislocation block 19 20 15 35 24.4 25.4 units box
group      5 region dislocation //creates a vertical defect
delete_atoms group 5

timestep   0.002 //sets the timestep for subsequent simulations
pair_style eam/alloy //interaction between two atoms Embedded Atomic Method,
           calculates pair wise interaction

```



```
pair_coeff      * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                                     potential file
```

```
# Energy Minimization
```

```
minimize      1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state
```

```
fix 23 all nvt temp 50 50 0.01      //fixes temperature for energy minimization of atoms
```

```
run          1000
```

```
compute      csym all centro/atom fcc
```

```
compute      peratom all pe/atom
```

```
variable     tmp equal ly
```

```
variable     lo equal ${tmp}
```

```
variable     strain equal (ly-v_lo)/v_lo
```

```
variable     p1 equal "-pxx/10000"
```

```
variable     p2 equal "-pyy/10000"
```

```
variable     p3 equal "-pzz/10000"
```

```
variable     p12 equal "-pxy/10000"
```

```
variable     p23 equal "-pyz/10000"
```

```
variable     p13 equal "-pxz/10000"
```

```
variable     fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
```

```
variable     fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-  
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" ##### Von Mises Stress
```

```
variable     t equal "v_fm/v_fv"
```

```
variable     fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm))-(v_p12)^2*(v_p3-v_fm)-  
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-  
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress
```

```
# principal stresses
```

```
variable     I1 equal "(v_p1+v_p2+v_p3)"
```

```
variable     I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-  
(v_p23)^2-(v_p13)^2"
```

```
variable     I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-  
((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
```

```
variable     A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-  
(3*(v_I2)))^(3/2)))))/3"
```

```
variable     s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
```

```
variable     s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
```

```

variable      s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos       10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style  custom step temp vol press pekeetotal

dump          1 all custom 10000 Cu_defect_vertical_tensile_50K.lammpstrj id type x y z
//dumps snapshot of atom quantities every 10000 timesteps to the specified
//file
dump          2 all cfg 10000 Cu_defect_vertical_tensile*.cfg id type xsyzszc_csyz
c_peratom

#dump         3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
c_1[5] c_1[6]

log           NVTlog_compress_al.data

velocity      all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

fix           2 all deform 1 y erate 0.0001 units box //application of tensile deformation
force of 0.0001ps-1

fix           3 all print 10 "${strain} ${p2}" file
stress_strain_data_Cu_defect_vertical_tensile_50K.txt //gives the stress-strain
data

# temperature controller

fix           1 all nvt temp 50 50 0.01 //fixes the temperature (50 K)and pressure of the
given system
fix          def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
Cu_defect_vertical_tensile_von.txt

run           6000000 //number of iterations

```

5.1.3 Program for horizontal defect

```

units         metal //determines units of all quantities used in the program
echo          both //finds fault and displays error messages
atom_style    atomic
dimension     3
boundary      s p s
region        box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40

```

```

create_box      1 box

lattice         fcc 3.61 //lattice parameter for Cu crystal
region         Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms   1 region Cu units box

region         dislocation block 18 20 23 25 10 30 units box
group          5 region dislocation
delete_atoms   group 5 //creates horizontal defect

timestep       0.002 //sets the timestep for subsequent simulations
pair_style     eam/alloy //interaction between two atoms Embedded Atomic Method,
                calculates pair wise interaction
pair_coeff     * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                potential file

# Energy Minimization
minimize       1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state

fix 23 all nvt temp 50 50 0.01 //fixes temperature for energy minimization of atoms
run           1000

compute        csym all centro/atom fcc
compute        peratom all pe/atom

variable       tmp equal ly
variable       lo equal ${tmp}
variable       strain equal (ly-v_lo)/v_lo

variable       p1 equal "-pxx/10000"
variable       p2 equal "-pyy/10000"
variable       p3 equal "-pzz/10000"

variable       p12 equal "-pxy/10000"
variable       p23 equal "-pyz/10000"
variable       p13 equal "-pxz/10000"
variable       fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
variable       fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" ##### Von Mises Stress

variable       t equal "v_fm/v_fv"
variable       fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm))-(v_p12)^2*(v_p3-v_fm)-
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress

```

```

# principal stresses

variable      I1 equal "(v_p1+v_p2+v_p3)"
variable      I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-
                (v_p23)^2-(v_p13)^2"
variable      I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-
                ((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
variable      A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-
                (3*(v_I2))))^(3/2))))/3"

variable      s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
variable      s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
variable      s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos       10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style  custom step temp  vol press pekeetotal

dump          1 all custom 50 Cu_defect_horizontal_tensile_50K.lammpstrjid type x y z
//dumps a snapshot of atom quantities every 50 timesteps to the specified file
dump          2 all cfg 10000 Cu_defect_horizontal_tensile*.cfg id type xsyzszc_csym
                c_peratom

#dump         3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
                c_1[5] c_1[6]

log           NVTlog_compress_al.data

velocity      all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

fix           2 all deform 1 y erate 0.0001 units box //application of tensile deformation
                force of 0.0001ps-1
fix           3 all print 10 "${strain} ${p2}" file
                stress_strain_data_Cu_defect_horizontal_tensile_50K// gives the stress-strain
                data

# temperature controller

fix           1 all nvt temp 50 50 0.01 //fixes the temperature (50 K)and pressure of the
                given system
fix           def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
                Cu_defect_horizontal_tensile_von.txt

run           6000000 //number of iterations

```

5.2 Tensile tests at 10K :

5.2.1 Program for perfect crystal

```
units          metal //determines units of all quantities used in the program
echo          both //finds fault and displays error messages
atom_style    atomic
dimension     3
boundary      s p s
region        box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40
create_box    1 box

lattice       fcc 3.61 //lattice parameter for Cu crystal
region        Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms  1 region Cu units box

timestep      0.002 //sets the timestep for subsequent simulations
pair_style    eam/alloy //interaction between two atoms Embedded Atomic Method,
                  calculates pair wise interaction
pair_coeff    * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                  potential file

# Energy Minimization
minimize      1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state

fix 23 all nvt temp 10 10 0.01 //fixes temperature for energy minimization of atoms
run          1000

compute       csym all centro/atom fcc
compute       peratom all pe/atom

variable      tmp equal ly
variable      lo equal ${tmp}
variable      strain equal (ly-v_lo)/v_lo

variable      p1 equal "-pxx/10000"
variable      p2 equal "-pyy/10000"
variable      p3 equal "-pzz/10000"

variable      p12 equal "-pxy/10000"
variable      p23 equal "-pyz/10000"
variable      p13 equal "-pxz/10000"
variable      fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
```

```

variable      fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" #####Von Mises Stress

variable      t equal "v_fm/v_fv"
variable      fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm))-(v_p12)^2*(v_p3-v_fm)-
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress

# principal stresses

variable      I1 equal "(v_p1+v_p2+v_p3)"
variable      I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-
(v_p23)^2-(v_p13)^2"
variable      I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-
((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
variable      A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-
(3*(v_I2)))^(3/2))))/3"

variable      s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
variable      s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
variable      s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos       10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style  custom step temp vol press pekeetotal

dump          1 all custom 10000 Cu_perfect_tensile_10K.lammpstrj id type x y z //dumps a
snapshot of atom quantities every 10000 timesteps to the specified file
dump          2 all cfg 10000 Cu_defect_tensile*.cfg id type xsyzszsc_csymc_peratom

#dump         3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
c_1[5] c_1[6]

log           NVTlog_compress_al.data

velocity      all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

fix           2 all deform 1 y erate 0.0001 units box //application of tensile deformation
force of 0.0001ps-1
fix           3 all print 10 "${strain} ${p2}" file
stress_strain_data_Cu_perfect_tensile_10K //gives the stress-strain data

# temperature controller

```

```

fix          1 all nvt temp 10 10 0.01 //fixes the temperature (10 K)and pressure of the
                                     givensystem
fix    def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
        Cu_defect_tensile_von.txt

run          6000000      //number of iterations

```

5.2.2 Program for vertical defect

```

units        metal //determines units of all quantities used in the program
echo         both  //finds fault and displays error messages
atom_style   atomic
dimension    3
boundary     s p s
region       box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40
create_box   1 box

lattice      fcc 3.61 //lattice parameter for Cu crystal
region       Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms 1 region Cu units box

region       dislocation block 19 20 15 35 24.4 25.4 units box
group        5 region dislocation //creates a vertical defect
delete_atoms group 5

timestep     0.002 //sets the timestep for subsequent simulations
pair_style   eam/alloy //interaction between two atoms Embedded Atomic Method,
                       calculates pair wise interaction
pair_coeff    * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                                       potential file

# Energy Minimization
minimize     1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state

fix 23 all nvt temp 10 10 0.01 //fixes temperature for energy minimization of atoms
run          1000

compute      csym all centro/atom fcc
compute      peratom all pe/atom

variable     tmp equal ly
variable     lo equal ${tmp}
variable     strain equal (ly-v_lo)/v_lo

```

```

variable      p1 equal "-pxx/10000"
variable      p2 equal "-pyy/10000"
variable      p3 equal "-pzz/10000"

variable      p12 equal "-pxy/10000"
variable      p23 equal "-pyz/10000"
variable      p13 equal "-pxz/10000"
variable      fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
variable      fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" ##### Von Mises Stress

variable      t equal "v_fm/v_fv"
variable      fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm)-(v_p12)^2*(v_p3-v_fm)-
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress

# principal stresses

variable      I1 equal "(v_p1+v_p2+v_p3)"
variable      I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-
(v_p23)^2-(v_p13)^2"
variable      I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-
((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
variable      A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-
(3*(v_I2)))^(3/2))))/3"

variable      s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
variable      s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
variable      s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos       10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style  custom step temp vol press pekeetotal

dump          1 all custom 50 Cu_defect_vertical_tensile_10K.lammpstrj id type x y z //dumps
              a snapshot of atom quantities every 50 timesteps to the specified file
dump          2 all cfg 10000 Cu_defect_vertical_tensile*.cfg id type xsyzszc_csym
              c_peratom
#dump         3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
              c_1[5] c_1[6]

log           NVTlog_compress_al.data

velocity      all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

```



```

fix          2 all deform 1 y erate 0.0001 units box //application of tensile deformation
                                                    force of 0.0001ps-1
fix          3 all print 10 "${strain} ${p2}" file
stress_strain_data_Cu_defect_vertical_tensile_10K.txt //gives the stress-strain
                                                    data

# temperature controller

fix          1 all nvt temp 10 10 0.01 //fixes the temperature (10 K)and pressure of the
                                                    givensystem
fix          def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
Cu_defect_vertical_tensile_von.txt

run          6000000 //number of iterations

```

5.2.3 Program for horizontal defect

```

units        metal //determines units of all quantities used in the program
echo         both //finds fault and displays error messages
atom_style   atomic
dimension    3
boundary     s p s
region       box block 0 20 0 50 0 40 units box //creates a box of dimension 20x50x40
create_box   1 box

lattice      fcc 3.61 //lattice parameter for Cu crystal
region       Cu block 0 20 0 50 0 40 units box //creates Cu atoms in the given box
create_atoms 1 region Cu units box

region       dislocation block 18 20 23 25 10 30 units box
group        5 region dislocation
delete_atoms group 5 //creates horizontal defect

timestep     0.002 //sets the timestep for subsequent simulations
pair_style   eam/alloy //interaction between two atoms Embedded Atomic Method,
                    calculates pair wise interaction
pair_coeff    * * Cu_zhou.eam.alloy Cu //energy between two atoms is taken from the given
                    potential file

# Energy Minimization
minimize     1.0e-9 1.0e-6 1000 1000 //brings atoms to minimum energy state

```

```

fix 23 all nvt temp 10 10 0.01 //fixes temperature for energy minimization of atoms
run 1000

compute csym all centro/atom fcc
compute peratom all pe/atom

variable tmp equal ly
variable lo equal ${tmp}
variable strain equal (ly-v_lo)/v_lo

variable p1 equal "-pxx/10000"
variable p2 equal "-pyy/10000"
variable p3 equal "-pzz/10000"

variable p12 equal "-pxy/10000"
variable p23 equal "-pyz/10000"
variable p13 equal "-pxz/10000"
variable fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress
variable fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-
v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" #####Von Mises Stress

variable t equal "v_fm/v_fv"
variable fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm))-(v_p12)^2*(v_p3-v_fm)-
(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-
v_fm)+2*v_p12*v_p23*v_p13)#####Deviatoric Von Mises stress

# principal stresses

variable I1 equal "(v_p1+v_p2+v_p3)"
variable I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-
(v_p23)^2-(v_p13)^2"
variable I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-
((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"
variable A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2))+27*(v_I3))/(2*((v_I1)^2-
(3*(v_I2)))^(3/2))))/3"

variable s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"
variable s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"
variable s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermos 10 //computes and prints thermodynamic data after every 10 timesteps
thermo_style custom step temp vol press pekeetotal

```

```

dump      1 all custom 50 Cu_defect_horizontal_tensile_10K.lammpstrjid type x y z
//dumps a snapshot of atom quantities every 50 timesteps to the specified file
dump      2 all cfg 10000 Cu_defect_horizontal_tensile*.cfg id type xsyzszc_csym
c_peratom

#dump     3 all custom 50000 stress_peratom* id type x y z c_1[1] c_1[2] c_1[3] c_1[4]
c_1[5] c_1[6]

log       NVTlog_compress_al.data

velocity  all create 10 873847 rot yes mom yes distgaussian

# tensile deformation

fix       2 all deform 1 y erate 0.0001 units box //application of tensile deformation
force of 0.0001ps-1

fix       3 all print 10 "${strain} ${p2}" file
stress_strain_data_Cu_defect_horizontal_tensile_10K//gives the stress-
strain data

# temperature controller

fix       1 all nvt temp 10 10 0.01 //fixes the temperature (10 K)and pressure of the
givesystem
fix       def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}" file
Cu_defect_horizontal_tensile_von.txt

run       6000000 //number of iterations

```

6. Results and Discussions

6. Results and Discussions

MD simulation tensile studies on defect and defect free Cu single crystals are presented below.

6.1 Perfect Crystal at 10K

The stress-strain curve for the perfect crystal sample after tensile loading simulation at simulation temperature of 10K is as shown below.

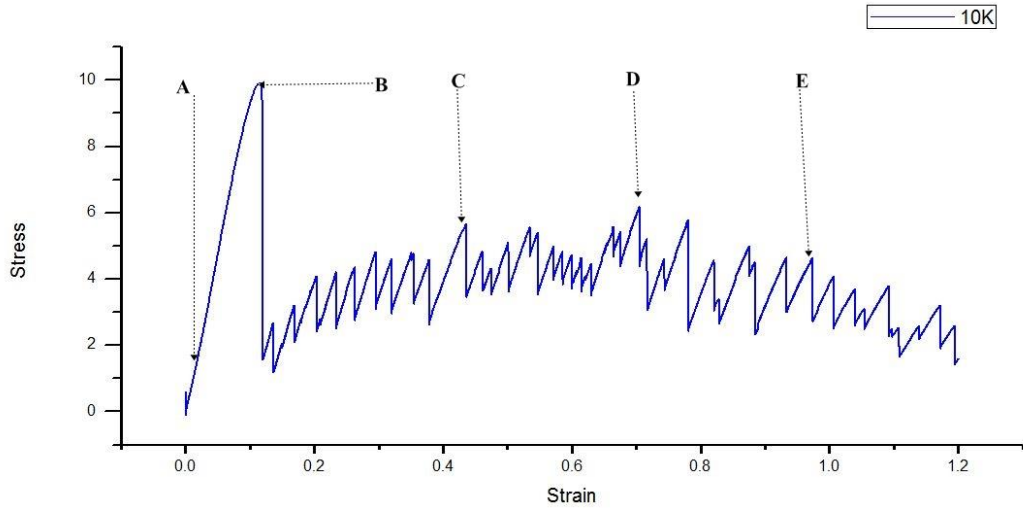


Fig.6.1

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.115. The region after the yield strain of 0.115 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%.

Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

At point A:

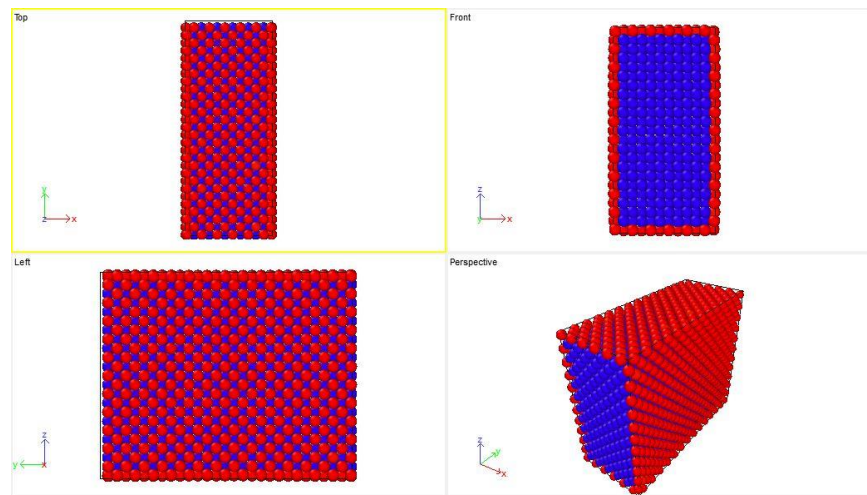


Fig 6.2 Atomic position snap shots of the perfect Cu single Crystal

At point B:

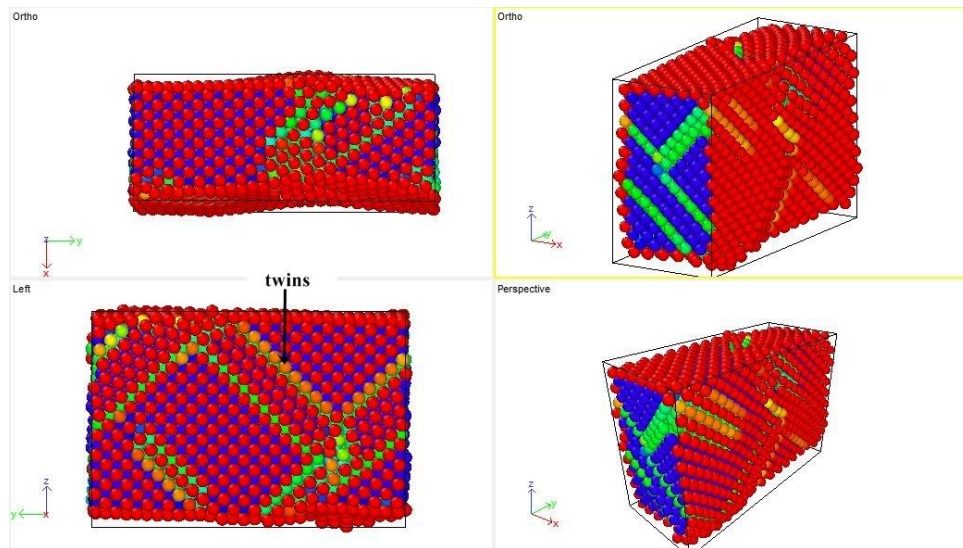


Fig 6.3

The formation of twins can be significantly seen. The fall in the curve represents deformation by twinning.

At point C:

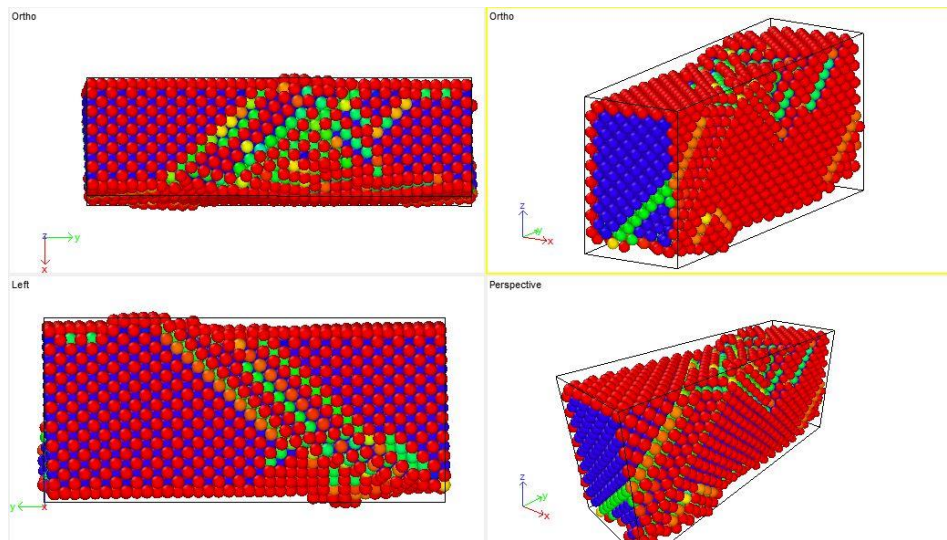


Fig 6.4

The formation of twins can be seen. The drop in the stress-strain curve represents plastic deformation by twinning

At point D:

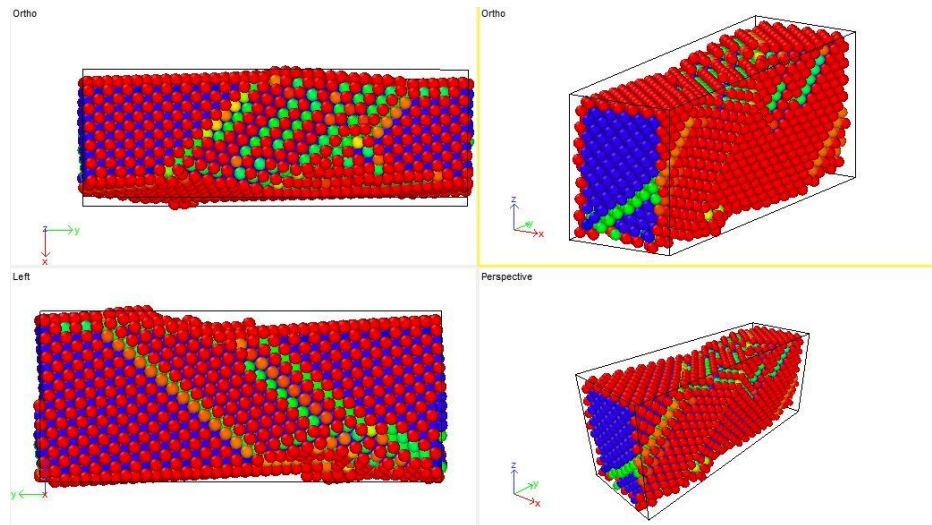


Fig 6.5

At point E:

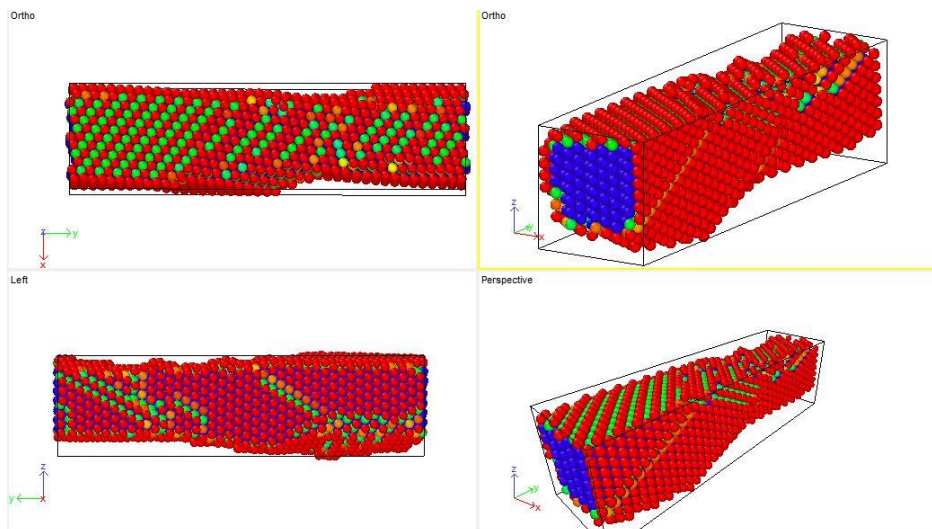


Fig 6.6

Elongation continues further with development of twin regions.

6.2 Perfect Crystal at 50K

The stress-strain curve for the perfect crystal sample at simulation temperature of 50K is as shown below.

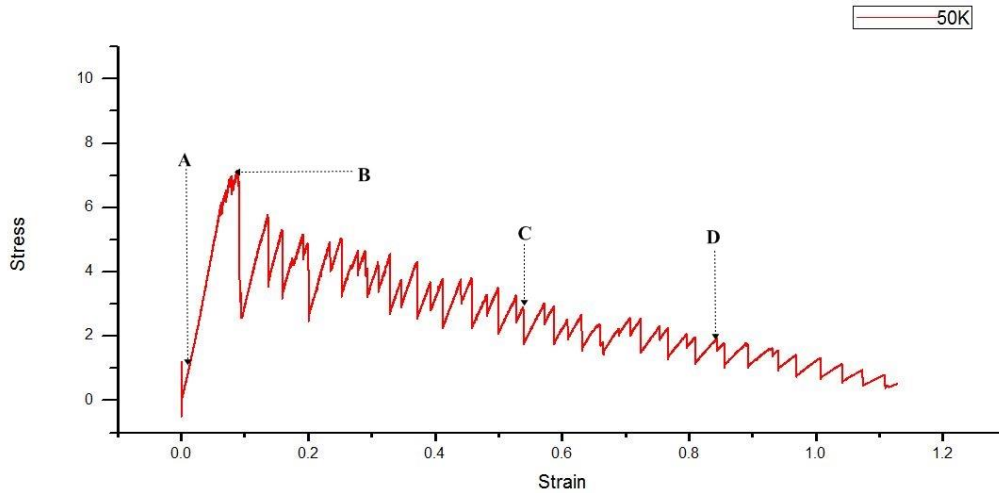


Fig 6.7

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.087. The region after the yield strain of 0.087 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%. Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

At point A:

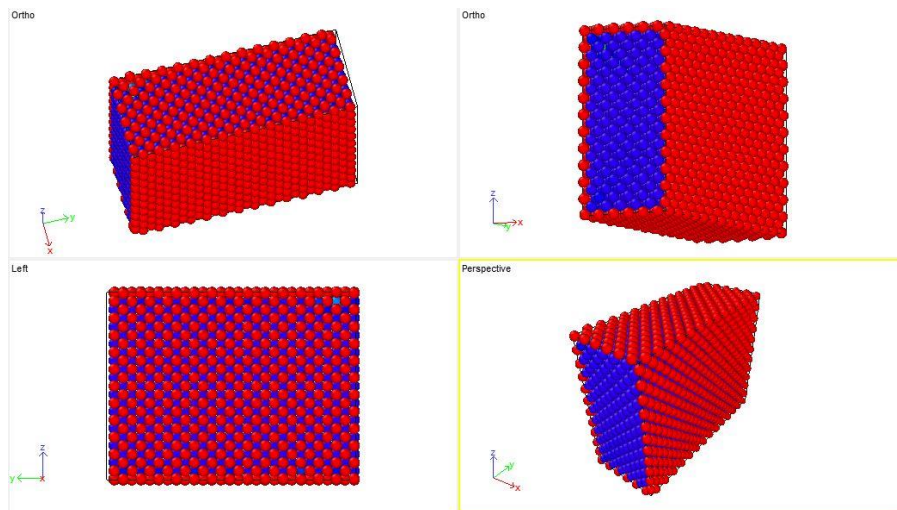


Fig 6.8 Atomic positions snap shots of perfect crystal at 50K

At point B:

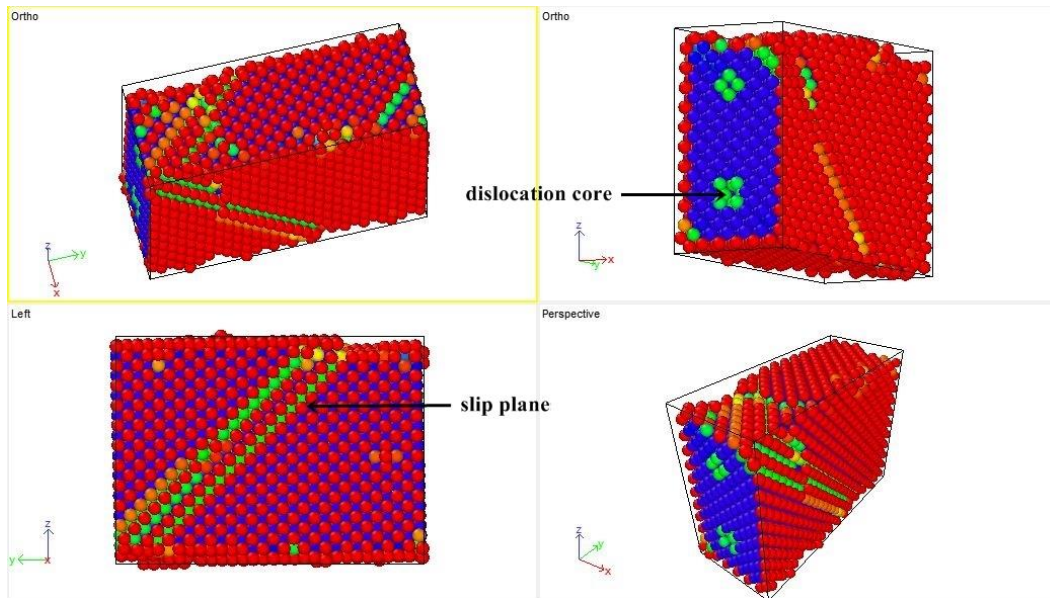


Fig 6.9

Formation of slip planes emanating from various dislocation cores in the crystal. Each fall in the curve represents movement of dislocation.

At point C

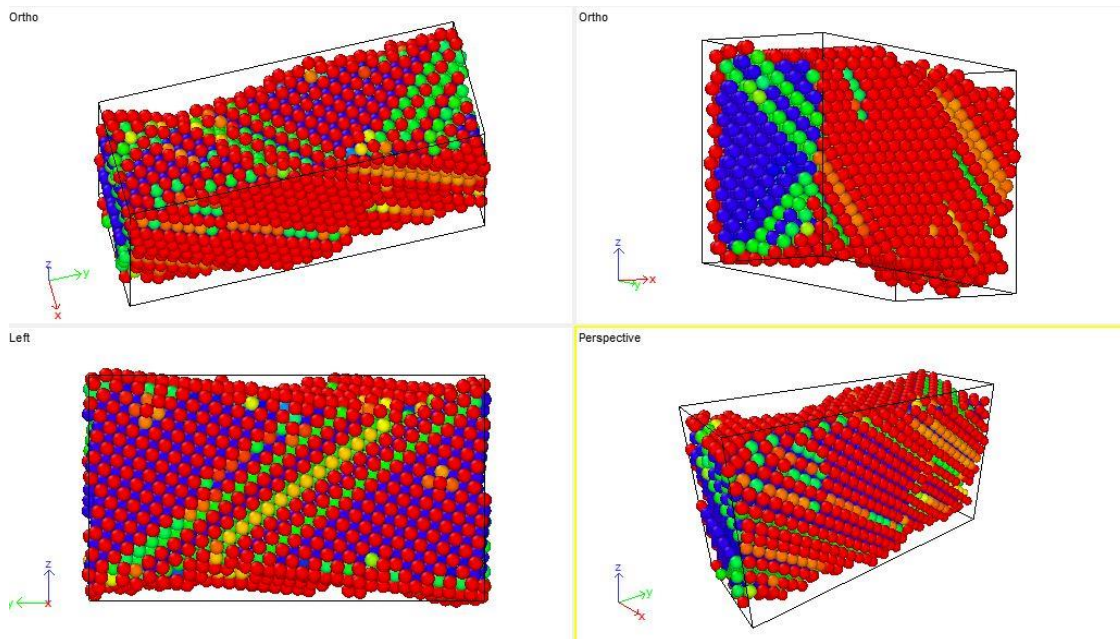


Fig 6.10

Elongation continues further with development of twin regions.

At point D

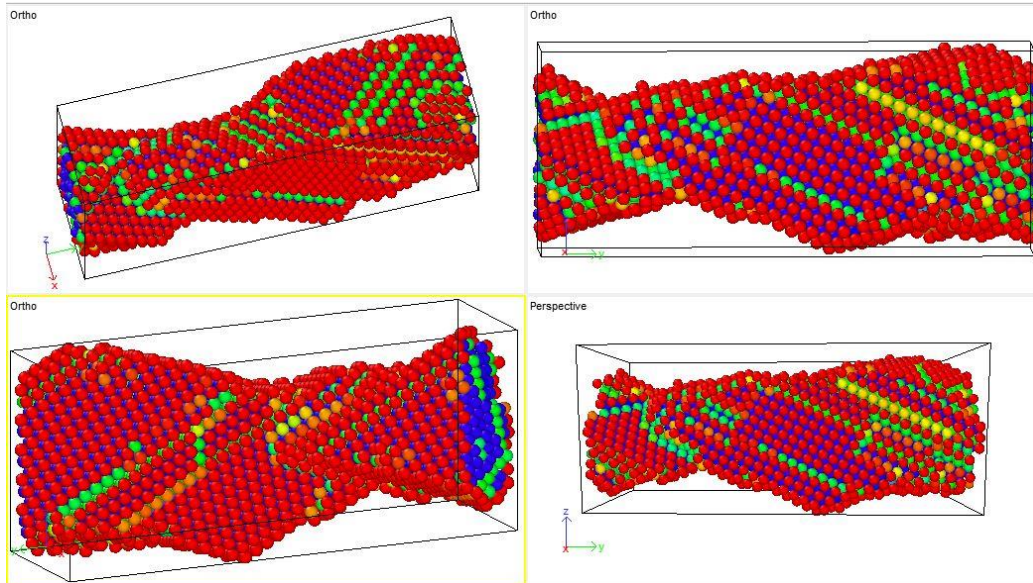


Fig 6.11

Elongation continues further with development of twin regions.

6.3 Crystal with horizontal defect at 10K

The stress-strain curve for the sample with horizontal defect after tensile test simulation at the simulation temperature of 10K is as follows.

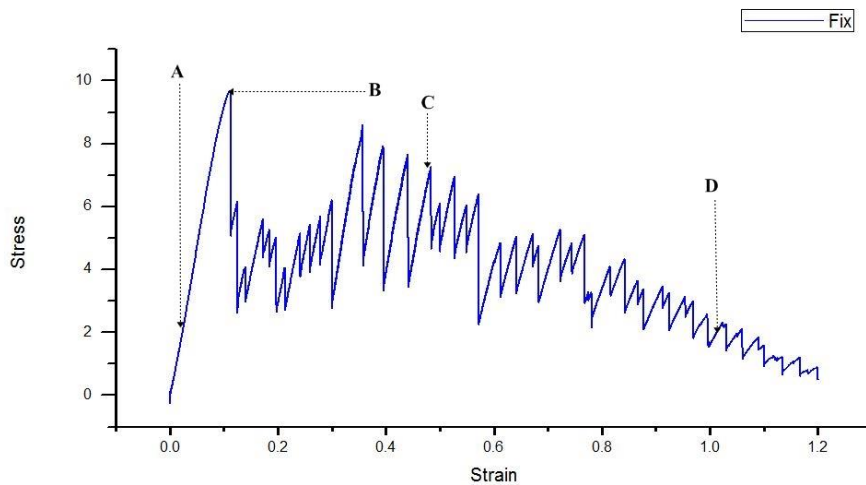


Fig 6.12

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.112. The region after the yield strain of 0.112 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%.

Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

Images of the sample with progress of time as shown in the above graph

At point A:

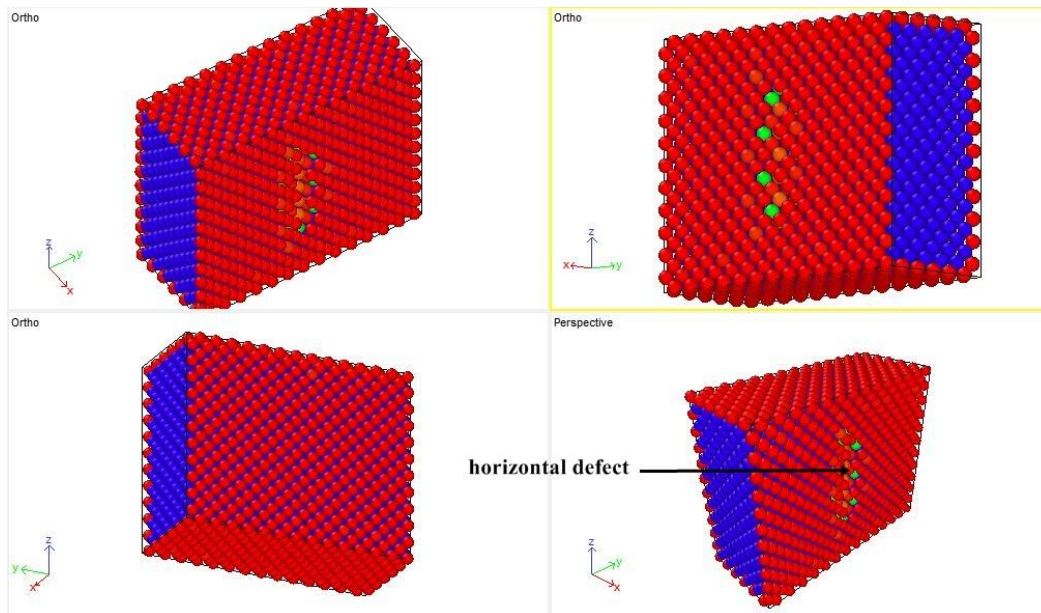


Fig 6.13 Atomic position snap shots of the Cu Crystal with horizontal defect showing the dislocation at 10K

Point B

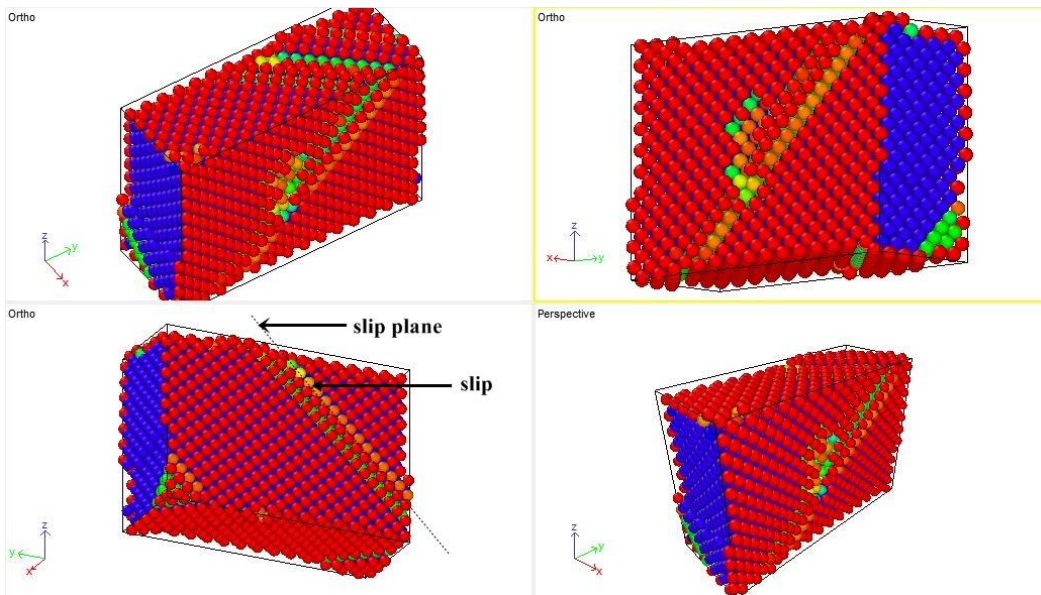


Fig 6.14 Atomic position snap shots of the Cu Crystal with horizontal defect showing the dislocation emanating from the edge of horizontal defect. slip plane is indicated by arrow

Point C:

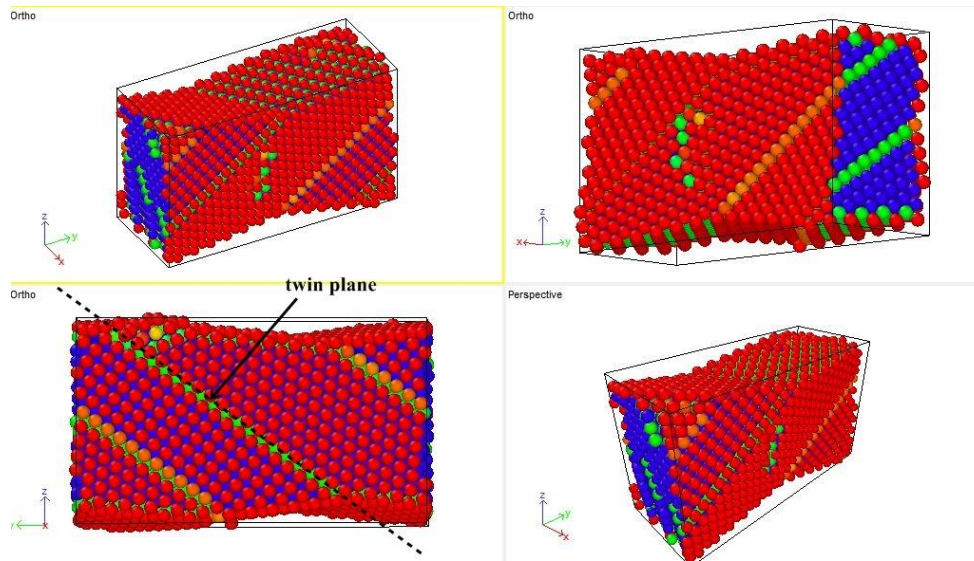


Fig 6.15

The formation of twins with twin planes can be seen significantly. The fall in the curve represents deformation by twinning.

Point D:

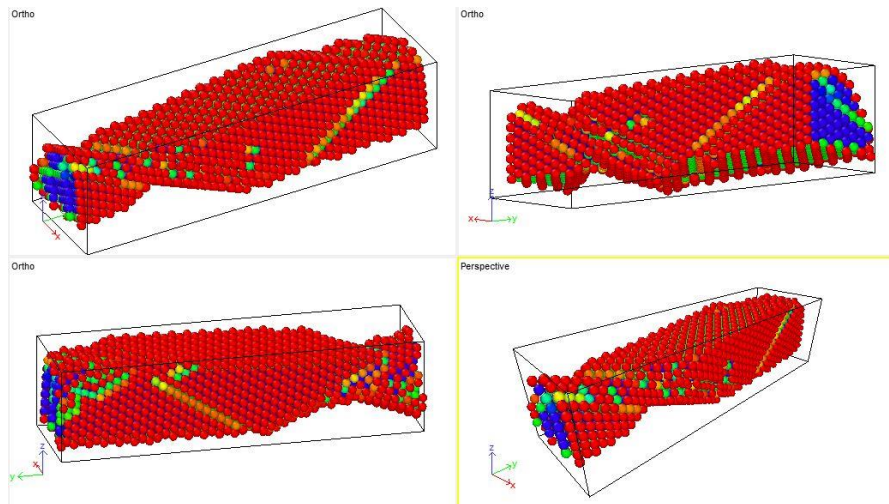


Fig 6.16

Elongation continues further with development of twin regions.

6.4 Crystal with horizontal defect at 50K

The stress-strain curve for the sample with horizontal defect after simulating at the temperature of 50K is shown below.

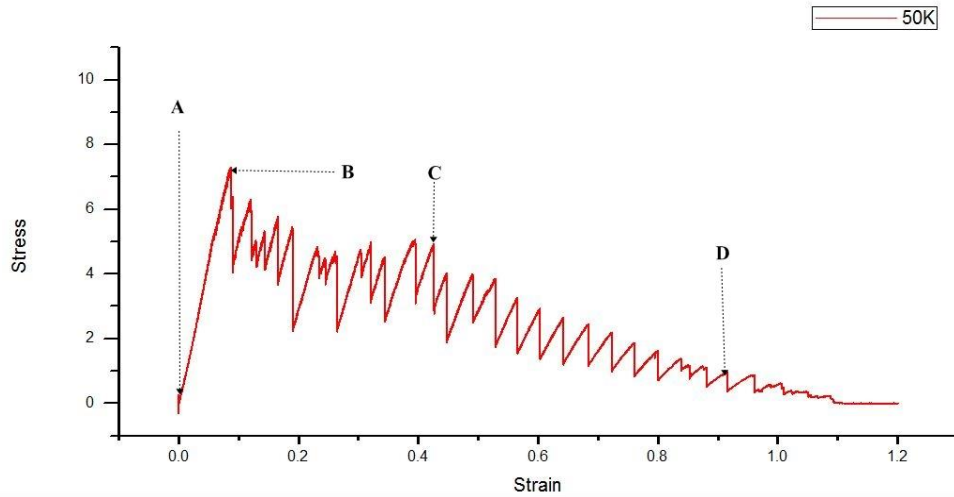


Fig 6.17

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.086. The region after the yield strain of 0.086 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%. Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

At point A:

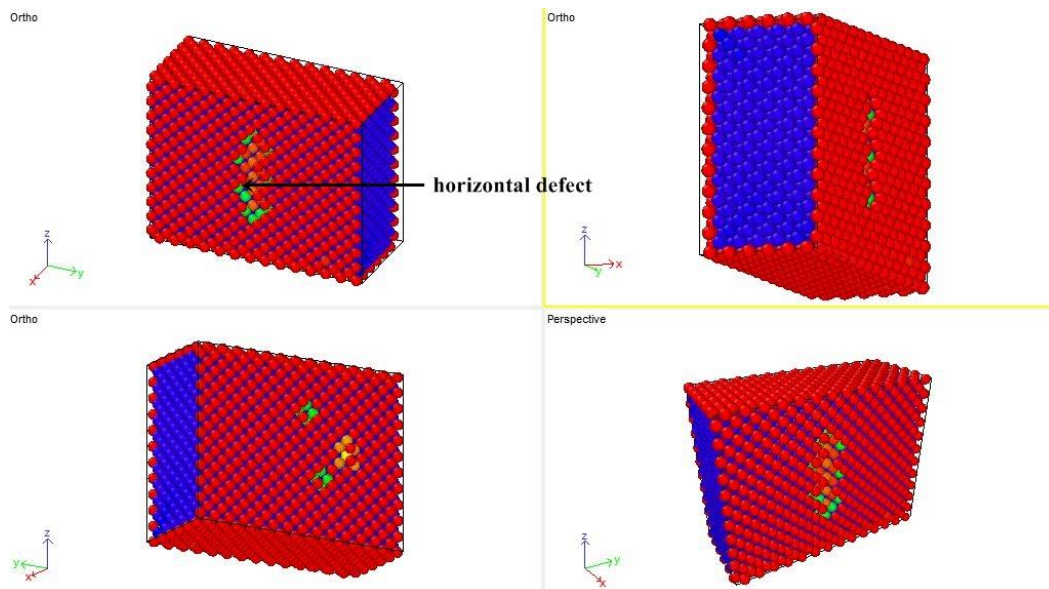


Fig 6.18 Atomic position snap shots of the Cu Crystal with horizontal defect showing the dislocation at 50K

At point B

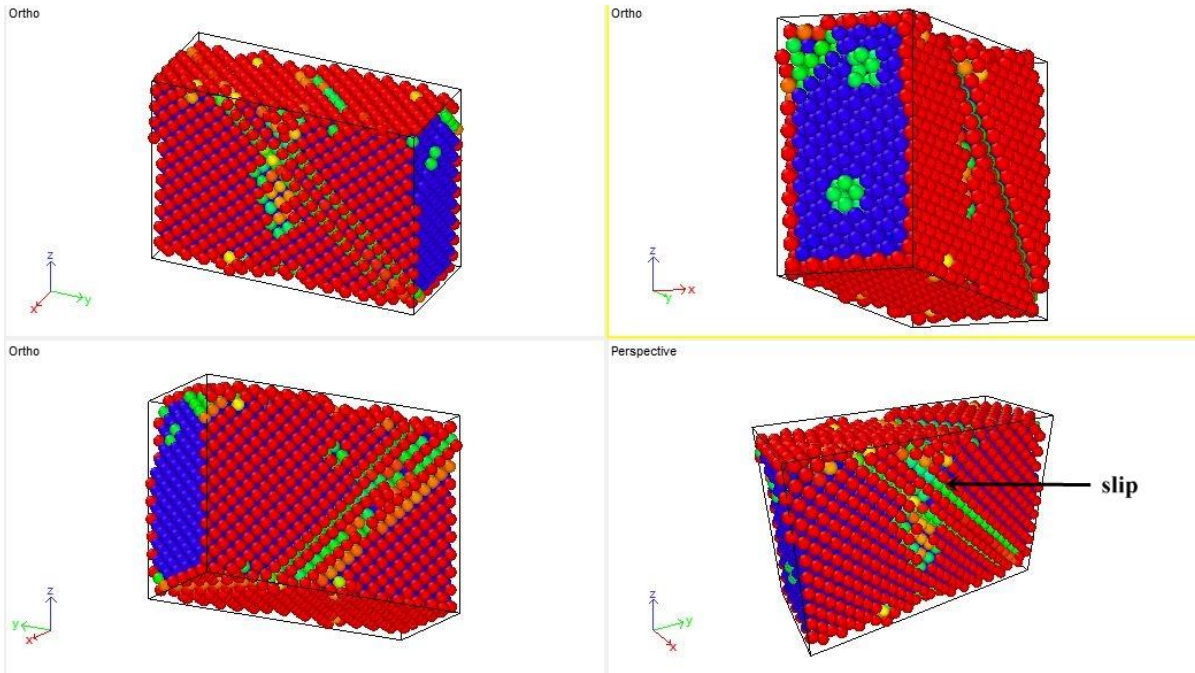


Fig 6.19 Atomic positions snap shots of the Cu Crystal with horizontal defect showing the dislocation emanating from the edge of horizontal defect

At point C

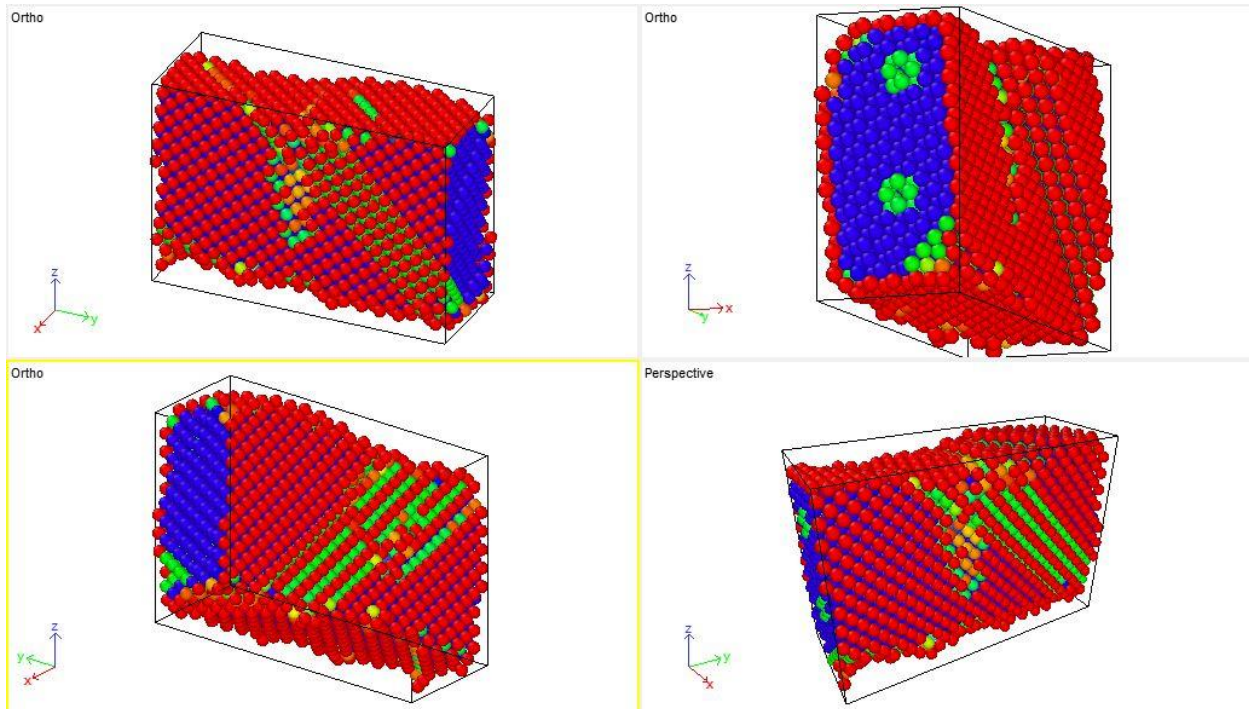


Fig 6.20

Elongation continues further with development of twin regions

At point D

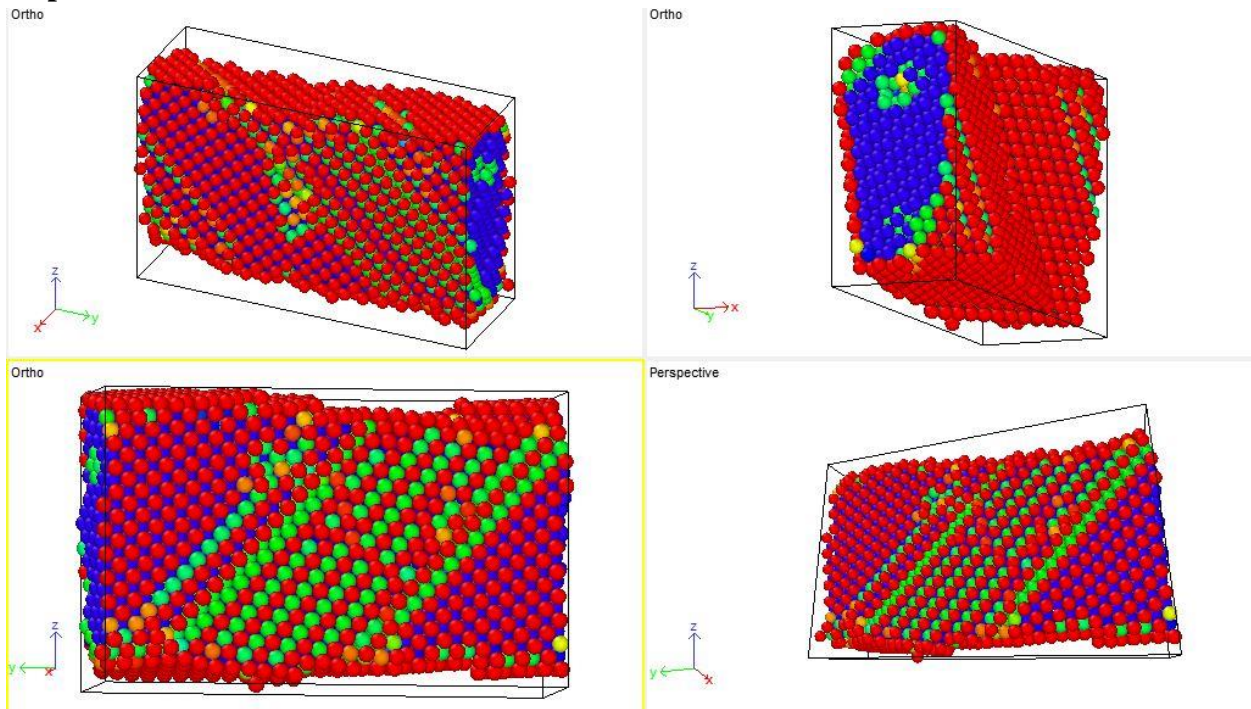


Fig 6.21

Elongation continues further with development of twin regions

6.5 Crystal with vertical defect at 10K

The stress-strain curve for the sample with vertical defect after simulating at a temperature of 10K is as follows.

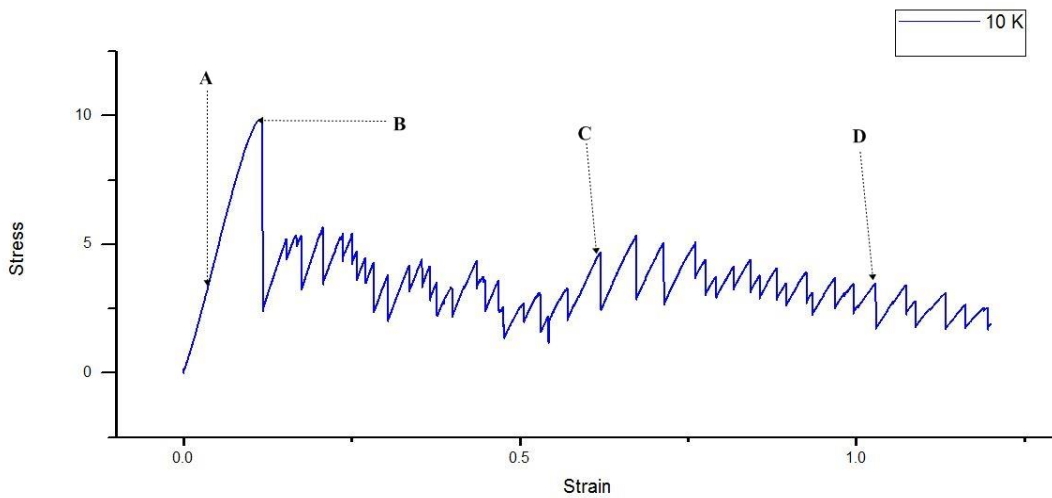


Fig 6.22

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.114. The region after the yield strain of 0.114 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%. Atomic position snapshots corresponding to the different regions of the stress- strain curve are shown below.

Atomic position snapshots corresponding to the different regions of the stress- strain curve are shown below.

At point A:

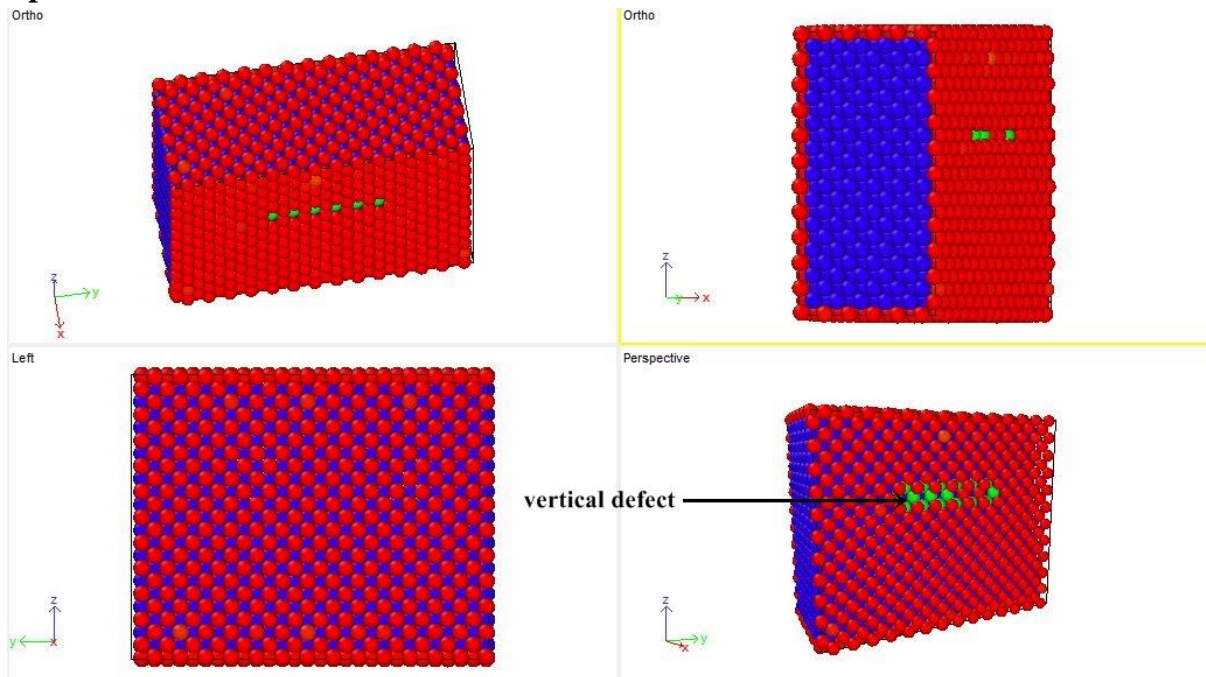


Fig 6.23 Atomic position snapshots of the Cu Crystal with vertical defect showing the dislocation at 10K

At point B

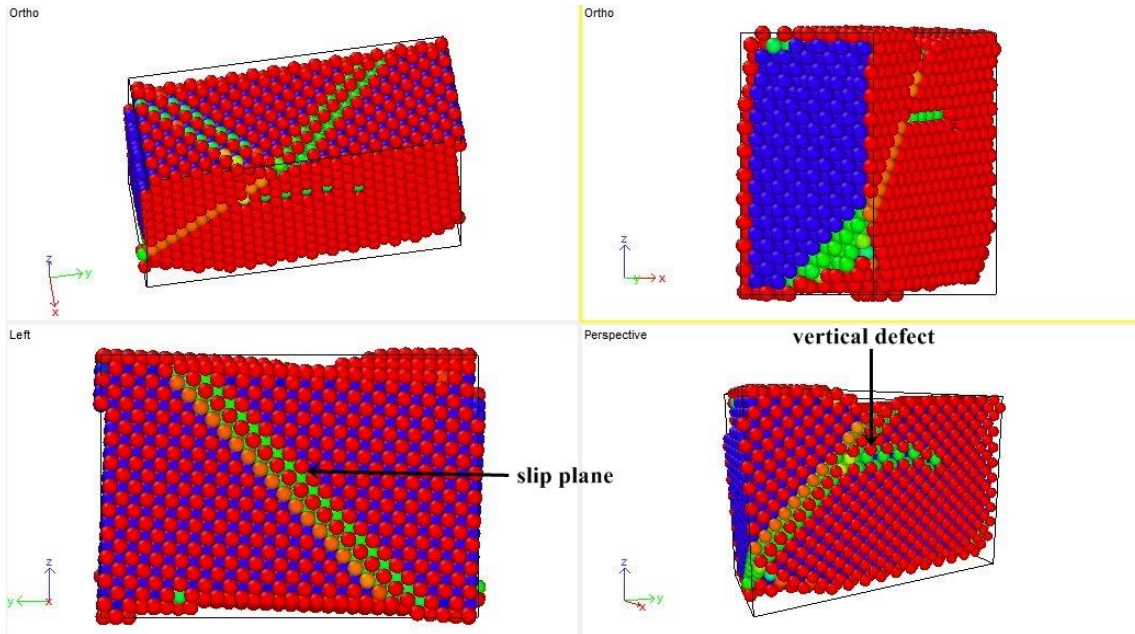


Fig 6.24 Atomic positions snap shots of the Cu Crystal with vertical defect showing the dislocation emanating from the edge of the vertical defect

At point C

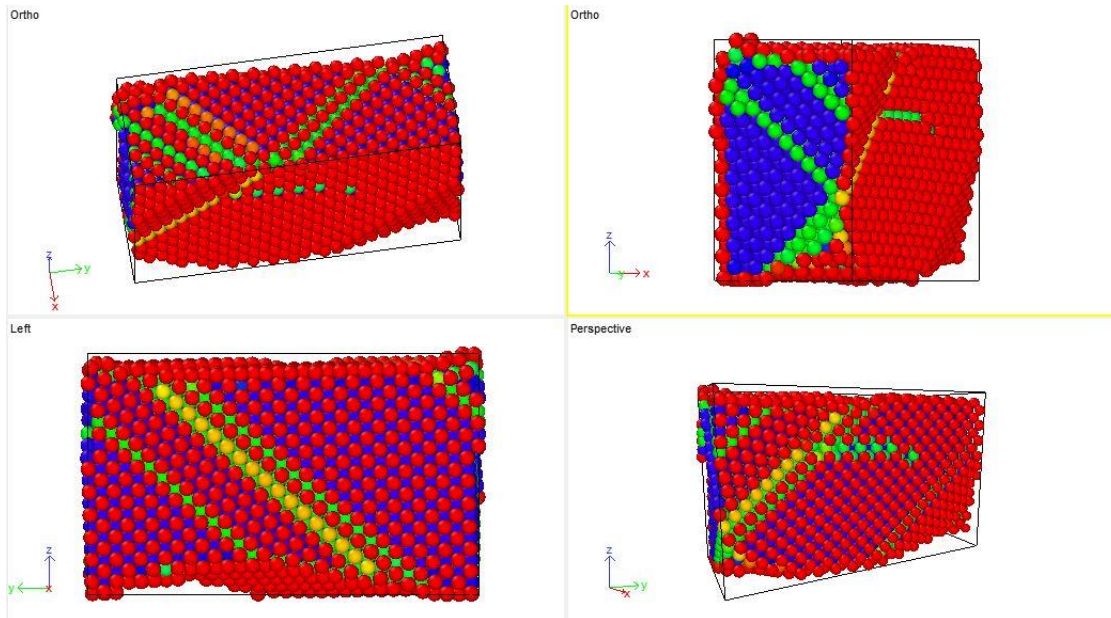


Fig 6.25

The formation of twins with twin planes can be seen significantly. The fall in the curve represents deformation by twinning.

At point D

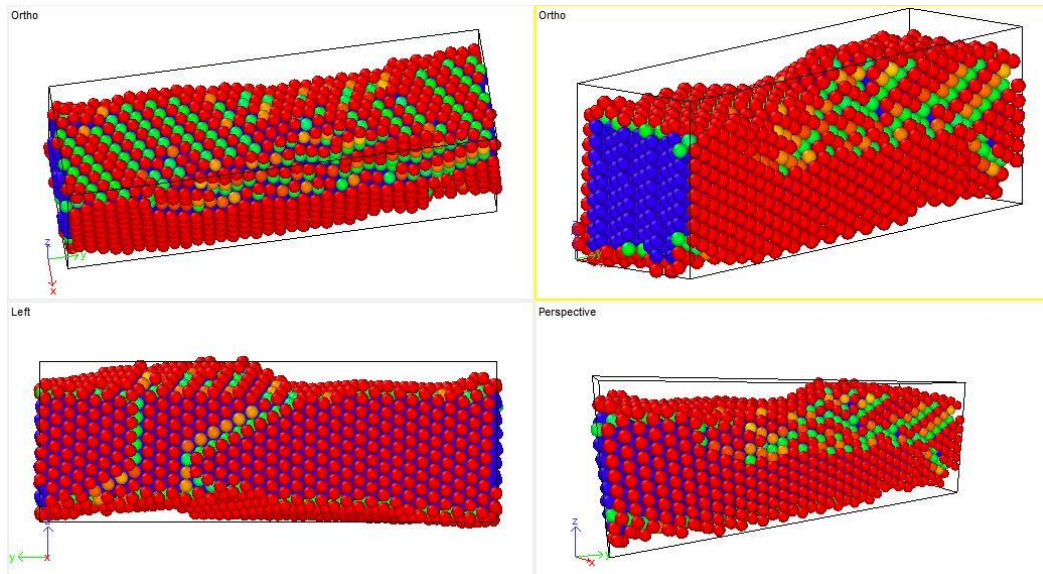


Fig 6.26

Elongation continues further with development of twin regions

6.6 Crystal with vertical defect at 50K

The stress-strain curve for the vertical defect sample after the tensile test simulation at a temperature of 50K is shown below.

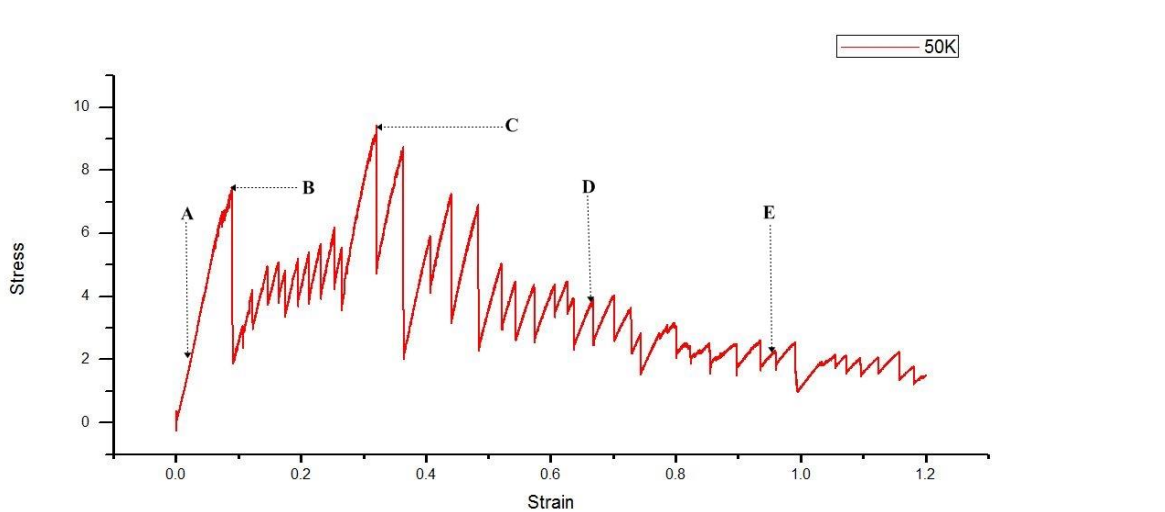


Fig 6.27

The graph shows two regions i.e. the elastic portion and the plastic region. As it can be seen from the plot, the yielding starts after a strain of 0.089. The region after the yield strain of 0.089 is the plastic region. The material did not undergo fracture even after loading to a strain of 120%.

Atomic position snap shots corresponding to the different regions of the stress- strain curve are shown below.

Images of the sample with progress of time as shown in the above graph

At point A:

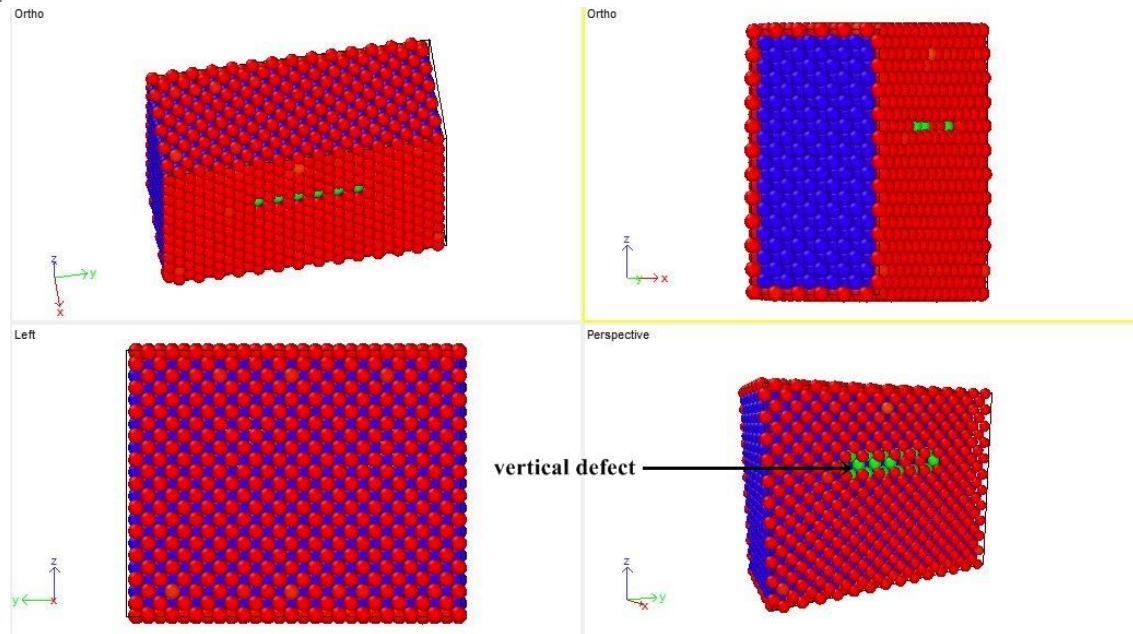


Fig 6.28 Atomic position snap shots of the Cu Crystal with vertical defect showing the dislocation at 50K

At Points B:

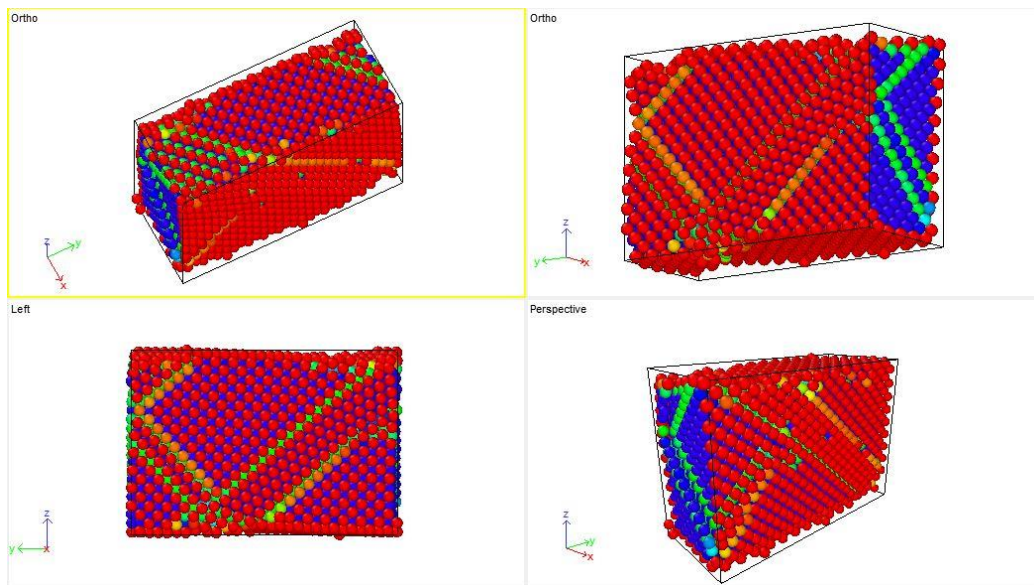


Fig 6.29

The formation of twins with twin planes can be seen significantly. The fall in the curve represents deformation by twinning.

At point C:

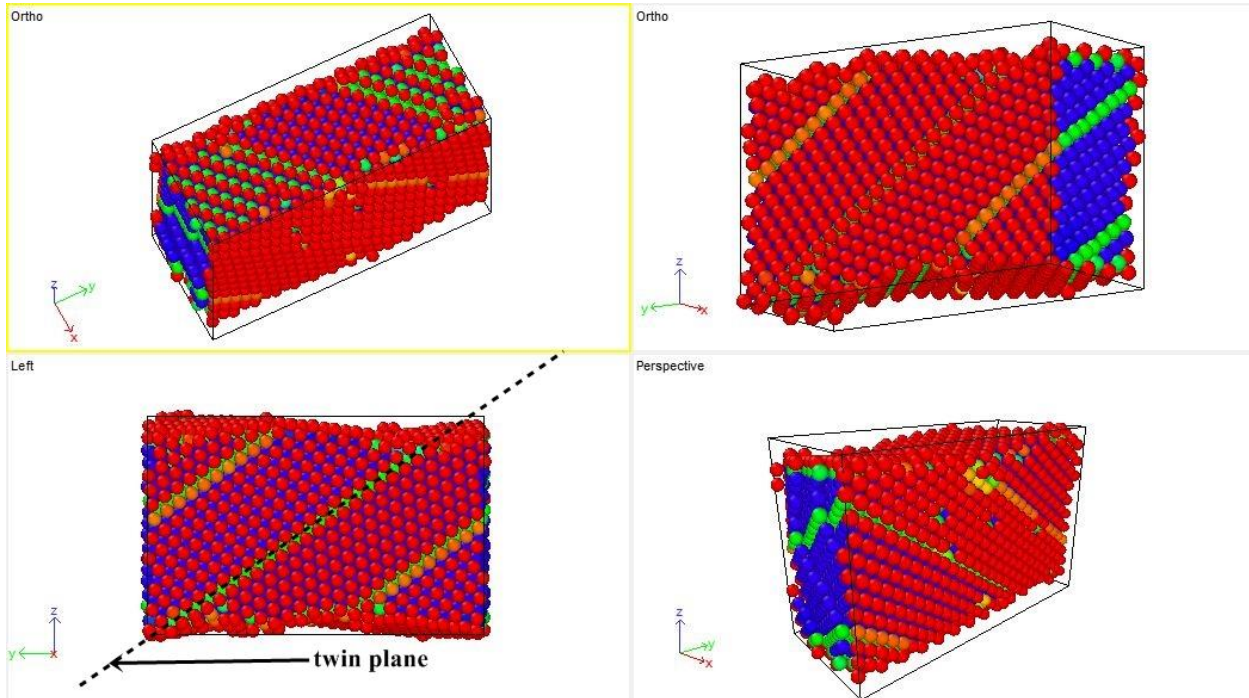


Fig 6.30

The formation of twins with twin planes can be seen significantly. The fall in the curve represents deformation by twinning.

At point D:

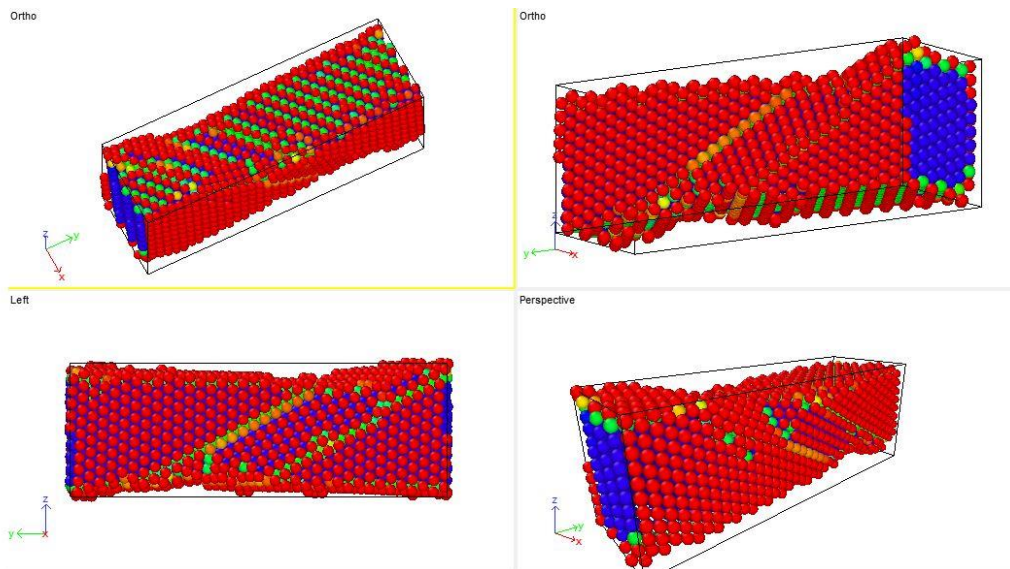


Fig 6.31

Elongation continues further with development of twin regions

At point E

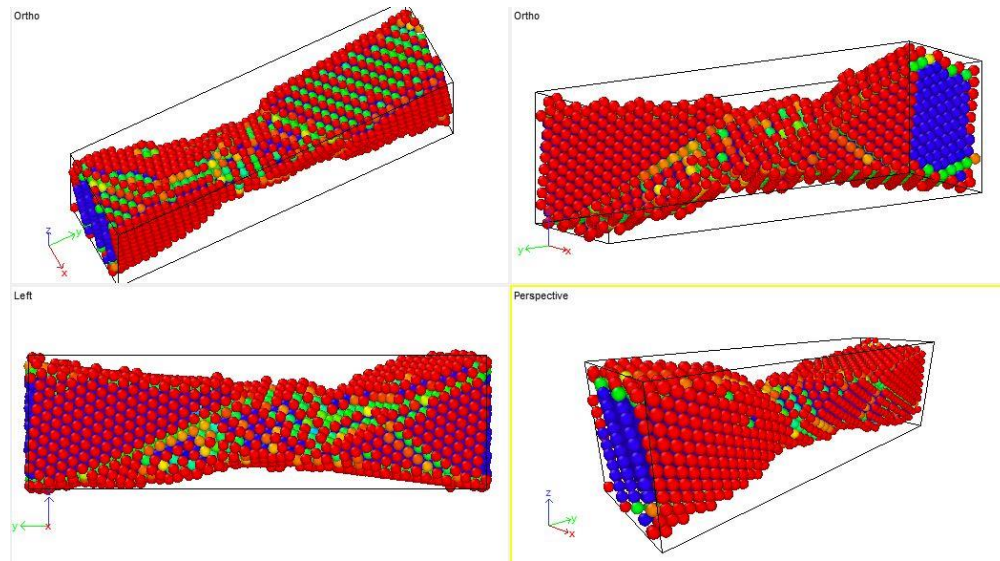


Fig 6.32

Elongation continues further with development of twin regions

6.7 Variation with defect

6.7.1 At 10K

The table below shows the values of the results obtained after the tensile test simulation for elastic moduli, yield strengths and ultimate tensile strengths for perfect crystal, crystal with horizontal defect and crystal with vertical defect at the simulation temperature of 10K.

Table 6.1

Defect type	Elastic Modulus in GPa	Yield Strength in GPa	Ultimate tensile Strength in GPa
Perfect	112.098	9.916	9.916
Horizontal	99.080	9.670	9.670
Vertical	101.709	9.8707	9.8707

The elastic modulus is calculated by calculating the slope of the linear region of the stress-strain curves drawn based on the data obtained after the simulation. It can be seen from the values obtained at a temperature of 10K that the elastic modulus obtained for perfect crystal is 112.098 which is higher than those obtained for crystals with defects. The crystal with horizontal defect shows the least value among the 3 kinds of samples taken for simulation while the crystal with vertical defect shows a slightly greater value than the crystal with horizontal defect.

The yield strength is given by the value of stress at the point where the first drop is seen in the stress-strain curves plotted. The perfect crystal sample shows the highest value of yield stress among the three samples. The sample with horizontal defect shows a yield strength of 9.670 which is the least among the three samples.

The Ultimate Tensile Strength (UTS) is given by the highest value of stress in the stress-strain curve plotted. The UTS of the perfect crystal sample is found to be highest which is close to the value obtained in case of sample with vertical defect while the sample with horizontal defect shows the least Ultimate Tensile Strength.

6.7.2 At 50 K

The table shows the values of elastic moduli, yield strength, ultimate tensile strength and fracture strengths for the different samples obtained at 50K.

Table 6.2

Defect type	Elastic Modulus in GPa	Yield Strength in GPa	Ultimate tensile Strength in GPa
Perfect	106.090	7.141	7.141
Horizontal	89.72	7.215	7.215
Vertical	96.090	7.465	9.428

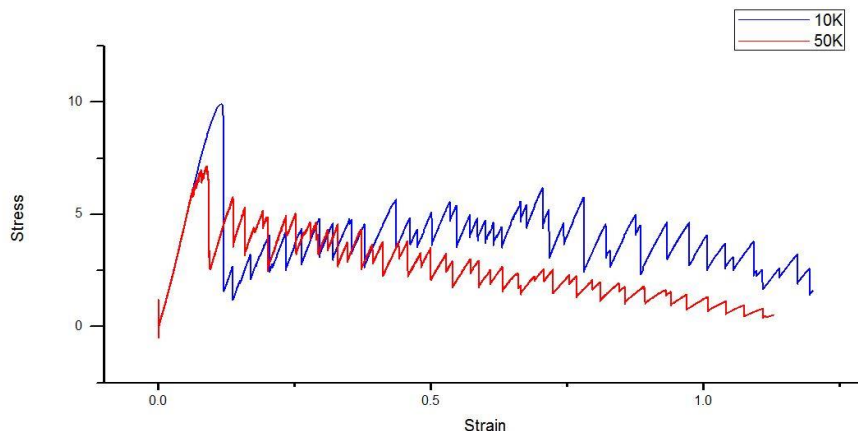
Similar procedure is followed at 50K to obtain the values of elastic moduli, yield strengths and Ultimate tensile strengths of the various samples. At 50K, the modulus of elasticity showed a similar pattern as that at 10K as modulus of elasticity of the perfect sample is found to be the highest among the three with its value for the vertical defect sample being higher than that of the horizontal defect sample.

The yield strengths and Ultimate tensile strengths however showed a different pattern at 50K. The yield strength of the vertical defect sample is highest at 50K and it is least for the perfect crystal sample. The UTS showed a similar pattern of variation as that of yield strength at 50K. Vertical defect sample is found to have the highest UTS i.e 9.428.

6.8 Variation with temperature for each crystal

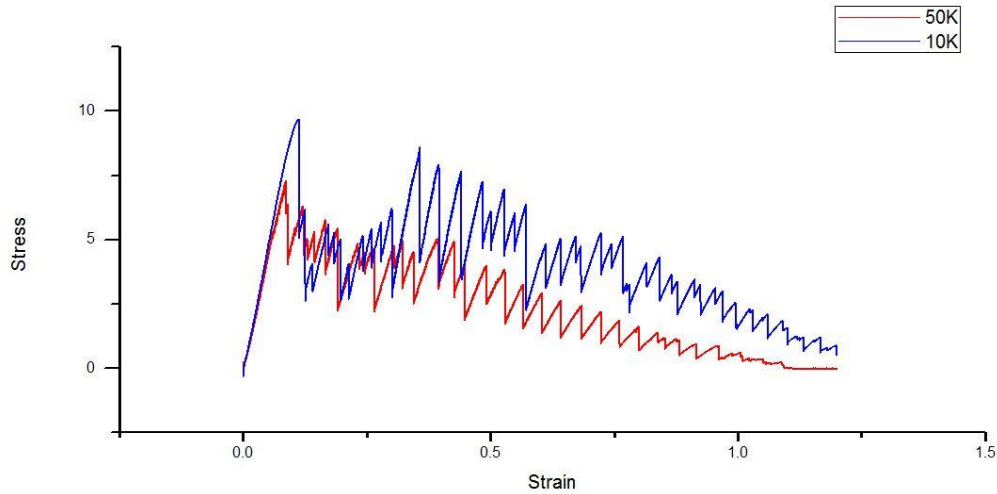
The variation of the modulus of elasticity, yield strength, ultimate tensile strength and fracture strength with temperature for a particular sample is also studied.

6.8.1 Perfect Crystal



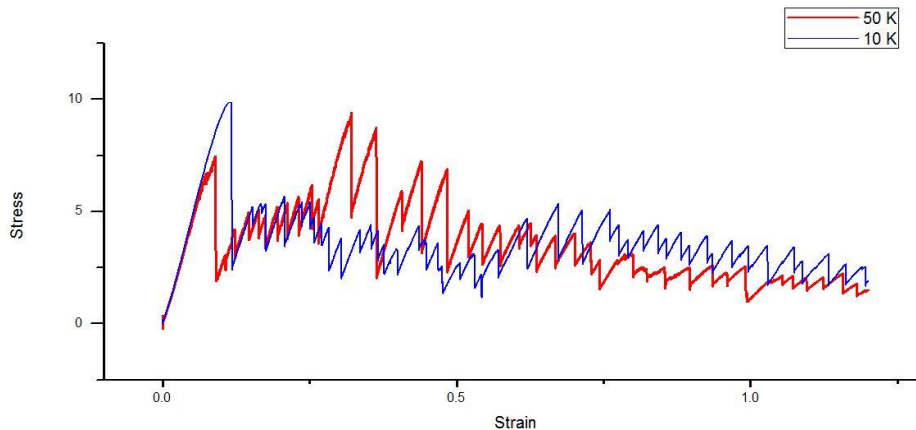
In case of the perfect crystal there is a significant drop in the values of the above mentioned when the temperature of simulation is increased to 50K from 10K.

6.8.2 Horizontal defect



A similar trend in data is observed for the sample with horizontal defect, i.e with increase in simulation temperature there is a prominent drop in the values of elastic modulus, yield strength and ultimate tensile strength.

6.8.3 Vertical Defect



In case of sample with vertical defect, the same trend is observed too. The values of the parameters calculated are seen to decrease with an increase of temperature of simulation.

Thus it can be generalized for a given sample, the values of elastic of modulus, yield strength and ultimate tensile strength decrease with an increase of temperature at which the tensile test simulation is done. As temperature increases, the inter-atomic bond strengths decrease and it leads to softening of the material. Softening of the material leads to decrease in yield strength and ultimate tensile strength.

7. Conclusions

Based on the MD simulation done on the Cu single crystal with various surface defects at strain rate of 0.0001ps^{-1} and temperatures of 10K and 50K, the following conclusions were drawn

- 1) The dominant deformation mechanism is by twinning.
- 2) The defects act as a source of dislocations.
- 3) The presence of defects lowers the Yield Strength and Ultimate strength of Cu single crystal specimens.
- 4) Young's Modulus, Yield Strength and Ultimate strength decrease with increase in temperature from 10K to 50K for all specimens.

Scope for future work

1. Indexing the slip planes and directions.
2. Dislocation reactions in the crystal during deformation.

8. References

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