DEFORMATION BEHAVIOR OF RADIATION DAMAGED NANO COPPER SINGLE CRYSTAL: A MOLECULAR DYNAMICS SIMULATION STUDY

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by

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under the guidance and supervision of
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May 2016

Supervisor's Certificate

This is to certify that the work presented in this dissertation entitled **"Deformation Behavior of Radiation Damaged Nano Copper Single crystal:A Molecular Dynamics gSimulation Study"** by **"Krishna Chaitanya Katakam"** Roll No. **214MM2499** is a record of original research carried out by him under my supervision and guidance in partial fulfilment of the requirements of the degree of **Master of Technology** in the **Department of Mechanical Engineering**. Neither this dissertation nor any part of it has been submitted for any degree or diploma to any institute or university in India or abroad.

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Prof. Natraj Yedla

DECLARATION OF ORIGINALITY

I, Krishna Chaitanya Katakam, Roll No. 214MM2499 hereby declare that this dissertation entitled "Deformation Behavior of Radiation Damaged Nano Copper Single crystal:A Molecular Dynamics Simulation Study" represents my original work carried out as a postgraduate student of NIT Rourkela and, to the best of my knowledge, it contains no material previously published or written by another person, nor any material presented for the award of any other degree or diploma of NIT Rourkela or any other institution. Any contribution made to this research by others, with whom I have worked at NIT Rourkela or elsewhere, is explicitly acknowledged in the dissertation. Works of other authors cited in this dissertation have been duly acknowledged under the section "References". I have also submitted my original research records to the scrutiny committee for evaluation of my dissertation.

I am fully aware that in case of any non-compliance detected in future, the Senate of NIT Rourkela may withdraw the degree awarded to me on the basis of the present dissertation.

Place: NIT Rourkela Krishna Chaitanya Katakam

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ABSTRACT

This project work presents a Molecular dynamics(MD) simulation study on radiation damage of Nano copper single crystal and its effect on the deformation behavior and underlying deformation mechanism. At first, perfect Nano copper models will be created using MD simulations. Then the models will be subjected to radiation and the damaged samples will be tested for mechanical characterization by tensile studies at a temperature 300K and strain rate 10^{10}s-1. The MD simulation was performed by using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). In this, we studied Irradiated Nano copper-cascade interactions caused by 0.2KeV to 3KeV primary knock-on atoms (PKA) respectively. We found the displacement of atoms(dpa) from its lattice structure that caused for the creation of various defects within the lattice structure. The mechanical properties of the Irradiated Nano copper single crystal are analyzed and both the elastic properties and yields under tension is analyzed. Defects like point(vacancy) and stacking faults, appears in the irradiated Nano copper depending on the incident energy. The Young modulus is significantly reduced by the incident irradiation energy, and the reduction magnitude depends on the vacancy number, which is determined by the incident radiation energy. The mechanism for these changes are also discussed.

Keywords: Molecular dynamics simulation, Irradiation damage, defects, Mechanical properties, Yield phenomenon.

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Introduction

1.1 Background

Radiation is the energy that generates from a source and travels through some matter or through space. Light, heat and sound are types of radiation and the ionizing radiation is produced by charged particles(ions) in matter. Ionizing radiation is produced by unstable atoms. Unstable atoms are different from that of the stable atoms and these unstable atoms have excess energy or mass or even both. To reach the stable position, these unstable atoms release or emits the excess energy or mass and these emissions are called as radiation[1] In the present environment we can observe the particles with kinetic energy greater than 1.0eV, and they exist in nature because of cosmic radiation that are generated from the manmade devices for his application. In the application side, ion implantation is one of the important technologies in the manufacturing of silicon chips and in treating cancer, electron accelerators are used. In the Nuclear reactors metals like copper, iron, nickel, zirconium, magnesium, and titanium are continuously subjected to different types of radiations like alpha, gamma, beta and neutrons. Some of these radiation causes significant damage to the crystalline structure of metals. Nuclear radiation having large amount of energy that strikes over the highly localized areas of metals. Due to this high radiation interactions, crystal structure is totally modified that results changes in the mechanical properties of metals. We can understand that the change of crystal structure starts with the displacement of atoms from its initial lattice site (vacancy) creating an atom at an interstitial site in front. This kind of defect formation generally takes place and at instance defect clusters, stacking faults, amorphous zones, dislocation loops are formed.

The temperature in a nuclear reactor is as high as 800 to 1000^0C or even more depending on the fission reaction. Due to the fission reactions a huge amount of radiation damage occurs inside the reactor that causes interaction of fission fragments with the nuclear reactor metals. As a consequence, these metals may degrade or fail by cracking, swelling, corrosion, embrittlement, flacking and blistering etc. These radiations induced defects greatly reduces and limit the reactor lifetime and can cause reactor accidents unknowingly. So there is a need to make reactor safer, and to reach the next generation reactors, metals with enhanced radiation tolerance are required. Towards this goal, we need depth understanding on the failure mechanism[24]. Hence our research should not only have limited to measure the macroscopic properties, but our studies need to reach microscopic details, and even atomic levels to design metals that can resist the radiation energy and can exist in that radiation environment. This requires an integration of modeling and experimental studies[5]. Particularly, due to limitation from current characterization tools[21], the knowledge on defect developments at a time scale and spatial scale beyond experiments are largely missing. Driven by this purpose, this thesis works is aimed to develop fundamental understanding by using atomic scale modeling using OVITO[11].

In this work I have irradiated Nano copper single crystal of size $5*10*5nm^3$ with different radiation energies ranging from 0.2KeV to 3KeV followed by tensile deformation. The moto behind this work is to investigate the mechanical properties of the Nano copper at different radiation energies. The mechanical properties of irradiated Nano copper, like Young modulus and

maximum tensile strength and yield stresses have not been quantitatively studied. It is observed that the properties of Nano copper are greatly influenced by defects[19], and the irradiation can induce various defects in Nano copper[6]. Therefore, we are using PKA to irradiate the Nano copper, and the effect of radiation on the mechanical properties should be considered. Till now, extensive studies have been done for understanding the deformation mechanisms of un-irradiated nanowires and their failure mechanisms of various metals[24] and nanotubes[18], and it is recognized that there is a lack of theoretical studies of the effect of irradiation on properties of Nano copper, and this is a subject that clearly needs additional theoretical and computational work.

1.2 Research objectives

(a) Inducing radiation to Nano copper single crystal at different radiation energies.

(b) Tensile deformation studies of the different radiation damaged samples at a particular strain rate and temperature to investigate the Mechanical properties.

(c) Using OVITO software, defect analysis should be done on the radiation damaged Nano copper samples to investigate different defects like vacancies, dislocations and stacking faults that occur during radiation and tensile deformation.

2. Literature Review

2.1 Introduction

Radiation is the energy that occurs from a source and travels through some material or through space. Irradiation is the exposure to penetrating radiation and this occurs when all or part of the body is exposed to radiation from an unshielded source. Interaction of high energy radiation particles like photons, neutrons, electrons etc. with crystalline materials causes the radiation damage in the displacement cascade. The damage and its consequence with time determine the macroscopic response of a material to radiation and this damage production can be divided into 2 categories as:

1. The Primary radiation damage that is formed immediately after radiation(within few picoseconds) by the impact of PKA/ion/electron/neutron to irradiated sample[28].

2. Radiation damage evolution caused by thermally activated process last for long period and is called as Long-time scale (nanoseconds to years).[28]

The radiation damage from neutron/electron was proposed by Norgett, Torrens and Robinson (NRT) in 1975 to evaluate the No. of Frankel pairs formed for a given energy transfer to the primary knock-on atom(PKA)[22] and that results in the number of "displacement per atom" (DPA).

In the present world energy from nuclear reactors, which currently provides 13 to 15% of the worlds electricity taking advantage of the fission of uranium nuclei by neutrons, material degradation associated with neutron irradiation damage is one of the important factor. Interaction of this high energy particles with materials results in the formation of defects[26]. We can understand that an atom can be displaced from its initial lattice site (or vacancy) behind and creating an atom at an interstitial site in front. This kind of defect formation generally takes place and at instance defect clusters, amorphous zones, dislocation loops or 3-D defects etc. are formed.

In a thermal nuclear reactor, under normal operating conditions the fuel center can reach a temperature as high as 800 to 1000^0C. A huge amount of radiation damage occurs inside the fuel due to interaction of fission fragments, alpha, beta and gamma rays and neutrons. The fission fragments have a kinetic energy of 170MeV and the neutrons have a typical kinetic energy of 5MeV. Such high level energies significantly alter the micro-structure[4] of the in-core components. As a consequence, these materials have serious degradation including cracking, swelling, embrittlement, corrosion, blistering and flacking etc. These radiations induced defects greatly limits the reactor lifetime and can cause reactor accidents. So for a better energy electricity conversion there should be some advancements in the design of reactors and reactor materials for safety operation and also for a longer life time.

Driven by the need to make reactor safer, and to reach the next generation reactors, materials with enhanced radiation tolerance are needed. Towards this goal, we need to develop in depth understanding on the failure mechanism. Not limited to measure the macroscopic properties, studies need to reach microscopic details, and even atomic levels, to develop understanding necessary for materials engineering. This requires an integration of modeling and experimental

studies. Particularly, due to limitation from current characterization tools, the knowledge on defect developments at a time scale and spatial scale beyond experiments are largely missing. Driven by this purpose, this thesis works is aimed to develop fundamental understanding by using atomic scale modeling. For this purpose, the MD program LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) will be used to study non-linear damage caused by cluster ions under different conditions. LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers. It was developed at Sandia National Laboratories. It is an open-source code, distributed freely under the terms of the GNU Public License (GPL). The accuracy of MD simulation is directly determined by the interatomic potential used.

2.2 Importance of copper metal in the Nuclear power plants.

In the present scenario, 13 to 15% of world electricity is contributed from nuclear power plants and this percentage is increasing day by day. In the nuclear power plants disposal of nuclear waste or keeping the radioactive waste out of environment is a serious issue and intense research and development has been taking place in many of 32 countries that operate the world's 442 commercial nuclear power plants [4]. The major problem in the commercial nuclear power plants is the disposal of nuclear waste. For the disposal of this nuclear waste a specially designed containers was made. Corrosion resistance is the important property requirement of the materials that are used in the manufacturing of burial containers. Copper plays an important role from this point of view [11]. Important. From the standpoint of selecting a container material [29], scientists have three choices:

1. Materials that can exist in the external environmental conditions without failure.
2. Materials that can form protective surface films, so that properties like corrosion resistance can be improved.
3. Materials that can last for a long period without any kind of degradation of its mechanical properties.

Considering the above conditions copper metal and its alloy plays an important role in the design and manufacturing of burial containers. The corrosion rate of copper and its alloys are known and the abundant evidence of copper's corrosion resistance made it the best choice for the scientists [21] It is proved that 'since decade copper plumbing tubes operates trouble free' and the we also observed the ancient coins made of copper remain intact centuries. Being ductile, copper can easily rolled into thin sheets and fine wires. At low temperatures copper remains ductile and it can tolerate impact type loads without any kind of vibrations. Copper is generally casted, forged and rolled into a variety complex designs. Its's extraordinary mechanical and thermal properties made it to be the suitable candidate for the radioactive waste burial containers. Due to its excellent properties it remains forever without corroding, cracking, permitting radioactive release from a repository into the environment.

2.3 Theory and Background

2.3.1 Introduction to the displacement-per-atom concepts

Displacement per atom concepts can be understood and visualized by a series of elastic collisions initiated when a high energy particle strikes an atom. The initially struck atom is called as the primary knock on atom and simply called as PKA. When this PKA got displaced from its original lattice site, and got occupied at some interior lattice site of atoms creation of vacancies takes place. This also results in the formation of interstitial defects called as point defects. A point defect is formed when the original lattice site remains vacant and this is called vacancy. In this manner PKAs, causes for the creation vacancies and interstitial defects within the lattice. When this interstitial and vacancy remain stable within the lattice it is known as a Frenkel Pair. An illustration of typical PKA event in a simple lattice is given in Fig.2.3.1.

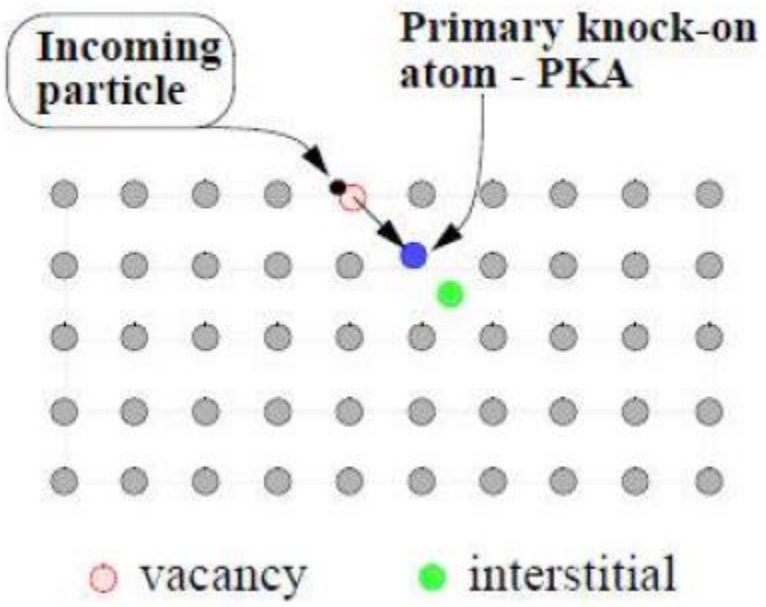


Fig.2.3.1 Mechanism of vacancy and interstitial creation due to primary-knock on atom(PKA)[29]

The displacement cascade theory is proposed on the assumption that an atom in a lattice struck by a PKA, must receive a minimum amount of energy in the collision, so that the displacement of atom can takes place. The minimum amount of energy is taken as E_d and is known as displacement threshold energy. During collision if the lattice atom receives energy less than E_d then the struck atom undergoes a large amplitude vibration within its potential but remains in it lattice position. If the collisions continue till the energy received by the struck atom is greater than E_d (typically after 10ps) then the atom can be expected to become a recoil that makes it to move through the lattice and produces more defects. If the energy given to the atom is higher than the E_d, then the equation 2.3.1 is the basic equation that can be used to calculate the No of displaced atoms in any material for which E_d is known and the damage energy T_d can be calculated.

dpa = (No of displaced atoms in volume from NRT equation) / (No. of materials atoms in same volume). ……2.3.1

The dpa concept and NRT equations are usually used in estimating the amount of radiation damage in materials. The Norgett Robinson Torrens (NRT) model was developed as a means of predicting the number of displacements (N_d) created by a PKA atom carrying potential energy *EPKA*. The NRT model is governed by the following equation:

$$N_d(T_d) = \begin{cases} 0 & T_d < E_d \\ 1 & E_d \leq T_d < 2E_d/\beta \\ \frac{\beta T_d}{2E_d} & 2E_d/\beta \leq T_d < \infty \end{cases}$$

E_d = Effective threshold displacement energy.

N_d = No of displacements created by PKA atom carrying potential energy, E_{PKA}

β = Scattering correction factor.

T_d = The damage energy.

2.3.1 Advantages of displacement-per-atom:

This concept is easy to understand and the No. of atoms displaced from its regular lattice can be clearly understood and explained by this concept. It can also be used for scaling radiation doses between different kinds of irradiation. Therefor it can estimate how much damage different irradiation causes. We can also recommend DPA especially in neutron transport calculation to make the transferable interpretation of different kinds of neutron irradiation condition.

2.4 Mechanical properties of copper nanowire with irradiation.

In the paper of 'Influence of ion irradiation induced defects on mechanical properties of copper nanowires, he has explained the mechanical properties and different defect formation that are generated during radiation and tensile, compression deformation of copper nanowire. The simulation details are as follows

We study <001> oriented nanowires which cut from bulk FCC Cu (see Fig.2.4.1(a)). In the simulation x, y, z axes are [1 0 0],[0 1 0] and [0 0 1] directions. Simulation size of the nanowire is 3*3*14.25 nm^3. The system is maintained at an equilibrium configuration of 300K. After the simulation we have irradiated the copper nanowire at different radiation conditions. The stresses are calculated using the virial theorem, which is equivalent to the Cauchy stress in the continuum theory [18]. The stress developed at part III of nanowire is taken to avoid any edge effect and has been averaged over 100 ps.

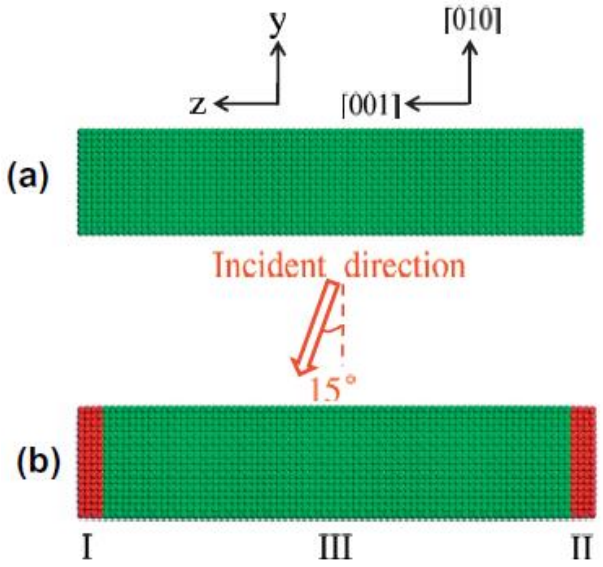


Fig. 2.4.1. Atomic pictures of the Cu nanowire. (a) The atomic configuration of the copper nanowire. (b) The incident direction of the ions in the irradiation simulation. Atoms at sides in (b) denote the fixed atomic layers at both ends.[1]

The aim of our work is to understand the basic damage mechanism of ion irradiation, that causes for the creation of vacancies and interstitials defects that severely damage the copper nanowire. The radiation energy is impinged in the [0 0 1] direction in the middle of<0 1 0> surface and separate each other by 1.2nm, which intends to avoid the irradiation damage of these three ions from overlapping. Defects created within the nanowire is due to the radiation energy, therefore we use ten kinds of incident ion energies ranging from 0.2 to 8 KeV. With the increase of ion irradiation energy, the defects in the nanowire also increased. During collisions NVE ensembles are used and when the ions stop transmitting inside the nanowire, the nanowire is relaxed at 300K under NVT ensembles for 50ps until equilibrium is achieved.

After irradiation the defects like vacancies and stacking faults are clearly shown in the fig.2.4.2. In this we observed due to irradiation the vacancy generation has been taken in all irradiated copper nanowire, but the stacking fault defect was formed in only 3, 4 and 8KeV irradiation. The number vacancies generated was increased with the increase of irradiation. The other conclusions which we come to know from this work are as follows:

- Defects like stacking fault, vacancies and interstitials are formed due to irradiation.
- Young's modulus is decreased in the irradiated Nano copper samples due to point defects and that is because of the relief of applied stresses by atomic relaxation near the defects.
- Due to smaller Young's modulus and yield strain, significant fall of yield stress takes place due to irradiation.
- Surface defects at the surface edge, advance the nucleation of partial dislocations, that results in the yield of the irradiated Nano copper at a smaller strain.

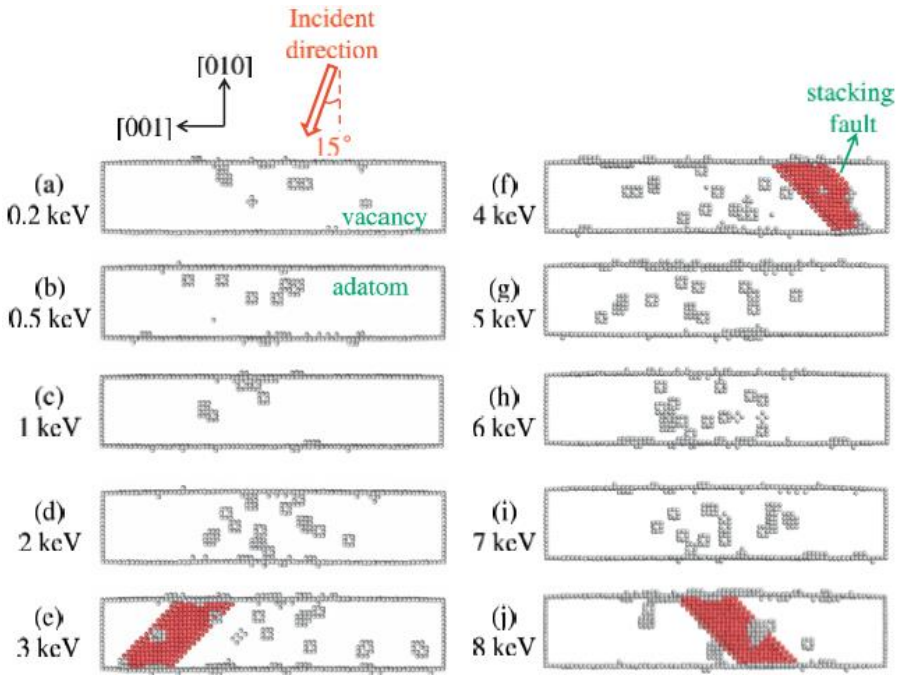


Fig. 2.4.2 Defects distribution in the nanowire after irradiation and the incident energies are given in front of each figure. Surface atoms (the outermost two atomic layers) and perfect FCC atoms are removed to visualize the stacking fault defects. At three incident energies, i.e., 3, 4 and 8 keV, besides point defects, the stacking faults are generated in the nanowire. [1]

Number of defects, the Young moduli (GPa) and yield stresses (GPa) of the irradiated nanowires.

	Vacancy No.	Interstitial No.	Adatom No.	E_t	E_c	σ_t
Unirradiated	0	0	0	61.89	55.27	6.59
0.2 keV	19	1	16	50.37	47.81	4.08
0.5 keV	33	7	16	48.63	45.69	4.40
1 keV	60	3	44	47.64	44.94	3.99
2 keV	41	5	14	47.95	45.63	4.08
5 keV	189	13	88	46.11	43.68	3.34
6 keV	75	10	29	46.55	44.57	3.80
7 keV	83	5	37	47.41	44.89	3.81

Table.2.4.1 Number of defects, the young moduli(GPa) and yield stress(GPa) of the irradiated nanowires. [1]

3.Theoretical and Computational method.

3.1 Molecular Dynamics(MD)

MD is an atomistic simulation method that can provide details of atomistic process in microstructural evolution. In the simplest physical term, MD can be characterized as a method of "particle tracking". Operationally it is a method for generating the trajectories of a system of N particles by direct numerical integration of Newton's equation[31] of motion with appropriate specification of Interatomic potentials and suitable initial boundary conditions.

The foundation of the MD simulation is the Newton's second law. In order to integrate Newton's equation, we can make such assumption that the position and the velocity of each atom can be calculated by Taylor's expansion.

$$r(t+\delta t) = r(t) + v(t)\delta t + (1/2)a(t)\delta t^2 + \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.1$$

$$v(t+\delta t) = v(t) + a(t)\delta t + (1/2)b(t)\delta t^2 + \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.2$$

$$a(t+\delta t) = a(t) + b(t)\delta t + \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.3$$

Where r is the position, v is the velocity and a is the acceleration. We can rewrite the displacementsat small timesteps as

$$r(t+\delta t) = r(t) + v(t)\delta t + (1/2)a(t)\delta t^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.4$$

$$r(t - \delta t) = r(t) - v(t)\delta t + (1/2)a(t)\delta t^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.5$$

Summing these two equations we obtain the following equation

$$r(t+\delta t) = 2r(t) - r(t - \delta t) + a(t)\delta t^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.6$$

This formula uses positions at time *t* and *t* - δt to calculate new positions at time *t+δt* (3.5, 3.6). One advantage by such calculation is that it largely reduces the errors introduced when a relatively larger time step is used. In most MD simulation, this formula is used as basic integration algorithms.

Fig.3.1 schematically shows MD simulation [10] procedure. At beginning, positions and velocities of all atoms are defined, then forces are calculated based on the potential gradients. Then, displacement equations are solved for all atoms in the system over time step δt and physical quantities of interest are extracted, such as temperature, energy, pressure etc. If the total computational time satisfies $t < t_{max,}$ the program will go back to the stage of calculating forces, so on repeating the steps within the loop, until finally $t = t_{max}$.

In explaining the mathematical, chemical, and thermodynamic behavior of solid and fluid materials MD simulation is the best method.in a rigorous manner. The material is modeled as a large collection of point masses (atoms) whose motion is tracked by integrating the classical equation of motion to obtain the positions and velocities of the atoms at large No. of timesteps. The force on the atoms are specified by interatomic potentials that defines the potential energy of the system as a function of the atom positions.

3.1.1 Flow chart of MD simulation.

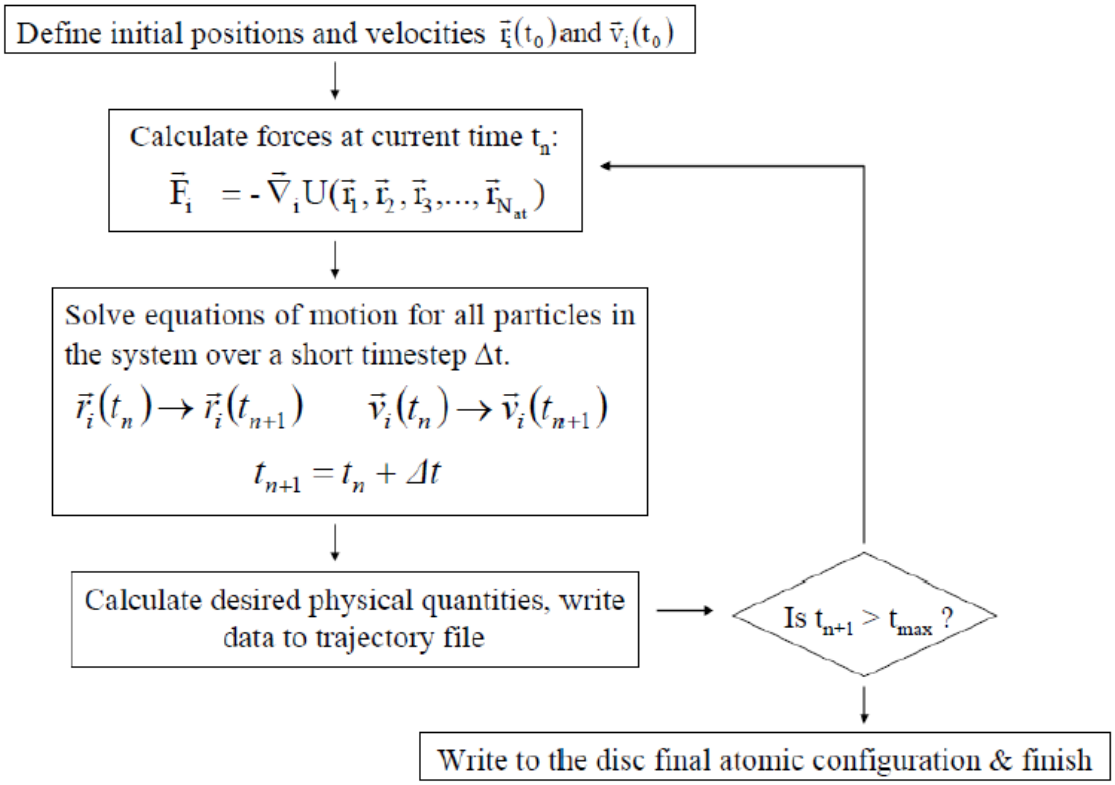


Fig 3.1.1. The simulation proceeds of molecular dynamics simulation

3.1.2 Properties that made MD unique

MD is a useful simulation technique and in this one follows the atomic motions according to the principles of classical mechanics as formulated by Newton and Hamilton [8]. Because of this the results are physically as meaningful as potential U that is used.

We can name MD simulation as 'Atomic video' of the particle motion.

3.1.3 Advantages of MD simulation

Useful study of all physical properties: Using MD, one can obtain the thermodynamic, structural, mechanical, dynamic, and transport properties of a system of particles that can be studied in solid, liquid or gas. One can even study chemical properties and reactions that are more difficult and will require quantum MD.

Several hundred particles are sufficient to simulate bulk matters.

The MD simulation is providing the link between potential models and physical properties of the components. We ca control the input, initial and the boundary conditions of the systems during simulation, so that the physical insight into the behavior of complex systems and we can have detailed atomic trajectories.

3.1.4 Limitations of MD simulation

Computational-capability constraints: The major challenge in MD simulation is in the time scale, because most of the processes of interest and experimental observations are at or longer than the scale of millisecond.

3.2 Interatomic Potential

The critical part of MD simulation is the force calculation, which depends on potentials. The accuracy of a MD simulation is determined by how accurate the interatomic potentials are. These potentials must come from more complicated quantum mechanics treatments. In many cases, even the most advanced calculations cannot serve the purposes well and a combination with experimental data is necessary to reflect the intrinsic properties of the materials. The primary approaches to get interatomic potentials include ab initio method, empirical method, semi-empirical method and embedded atomic method.

Interatomic potentials are mathematical functions for calculating the potential energy of a system of atoms with given positions in space. For understanding Interatomic potential, U can be represented as the sum of two body interactions as

$$U(r_1,r_2,\ldots\ldots\ldots\ldots\ldots r_N) = \sum V(r_{ij}) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.2.1$$

Where $(r_{ij}) = |r_i - r_j|$ is the separation distance between particle i and j. V is the pairwise additive interaction and a central force potential that is a function of only the scale separation distance between two particles r_{ij}.

A two body interaction energy commonly used in atomistic simulation is the Lenard-Jones potential.

$$V(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.2.2$$

ε and σ are potential parameters that set the scales for energy and separation distance.

The above fig shows the interaction energy rising sharply when the particles are close to each other showing a minimum at intermediate separation and decaying to zero at large distances.

The interatomic force is given as $F(r) = -(dv(r)) / (dr) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3.2.3$

The particles repel each other when they are too close and at large separation they attract. Repulsion is due to overlap of electron clouds, whereas attraction between the induced dipole in each atom.

3.2.1. Embedded atom method (EAM)

Embedded atom method (EAM)[7] is a semi-empirical, many atom potentials to calculate the total energy of metallic system. Embedded atom method [33] is an approximate description of energy between two atoms. The energy is a function of sum of function of the separation between an atom and its neighbors. EAM is very closed to the second moment approximation to tight binding theory, also known as the Finnis-Sinclair model. These model are particularly appropriate for metallic system. EAM is widely used in MD simulations

In a simulation, the potential energy of an atom i, is given by

$$E_i = F_\alpha\left(\sum_{i\neq j}\rho_\beta\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}\left(r_{ij}\right)$$

Where r_{ij} is the distance between atoms i and j.

$\phi_{\alpha\beta}$ is a pair-wise potential function

ρ_β is the contribution to the electron charge density from atom j of type β at the location of atom i and F is an embedding function that represents the energy required to place atom i of type α into the electron cloud.

3.2.2 Ab-initio method

Ab-initio methods[6] totally rely on the quantum mechanics. The potentials are created by the quantum mechanical calculation based on solving a multi body Schrödinger equations. The advantage of the method is that almost everything starts from the first principles. However, certain errors exist due to necessary assumptions and approximated used to simplify the process. Also certain details are not completely clear such as electron-electron interactions in heavy atoms.
Semi empirical potentials are also based on quantum mechanics calculation, but certain items are neglected in the calculation, For example, in Hartree-Fock calculations the overlapping of specific atomic orbitals are neglected, and the corresponding contribution is replaced by experimental results, in such a way the computations are less costly. For empirical potentials, the overlap of specific atomic orbitals are totally neglected and many free parameters are introduced to predict experimental observations.

3.3 LAMMPS

3.3.1 Background and Features of LAMMPS.

LAMMPS (Large scale Atomic/Molecular Massively parallel Simulator) [26] is a powerful MD simulator. It was developed at Sandia National, which is under the United States Department of Energy. LAMMPS is very easy to be use as it is compiled in a specific computational language. Three basic files are needed to run the MD code on LAMMPS platform: input script, a potential file and an exe. File. LAMMPS input script has basically four parts:

1.) Initialization

2.) Atom definition

3.) Setting

4.) Run a simulation

This software is free and distributed under the general public license(GPL). It is operated by codes and the code is easy to modify or extend with new functionality. Features of LAMMPS:

- runs on single processor or in parallel
- distributed –memory message-passing parallelism(MPI)
- open-source distribution
- optional libraries used: MPI and single-processor FFT
- runs from an input script
- highly portable C++
- syntax for defining and using variables and formulas
- syntax for looping over runs and breaking out of loops
- easy to extend with new features and functionality

There are many commercial softwares available for MD simulation. LAMMPS is one widely used in many areas. In order to make MD simulation run on LAMMPS, input file, potential file, and executable file are needed. However, to utilize LAMMPS for damage calculations, modification and extra cares are needed. Although LAMMPS provides many default potentials which predict bulk properties very well, they are not suitable for short range atomic interactions like those encountered in ion solid interactions. Self-made software is needed to extract defect information. Furthermore, LAMMPS does not provide visualization capability, though this can be readily solved by using other software such as OVITO and VMD.

3.3.2 Ensembles and boundary conditions

Three different ensembles are used in LAMMPS.

1. Micro canonical or NVE ensembles.
2. Canonical or NVT ensembles.
3. Isothermal – Isobaric or NPT ensemble.

Four boundary conditions are used in LAMMPS. These are p, f, s, m.

p is periodic
f is non-periodic and fixed
s is non-periodic and shrink wrapped.
m is non-periodic and shrink wrapped with a minimum value.

3.3.3 Output

Output file is generated after completion of running the MD code. Two files are generated.

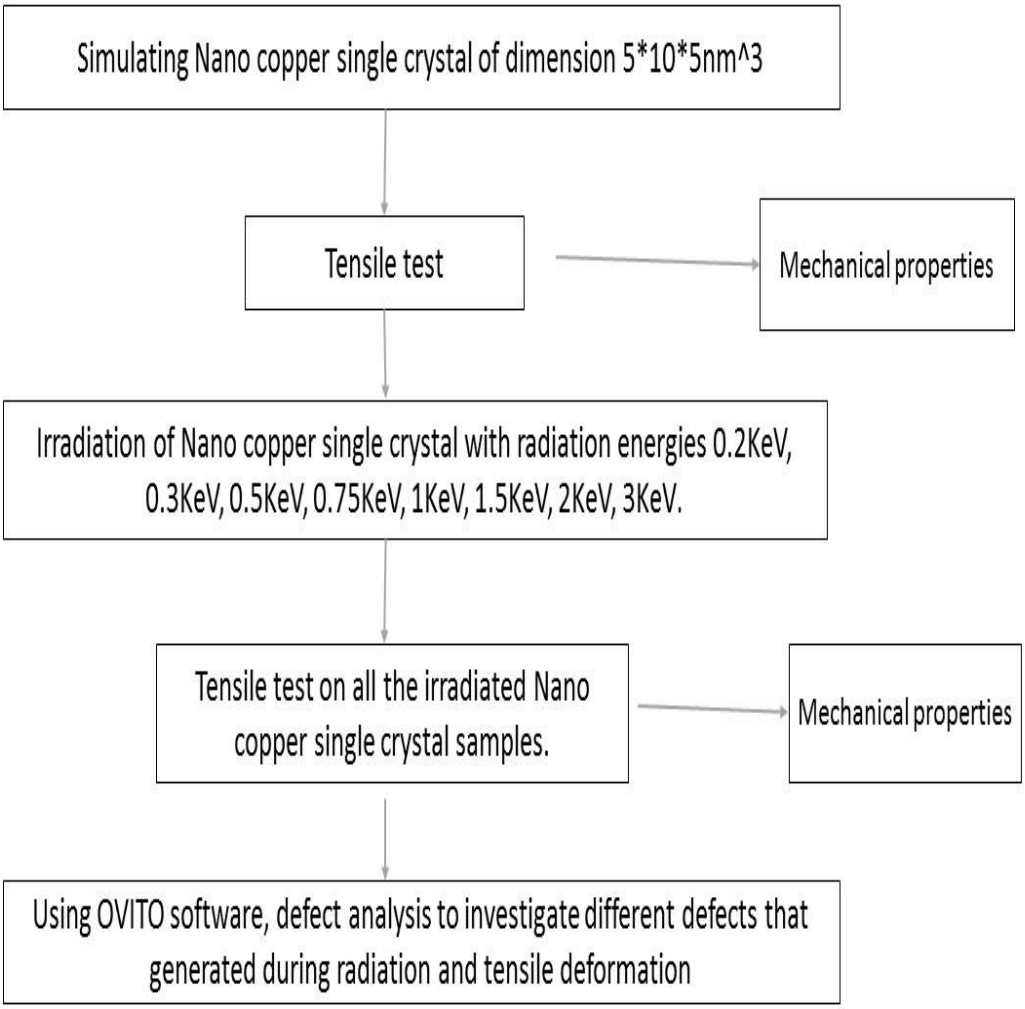
1) DUMP file: this file gives the atoms position in all three directions and respective their velocity.

2) Log file: This file contents the thermodynamic information of atoms like temperature, pressure, volume, and total energy.

3.4 OVITO (Open Visualization tool)

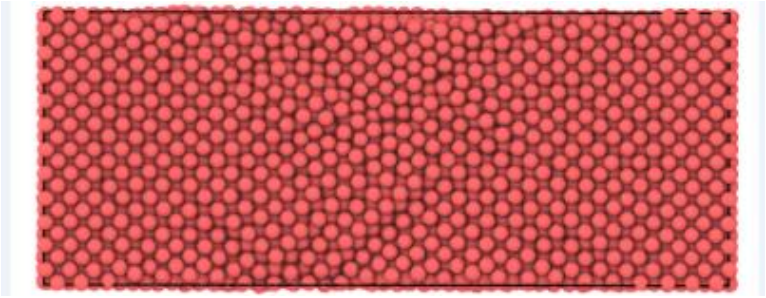
OVITO[11] is a molecular visualization package for displaying, animating, and analyzing large atoms/molecules using 3-D graphics and built-in scripting. In the present study all the atomic snapshots are taken by OVITO software [33]. Using OVITO software we have done defect analysis on the radiation damaged Nano copper samples to investigate different defects like vacancies, displacement of atoms and stacking faults that occur during radiation and tensile deformation.

Work plan


Simulating Nano copper single crystal of dimension 5*10*5nm^3
Tensile test
Mechanical properties
Irradiation of Nano copper single crystal with radiation energies 0.2KeV, 0.3KeV, 0.5KeV, 0.75KeV, 1KeV, 1.5KeV, 2KeV, 3KeV.
Tensile test on all the irradiated Nano copper single crystal samples.
Mechanical properties
Using OVITO software, defect analysis to investigate different defects that generated during radiation and tensile deformation

4. Results and Discussions

In the present study, classical molecular dynamics code LAMMPS was used to examine the interaction of atoms in the damaged cascades spaced in closed proximity. In simulation we have created FCC Nano copper [22] single crystal sample in x, y, z axes as [1 0 0], [0 1 0] and [0 0 1] directions. The sample have the shape of a rectangular parallelepiped with size of 5*10*5 nm^3. The size is evaluated from the equilibrium configuration at 300K. Periodic boundary conditions 'p' are applied in all dimensions to simulate the copper sample during irradiation and non-periodic shrink wrapped 's' are applied to radiated copper sample during tensile test. To describe the atomic interaction of Nano copper, embedded atom method(EAM) potential developed by Mishin at al is employed. The simulated Nano copper sample having 21952 atoms is equilibrated at 300K using Nose-Hoover thermostat for 30ps with timestep of 0.001ps and the equilibrium configuration is as shown in fig.4. Then both ends part I and part II in fig.4 of the simulated copper sample are fixed.



I III II

Fig.4 Atomic picture of irradiated Nano copper single crystal under investigation. Part I is fixed and part II is displaced repeatedly. Part III is under continuous deformation of given strain.

In the process of simulation, one copper atom which is treated as primary knock-on atom (PKA) is given a velocity ranging energies from 0.2KeV to 3KeV. The impact of this PKA on the rest of the Nano copper atoms is high enough to cause significant changes in the mechanical properties of the copper sample. Since the number of defects caused depends on the energies of the PKA, therefore we used different kinds of incident radiation energies in our simulation ranging from 0.2KeV to 3KeV. Due to irradiation effect by the PKA[23], displacement of atoms was taken in a large amount. During irradiation few copper atoms was displaced from their regular lattice to out of simulation box. To control this, we have simulated the copper box into two regions as interior and exterior regions and by fixing the exterior region of the simulation box we can control the atoms.

After irradiation, the copper sample is strained by displacing part II repeatedly. At each strain step, part II is moved along the y-axis while part I is fixed. Then the part III of Nano copper single crystal is relaxed at 300K NVT ensemble for 100 ps, with part II and part I is fixed. The stresses are calculated using the virial theorem, which is equivalent to the Cauchy stress in the continuum theory. In the stress analysis and in the atomic visualization, open visualization tool(OVITO) is used. The No of defects created after irradiation are analyzed with Wigner-Seitz cell method of OVITO visualization tool.

4.1 Mechanical properties of simulated Nano copper single crystal

4.1.1 Mechanical properties of simulated Nano copper single crystal without irradiation

To study the mechanical properties of Nano copper single crystal without irradiation, we have simulated copper and the tension is applied as described above. If we observe fig.4.1.1.1(a) the stress strain curve of Un-Irradiated Nano copper sample in tension is shown.

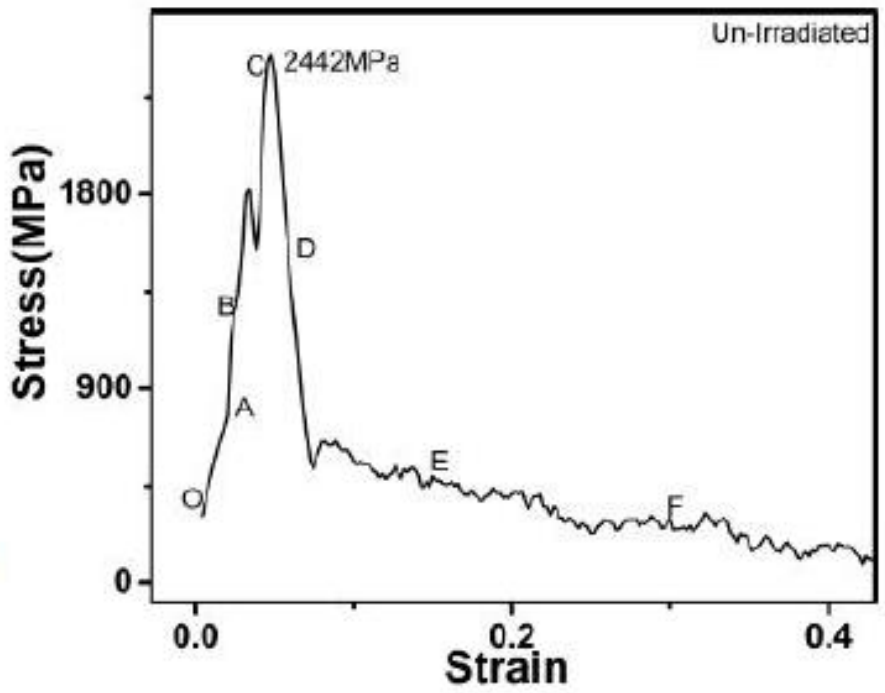


Fig.4.1.1.1(a)

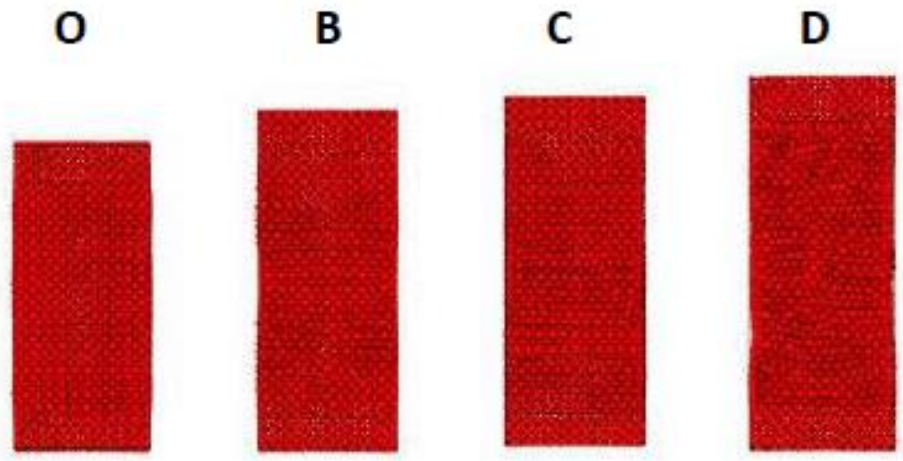


Fig.4.1.1.1(b)

Fig.4.1.1.1(a) Stress-Strain curve of Un-Irradiated Nano copper single crystal. Points O, A, B ,C,D,E and F represents different strian points during tension. Fig.4.1.1.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

During tension, the Un-irradiated Nano copper deforms elastically until a critical point is reached and then the sample yields until a permanent rupture is obtained. The stress just before the first

yield, i.e., the point B in fig.3(a) is taken as yield stress. The first yield results in a significant decrease in stress and then the stress increase linearly. The maximum yield stress that can be noted from the graph is 1.413GPa. From the graph we also observe the point A as the proportionality limit at which the curve deviates from the linearity. The slope in this region gives the modulus of elasticity. The point B is the elastic limit i.e., the stress up to which the curve follows the Hooke's law[27].

Fig.4.1.1.2(a)

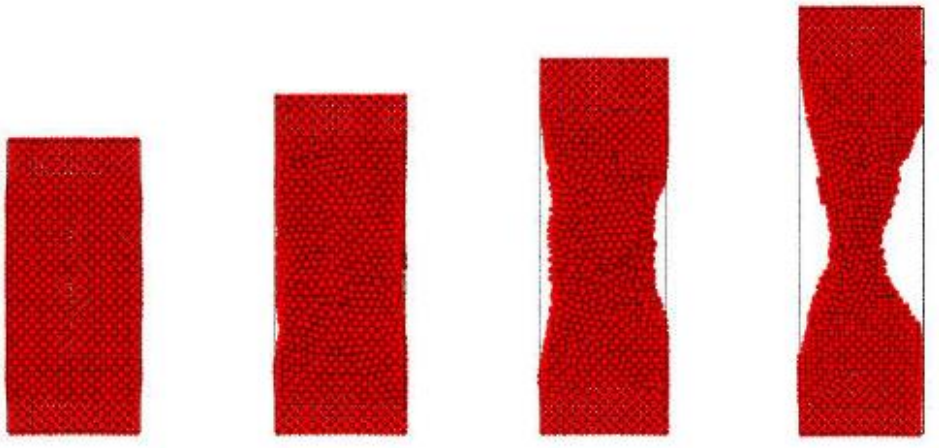


Fig.4.1.1.2(b)

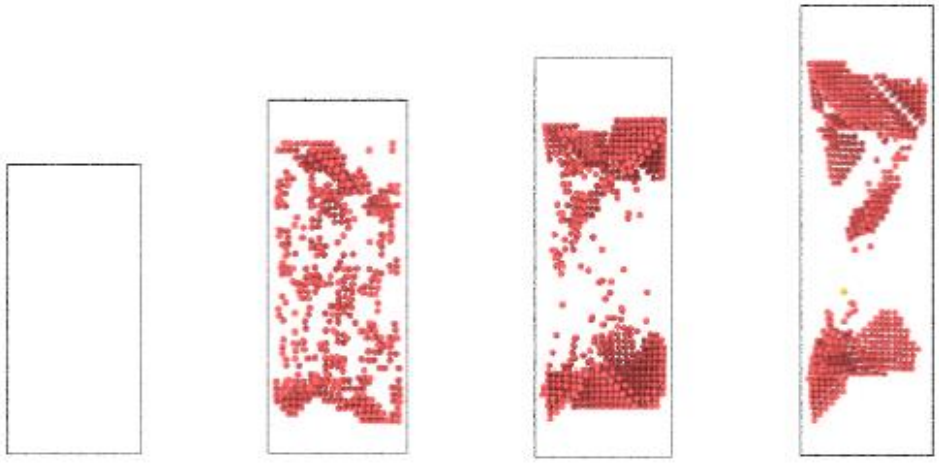


Fig.4.1.1.2(a) Atomic configuration of Un-Irradiated Nano-copper at points O, D, E, F corresponding to the stress-strain curve of Fig.4.1.1.1(a). Fig.4.1.1.2(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

In fig 4.1.1.2(a) and 4.1.1.2(b), we show the atomic configuration of the Un-irradiated Nano copper corresponding to the selected points on the stress-strain curve of Fig.4.1.1.1(a). By performing Common neighbor analysis (CNA) in OVITO[28] specifies the lattice structure type (FCC, BCC, HCP etc) for each atom. Atoms with unknown coordination structure are considered as other type of lattice structure. For instance, bulk atoms of the pristine Nano copper have the FCC structure and surface atoms are considered as other atoms by OVITO. By performing Common Neighbor Analysis, perfect FCC atoms and surface atoms are removed in Fig.4.1.1.2(b) to visualize the stacking faults generated by the {1 1 1}/<1 1 2> partial slip.

During tensile loading, the yield occurs via both the {1 1 1}/<1 1 2> partial slip and the {1 1 1}/<1 1 0> perfect slip. The {1 1 1}/<1 1 0> perfect slip happens when two {1 1 1}/(1 1 2) partial dislocation slip on the same {1 1 1} plane. The perfect slip removes stacking fault. Comparing the configurations at points C and D in Fig.4.1.1.2(b) there is a decrease in stacking fault with increase in tensile loading.

It is well known that at elastic regime, stress and strains relationship can be described by Hooke's law: $\sigma = E\varepsilon$ …….(4.1.1.1)

Where E is the young modulus. As the young's modulus depend on strain and its value can be calculated with the stress strain relationship. So the equation 2 should be written as:

$$\sigma = E(\varepsilon)\varepsilon = E_0\varepsilon + D\varepsilon^2, \quad \text{…….(4.1.1.2)}$$

where E_0 is the young modulus at zero strain and D is the higher order elastic modulus. In origin pro by using the quadratic fit to the stress-strain curve before the first yield, i.e., the section OA for tension, we got E = 136GPa. The maximum tensile strength of the copper sample of given dimensions without irradiation is 2442MPa.

Incident energy	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
Un-irradiated (0 KeV)	0	136.0	2442

Table.4.1.1.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the un-irradiated (0 KeV) Nano copper single crystal.

4.1.2 Mechanical properties of simulated Nano copper single crystal with irradiation

Case4.1.2.1: Study of 0.2KeV irradiated Nano copper single crystal.

Nano copper single crystal is irradiated by 0.2KeV PKA. After 0.2KeV irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.1.1(a).

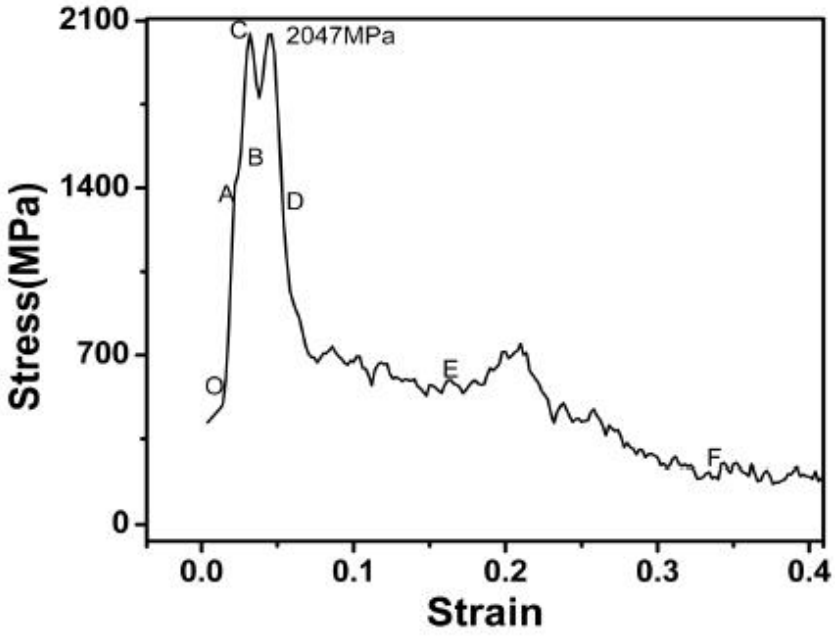


Fig.4.1.2.1.1(a)

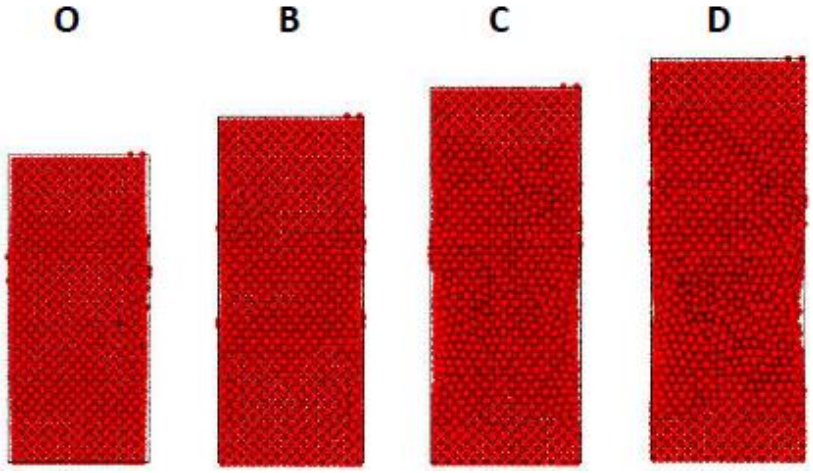


Fig.4.1.2.1.1(b)

Fig.4.1.2.1.1(a) Stress-Strain curve of 0.2KeV Irradiated Nano copper single crystal. Points O, A, B ,C,D,E and F represents different strian points during tension. Fig.4.1.2.1.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

We can observe the points O, A, B, C and D on the stress-strain graph. The corresponding atomic cofiguration of Nano copper strain points has been sketched in fig.4.1.2.1.1(b). The maximum tensile strength obtained by the 0.2KeV irradiated Nano copper is 2047MPa. This tensile strength is less than the un-irradiated Nano copper tensile strenth 2442MPa. The Young modulus is 108.26GPa and this Young modulus is also less than un-irradiated Nano copper Young modulus 136GPa. The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) due to 0.2KeV irradiation in Nano copper sample.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
0.2KeV	29	108.26	2047

Table.4.1.2.1.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 0.2KeV Irradiated Nano copper single crystal.

In fig.4.1.2.1.2 we can observe vacancies and displacement of atom from their regular lattice structure due to irradiation. The No. of vacancies generated due 0.2KeV Irradiation in the Nano copper is 29. With the increase in Irradiation the No. of vacancies generated within Nano copper sample also increases and this can be observed in following case studies.

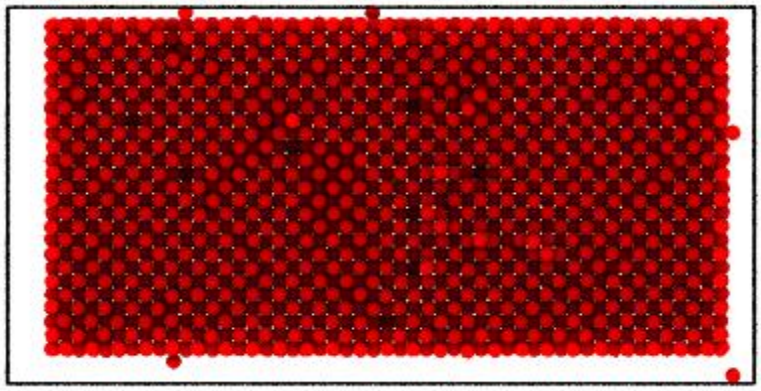


Fig.4.1.2.1.2 0.2KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

As we undergo tension after irradiation and when the sample reaches a plastic deformation zone, defects like stacking faults has been observed. This stacking fault is observed during plastic deformation only and the magnitude of these stacking faults has been increased with the increase in tension and it is explained with pictures by taking snap shots (from OVITO tool) of the Nano copper single crystal during tension as shown in Fig.4.1.2.1.3. The stacking faults results from the melting and recrystallizing of part of the Nano copper when the kinetic energy transferred from the incident PKA energy is high enough. Note that this stacking fault is observed in only some irradiation conditions and that to at a tension of higher than plastic strain of the copper Nano sample. In Fig.4.1.2.1.3(b) we can observe stacking fault generated by the {1 1 1}/{1 1 2} partial slip when the perfect fcc atoms and surface atoms are removed from the atomic configuration of

Nano copper. Upto yield point there is no sign of stacking fault and slowly there is a generation of stacking fault with tension in the Nano copper.

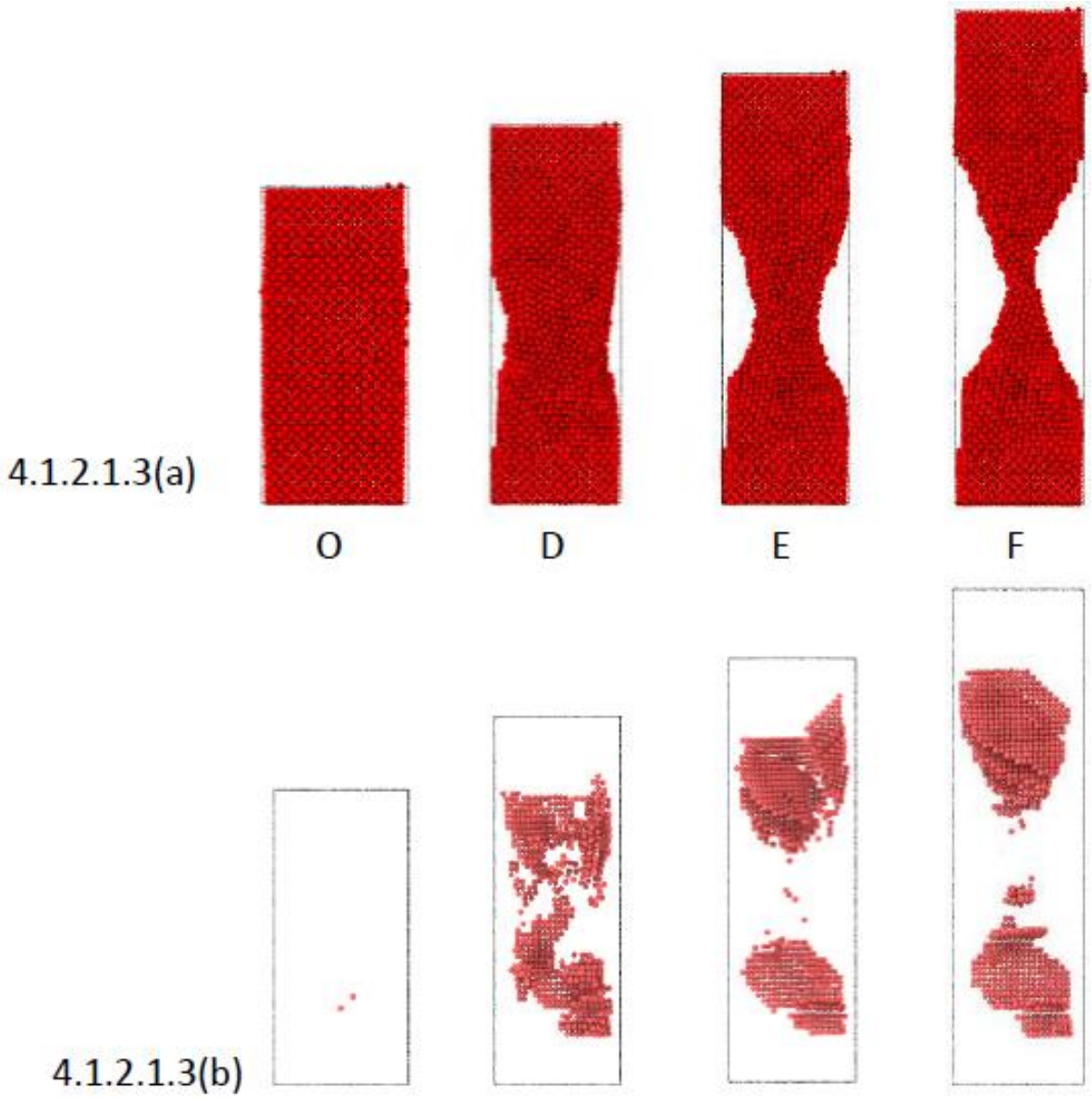


Fig.4.1.2.1.3(a) Atomic configuration of Nano-copper at points O, D, E, F corresponding to the stress-strain curve of Fig.4.1.2.1.1(a). Fig.4.1.2.1.3(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

Case4.1.2.2: Study of 0.3KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 0.3KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.2.1(a).

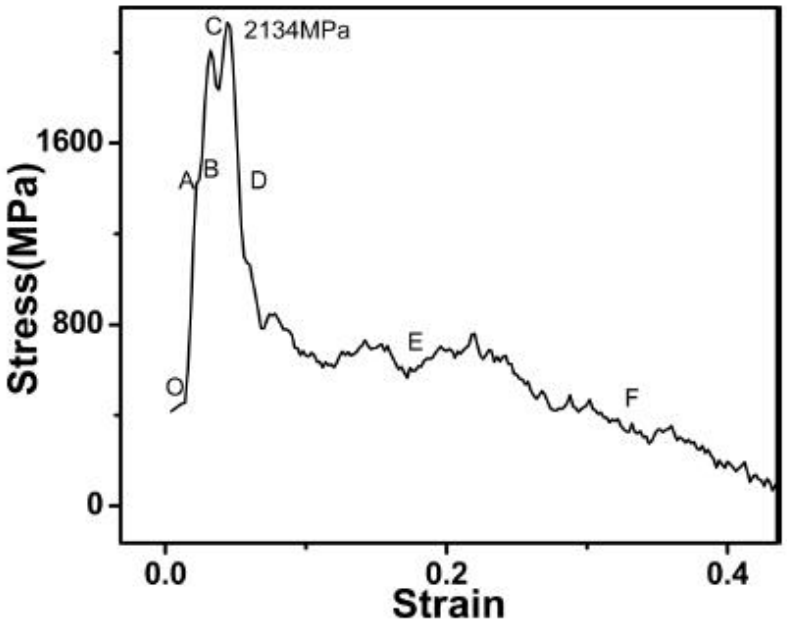


Fig.4.1.2.2.1(a)

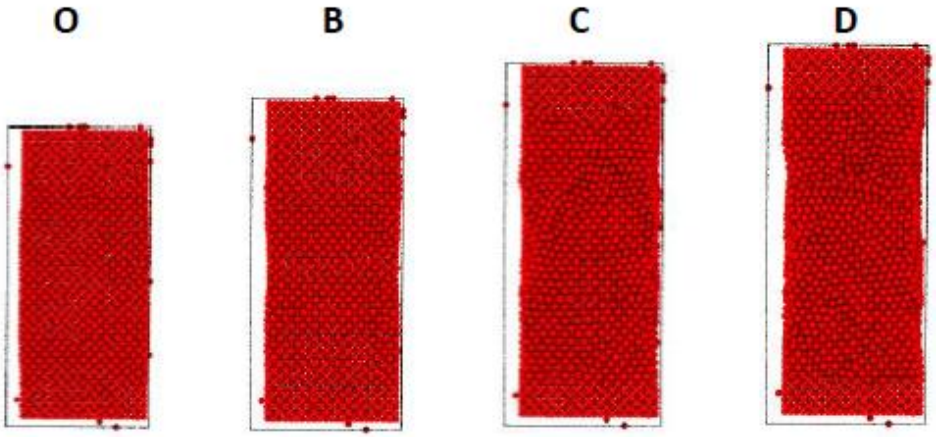


Fig.4.1.2.2.1(b)

Fig.4.1.2.2.1(a) Stress-Strain curve of 0.3KeV Irradiated Nano copper single crystal. Points O,A,B ,C,D,E and F represents different strian points during tension. Fig4.1.2.2.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

The maximum tensile strength obtained by the 0.3KeV irradiated Nano copper single crystal is 2134MPa. This tensile strength is greater than the 0.2KeV irradiated Nano copper tensile strength 2047MPa and less than un-irradiated Nano copper maximum tensile strength 2442MPa.

The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) due to 0.3KeV irradiation in Nano copper sample. The No. of vacancies generated during 0.3KeV irradiation in Nano copper sample is 35. As the incident irradiation energy increased from 0.2 to 0.3KeV, the No.of vacancies also increased from 29 to 35.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
0.3KeV	35	109.85	2134

Table.4.1.2.2.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 0.3KeV Irradiated Nano copper single crystal.

In fig.4.1.2.2.2 we can observe vacancies and displacement of atom from their regular lattice structure due to irradiation. The No. of vacancies generated by 0.3KeV Irradiation in the Nano copper is 35.

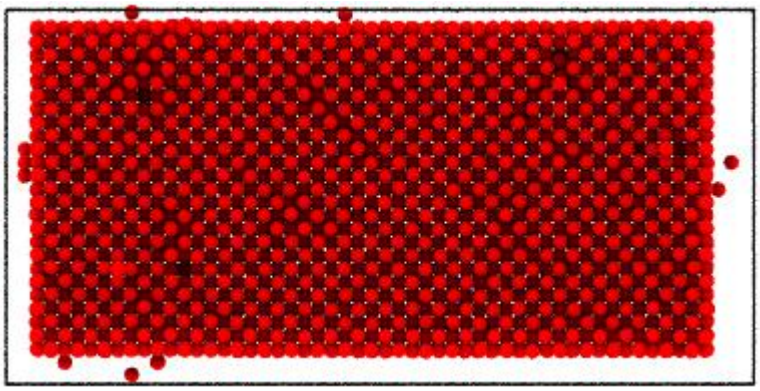


Fig.4.1.2.2.2 0.3KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

The stacking fault defect is observed during plastic deformation and the magnitude of these stacking faults has been increased with the increase in tension and it is explained with pictures by taking snap shots of the Nano copper single crystal during tension as shown in Fig.4.1.2.2.3(b). The stacking faults results from the melting and recrystallizing of part of the Nano copper when the kinetic energy transferred from the incident PKA energy is high enough. In Fig.12(b) we can observe stacking fault generated by the {1 1 1}/{1 1 2} partial slip when the perfect fcc atoms and surface atoms are removed from the atomic configuration of Nano copper. Upto yield point there is no sign of stacking fault and slowly there is a generation of stacking fault with tension in the Nano copper.

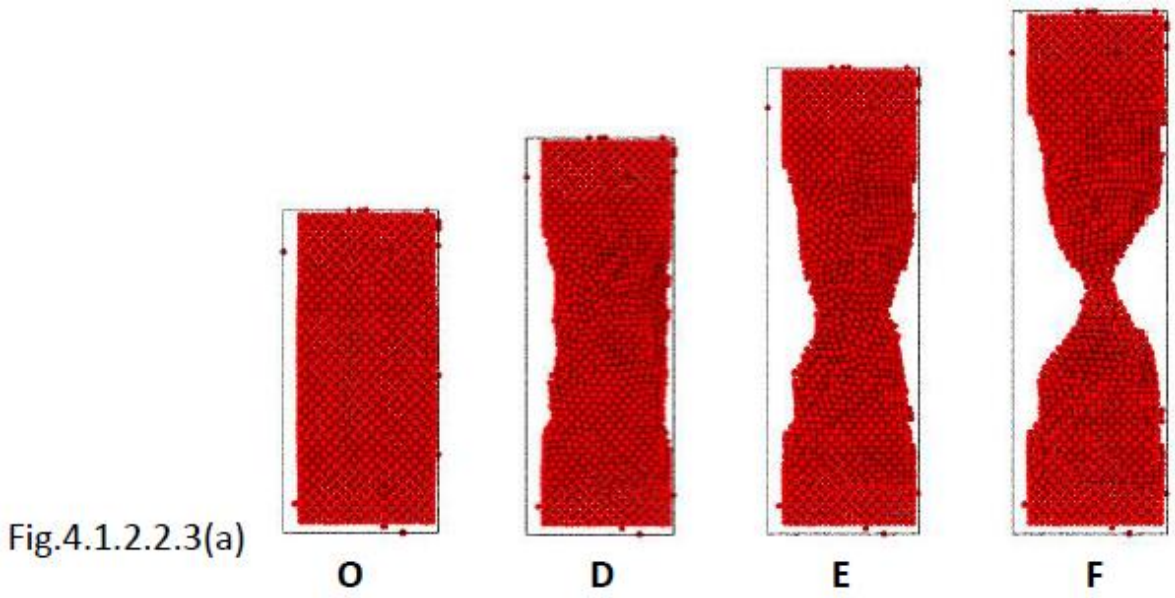


Fig.4.1.2.2.3(a) Atomic configuration of Nano-copper at points O, D, E, F corresponding to the stress-strain curve. Fig.4.1.2.2.3(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

Case4.1.2.3: Study of 0.5KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 0.5KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.3.1(a).

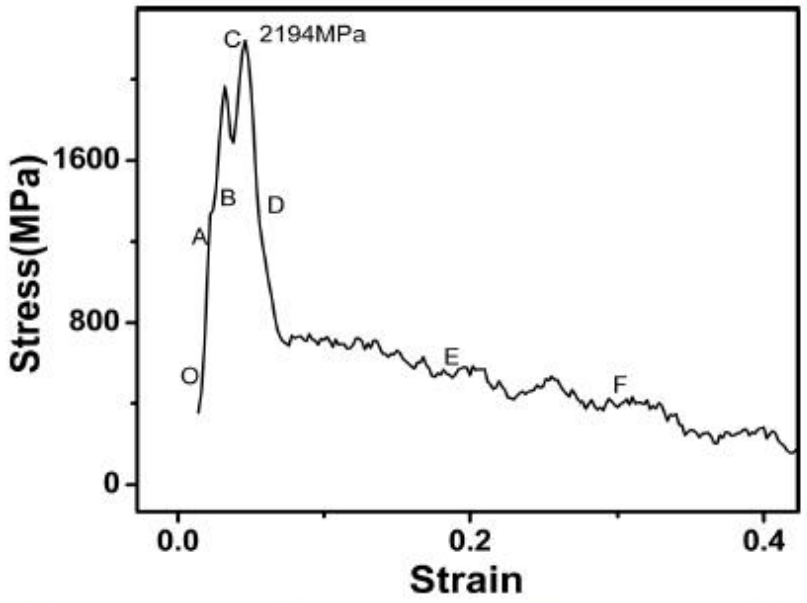


Fig.4.1.2.3.1(a)

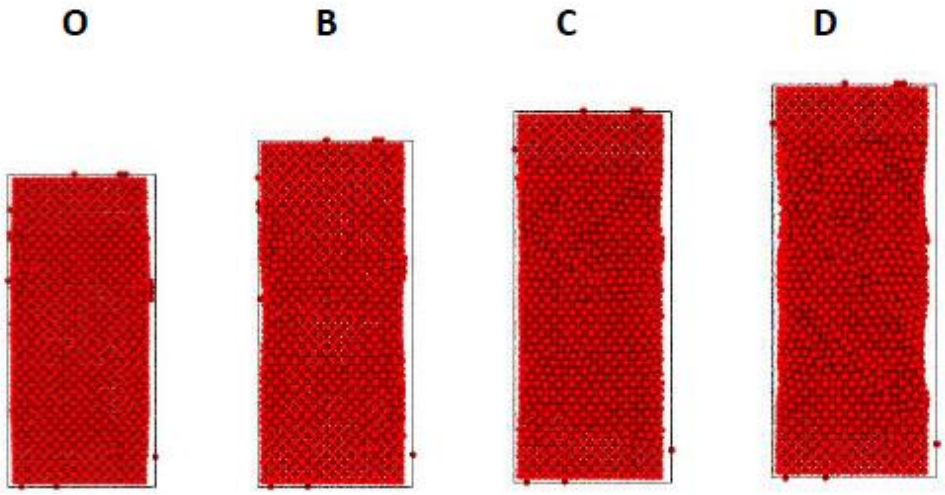


Fig.4.1.2.3.1(b)

Fig.4.1.2.3.1(a) Stress-Strain curve of 0.5KeV Irradiated Nano copper single crystal. Points O,A, B,C,D,E and F represents different strian points during tension. Fig.4.1.2.3.1(b)Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O,B,C, D.

The maximum tensile strength obtained by the 0.5KeV irradiated Nano copper single crystal is 2194MPa. This tensile strength is greater than the 0.2KeV and 0.3KeV irradiated Nano copper tensile strengths 2047MPa, 2134MPa and less than un-irradiated copper tensile strength 2442MPa.

The Young modulus is 114.185GPa and this Young modulus is less than un-irradiated Nano copper Young modulus 136GPa. The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) and displacement of atoms due to 0.5KeV irradiation in Nano copper sample. The No. of vacancies generated during 0.5KeV irradiation in Nano copper sample is 44. As the incident irradiation energy increased from 0.2 to 0.5KeV, the No.of vacancies also increased from 29 to 44. But the tensile strength and young modulus of 0.5KeV copper sample is greater than 0.2 and 0.3KeV copper samples.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
0.5KeV	44	114.185	2194

Table.4.1.2.3.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 0.5KeV Irradiated Nano copper single crystal.

In fig.4.1.2.3.2 we can observe vacancies and displacement of atom from their regular lattice structure due to irradiation. The No. of vacancies generated due 0.5KeV Irradiation in the Nano copper is 44.

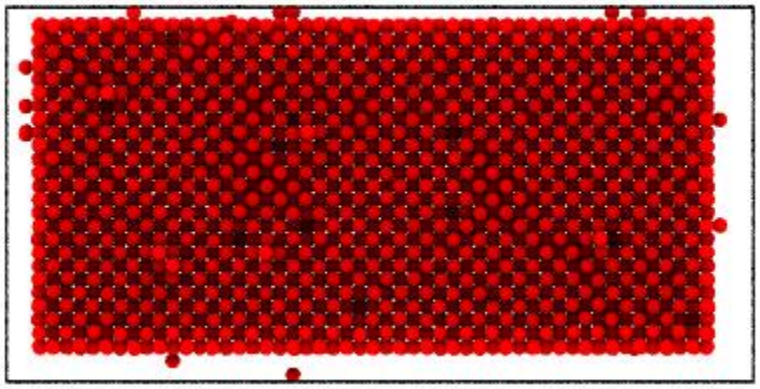


Fig.4.1.2.3.2 0.5KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

The stacking fault defect is observed during plastic deformation and the magnitude of these stacking faults has been increased with the increase in tension and it is explained with pictures by taking snap shots of the Nano copper single crystal during tension as shown in Fig.4.1.2.3.3(b). Stacking fault magnitude has been decreased from 0.2KeV to 0.5KeV. We can observe this in the above figures.

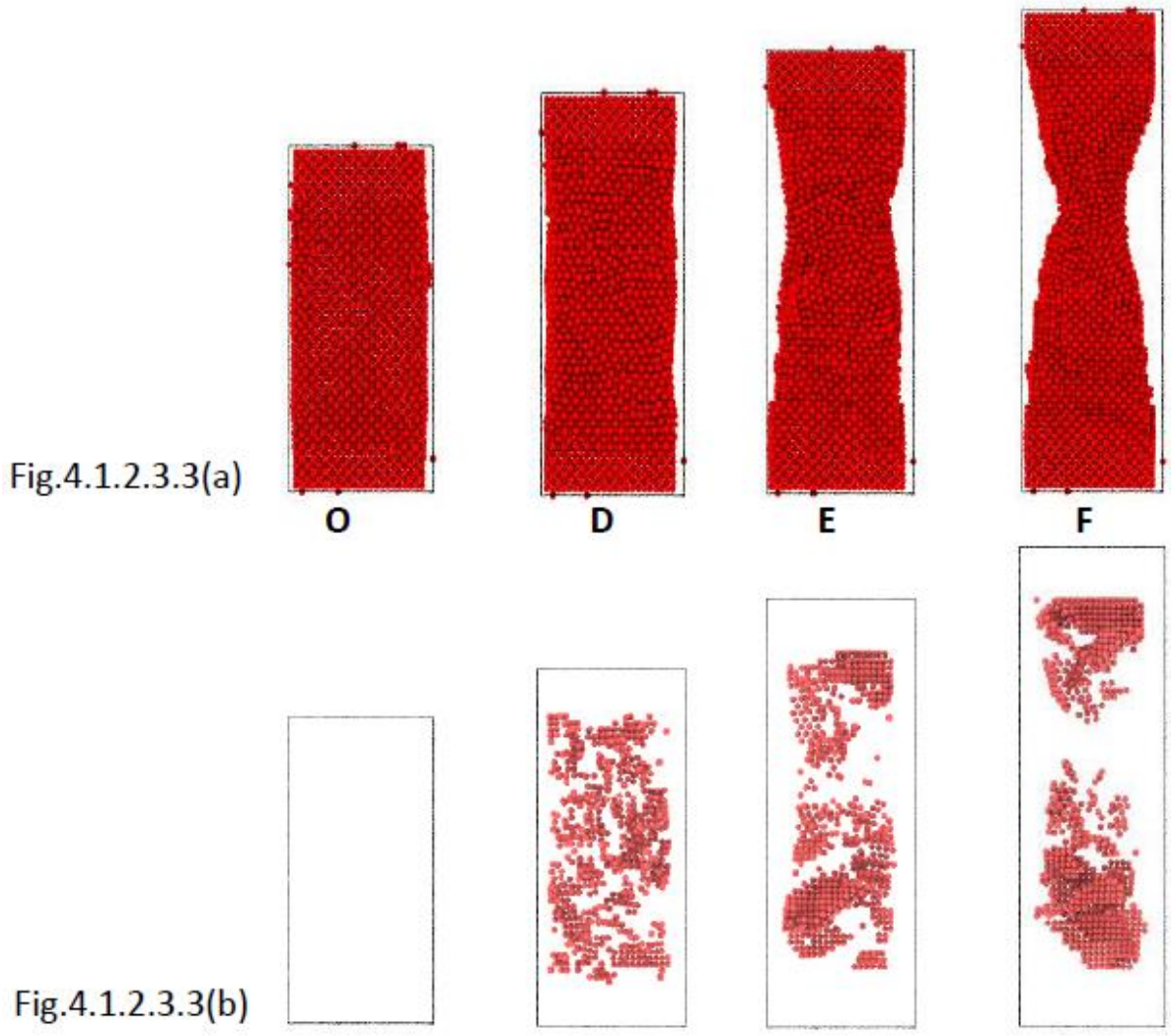


Fig.4.1.2.3.3(a) Atomic configuration of Nano-copper at points O, D, E, F corresponding to the stress-strain curve of Fig.4.1.2.3.1(a). Fig.4.1.2.3.3(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

Case 4.1.2.4: Study of 0.75KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 0.75KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.4.1(a).

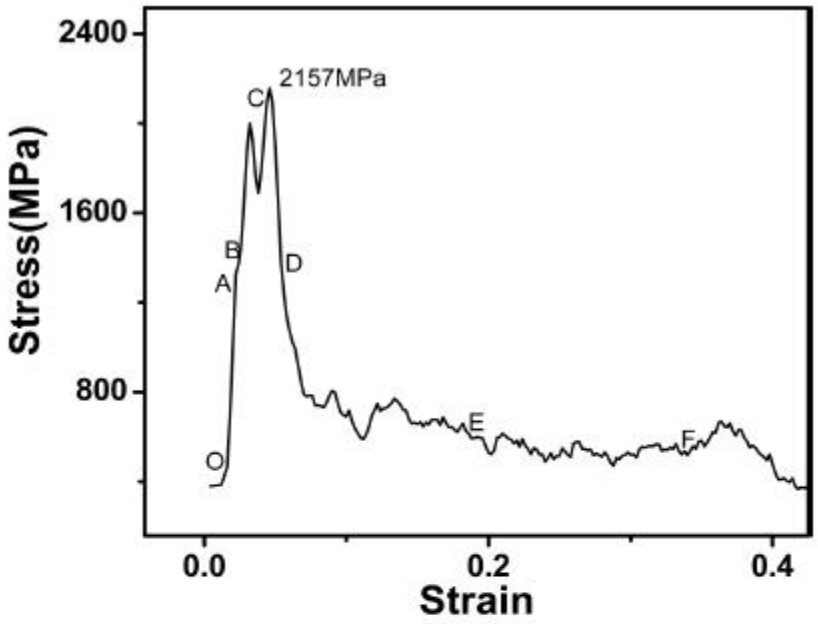


Fig.4.1.2.4.1(a)

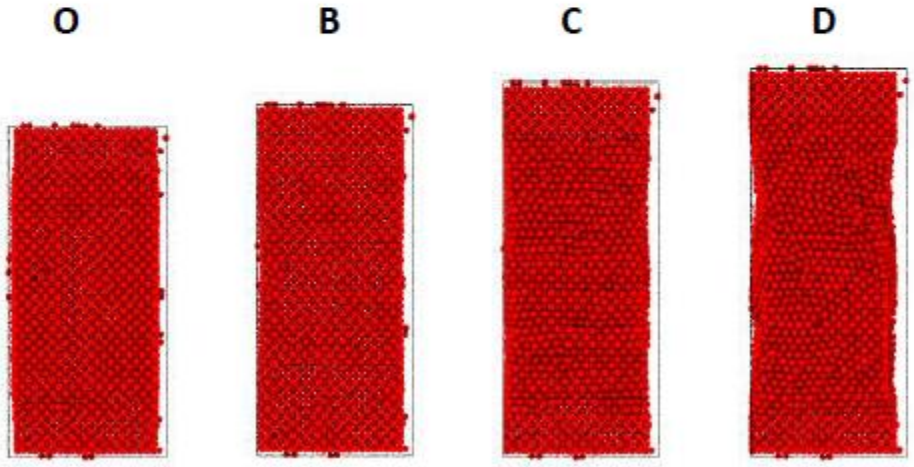


Fig.4.1.2.4.1(b)

Fig.4.1.2.4.1(a) Stress-Strain curve of 0.75KeV Irradiated Nano copper single crystal. Points O,A,B ,C,D,E and F represents different strian points during tension. Fig.4.1.2.4.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

The maximum tensile strength obtained by the 0.75KeV irradiated Nano copper single crystal is 2157MPa. This tensile strength is greater than the 0.2KeV and 0.3KeV irradiated Nano copper tensile strengths 2047MPa, 2134MPa but less than 0.5KeV and un-irradiated copper tensile strength 2194MPa and 2442MPa. The Young modulus is 113.126GPa and this Young modulus is less than un-irradiated Nano copper Young modulus 136GPa. The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) and displacement of atoms due to 0.75KeV irradiation in Nano copper sample. The No. of vacancies generated during 0.75KeV irradiation in Nano copper sample is 45. As the incident irradiation energy increased from 0.2 to 0.75KeV, the No.of vacancies also increased from 29 to 45.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
0.75KeV	45	113.126	2157

Table.4.1.2.4.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 0.75KeV Irradiated Nano copper single crystal.

In fig.4.1.2.4.2 we can observe vacancies and displacement of atoms from their regular lattice structure due to irradiation.

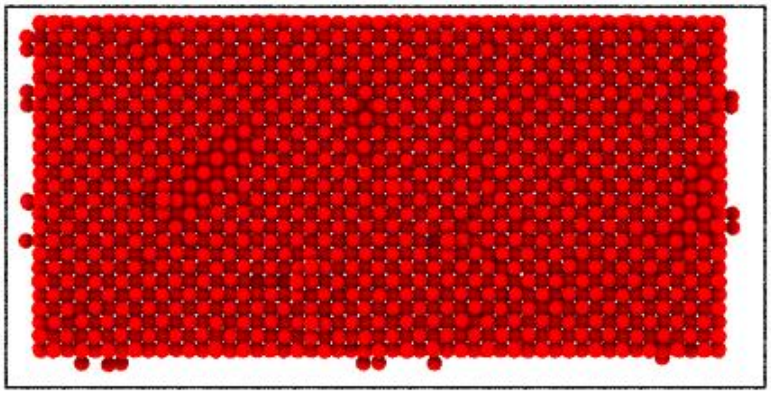


Fig.4.1.2.4.2 0.75KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

During tensile deformation of the Nano coper sample we haven't noticed the stacking fault defects. In the previous section as we observed that the magnitude of the stacking has been reduced with the incident irradiation energy.

Case 4.1.2.5: Study of 1KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 1 KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.5.1(a).

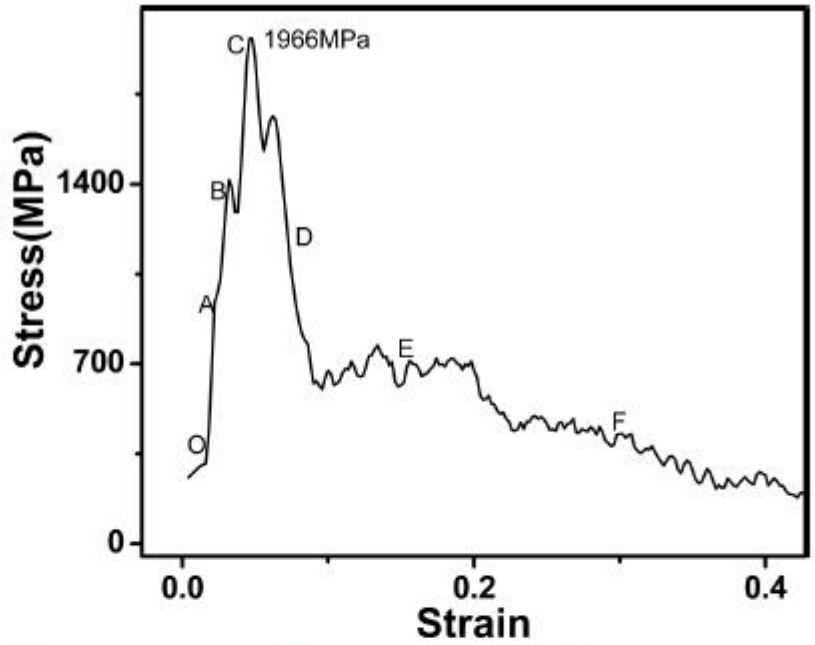


Fig.4.1.2.5.1(a)

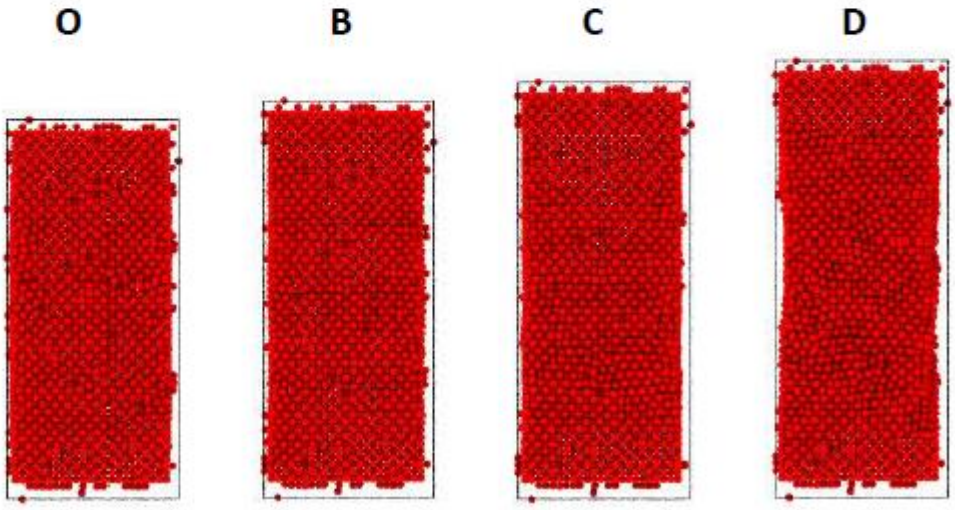


Fig.4.1.2.5.1(b)

Fig.4.1.2.5.1(a) Stress-Strain curve of 1KeV Irradiated Nano copper single crystal. Points O,A,B ,C,D,E and F represents different strian points during tension. Fig.4.1.2.5.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O,B,C, D.

The maximum tensile strength obtained by the 1KeV irradiated Nano copper single crystal is 1966MPa. This tensile strength is much less than the 0.2KeV, 0.3KeV, 0.5KeV, 0.75KeV irradiated Nano copper samples and un-irradiated copper tensile strength 2047, 2134, 2194, 2157

and 2442MPa. The Young modulus is 101.57GPa and this Young modulus is less than all irradiated copper samples and un-irradiated Nano copper Young modulus. The values are clearly depicted in the below table.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
1KeV	90	101.57	1966

Table.4.1.2.5.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 1 KeV Irradiated Nano copper single crystal.

The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) and displacement of atoms due to 1KeV irradiation in Nano copper sample. The No. of vacancies generated during 1KeV irradiation in Nano copper sample is 90. In 1KeV we have observed a maximum No. of vacancies generation and this defects has a major impact on the mechanical properties Nano copper sample.The following fig.18 clearly shows the defects creation in copper sample due to 1KeV irradiation.

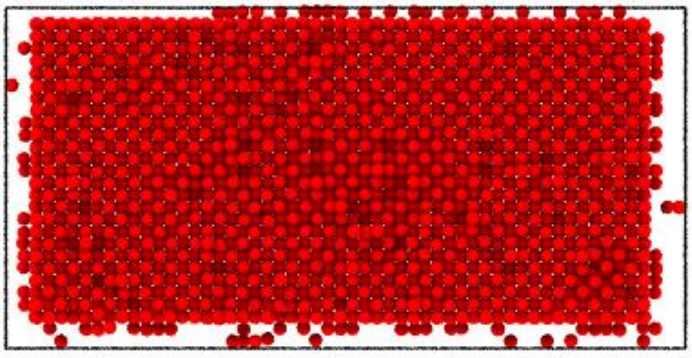


Fig.4.1.2.5.2 1KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

In 1KeV irradiation Nano copper sample, there is no generation of stacking faults has been taken place. Even at complete tension of irradiated copper sample, the magnitude of stacking fault is very less.

Case 4.1.2.6: Study of 1.5KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 1.5 KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.6.1(a).

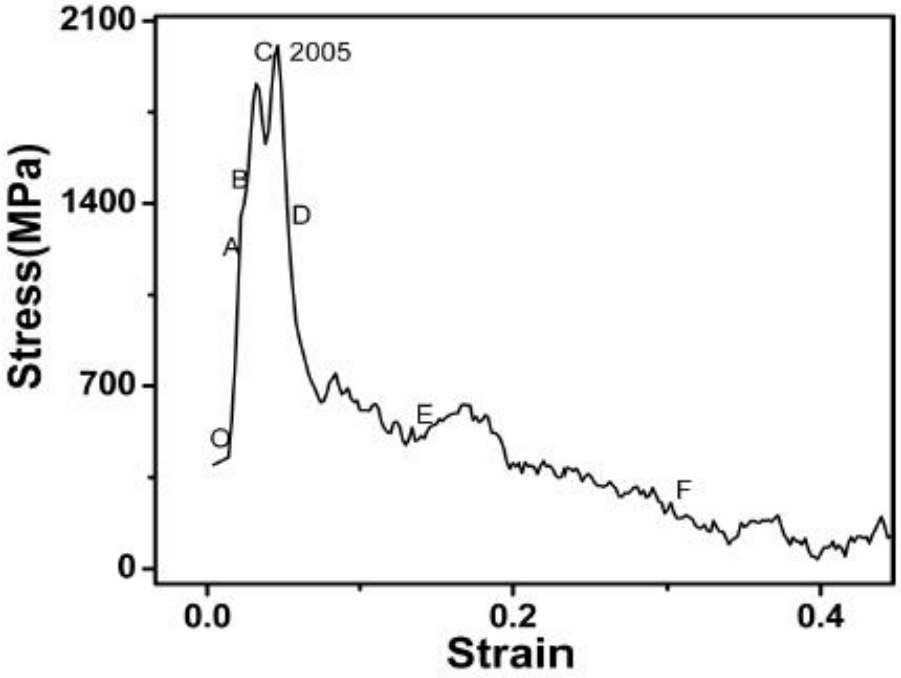


Fig.4.1.2.6.1(a)

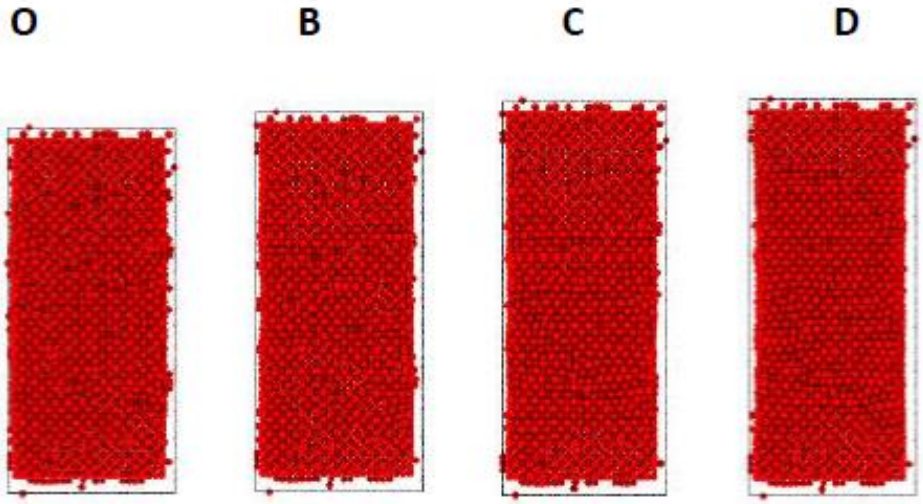


Fig.4.1.2.6.1(b)

Fig.4.1.2.6.1(a) Stress-Strain curve of 1.5KeV Irradiated Nano copper single crystal. Points O, A, B ,C,D,E and F represents different strian points during tension. Fig.4.1.2.6.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

The tensile strength and Young modulus of 1.5KeV irradiated copper sample is greater than 1KeV irradiated copper sample. The values are clearly depicted in the below table.4.1.2.6.1. The major cause for the fall of tensile strength and Young modulus is because of the creation of point defects(vacancies) and displacement of atoms due to 1.5KeV irradiation in Nano copper sample. The No. of vacancies generated by 1.5KeV irradiation in Nano copper sample is 58. The No. of defects generated are less than 1KeV irradiated copper sample and more than 0.2, 0.3, 0.5, 0.75KeV irradiated copper sample.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
1.5KeV	58	106.44	2005

Table.4.1.2.6.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 1.5KeV Irradiated Nano copper single crystal.

The following fig.4.1.2.6.2. clearly shows the defects creation in copper sample due to 1.5KeV irradiation.

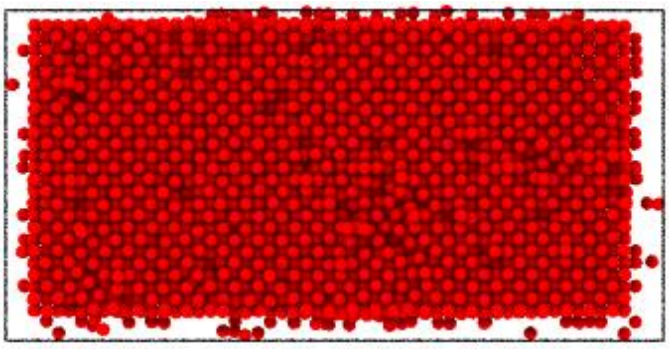


Fig.4.1.2.6.2 1.5KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

Case 4.1.2.7: Study of 2KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 2 KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.7.1(a).

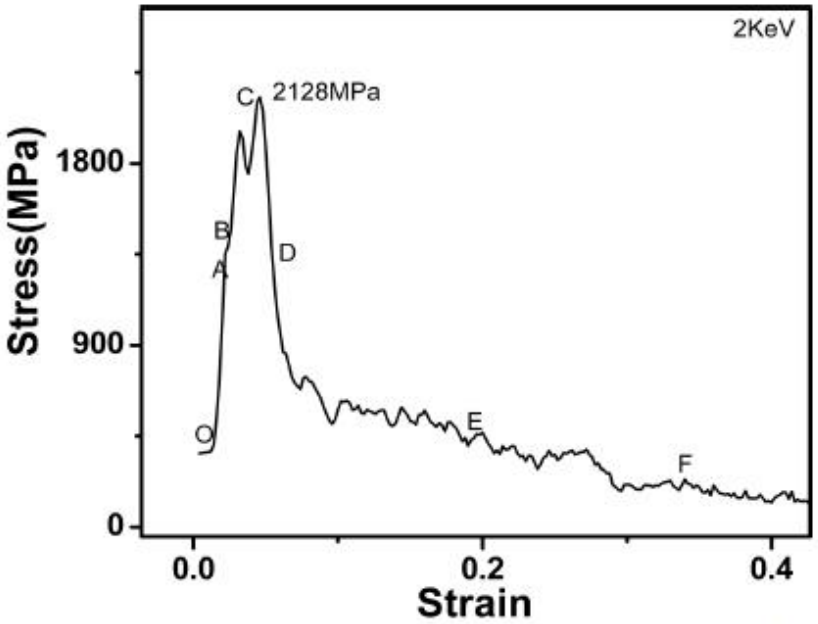


Fig.4.1.2.7.1(a)

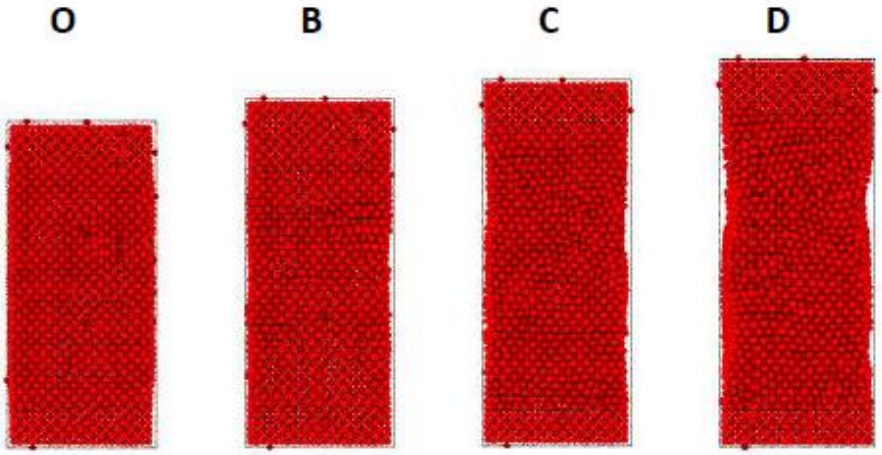


Fig.4.1.2.7.1(b)

Fig.4.1.2.7.1(a) Stress-Strain curve of 2KeV Irradiated Nano copper single crystal. Points O,A,B,C,D,E and F represents different strian points during tension. Fig.4.1.2.7.1(b) Atomic configuration of Nano copper single crystal correponding to stress-strain curve at points O, B, C, D.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
2KeV	65	109.44	2128

Table.4.1.2.7.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 2KeV Irradiated Nano copper single crystal.

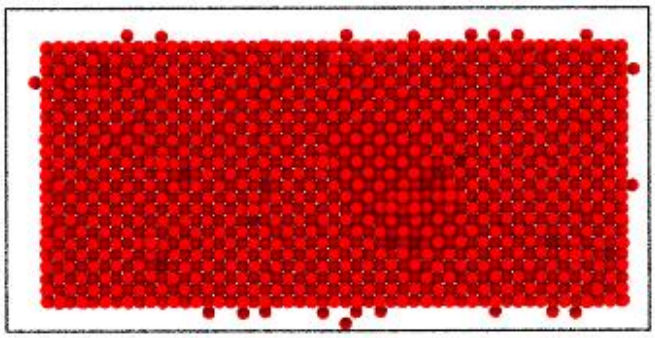


Fig.4.1.2.7.2 2KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

After 0.5KeV, again in 2KeV creation of stacking fault has been taken place during deformation.

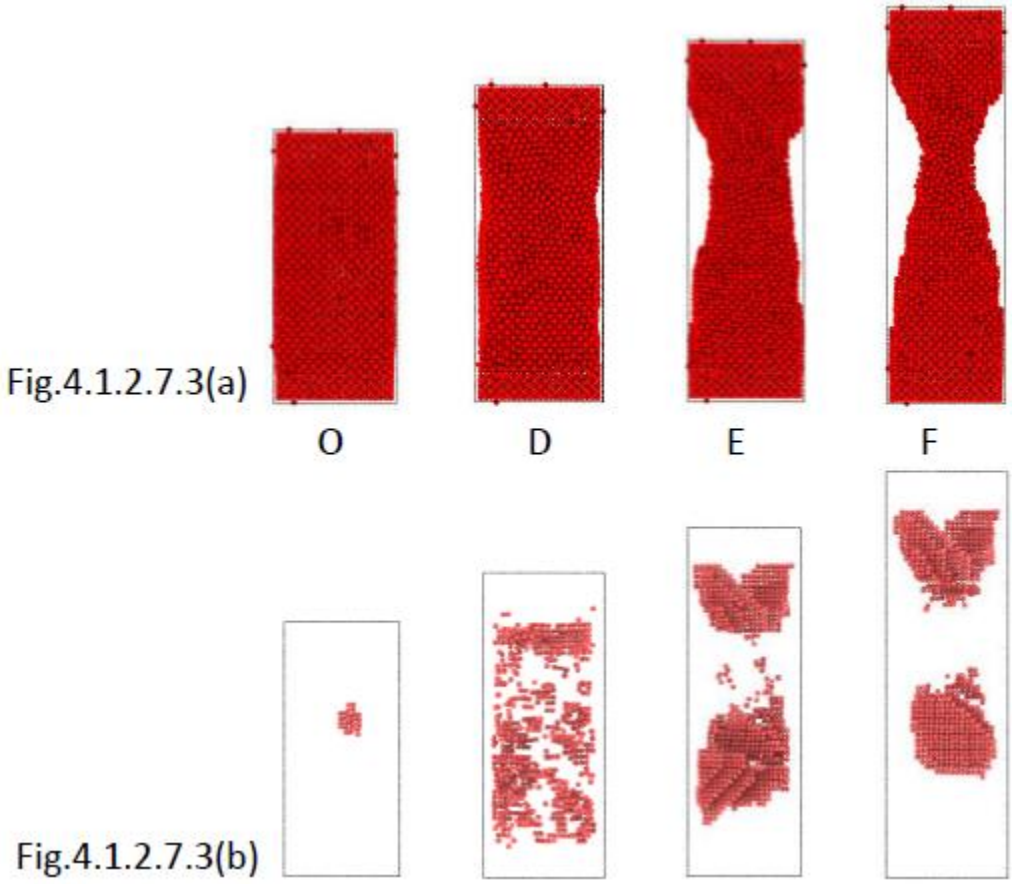


Fig.4.1.2.7.3(a) Atomic configuration of Nano-copper at points O, D, E, F corresponding to the stress-strain curve of Fig.4.1.2.7.1(a). Fig.4.1.2.7.3(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

Case 4.1.2.8: Study of 3KeV Irradiated Nano copper single crystal.

Nano copper single crystal has been irradiated by 3KeV PKA. After irradiation the irradiated copper sample has undergone tension at a strain rate of 10^10 /second. The crresponding stress-strain graph is plotted in the fig.4.1.2.8.1(a).

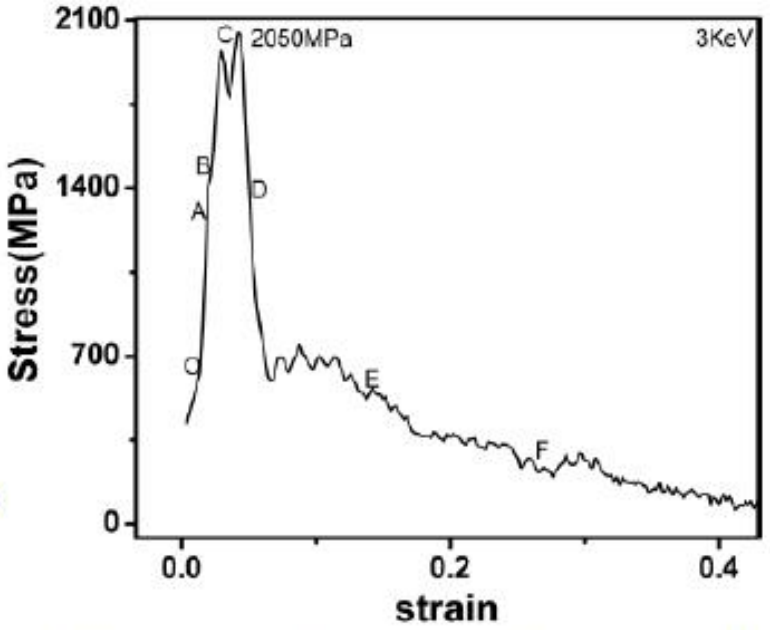


Fig.4.1.2.8.1(a)

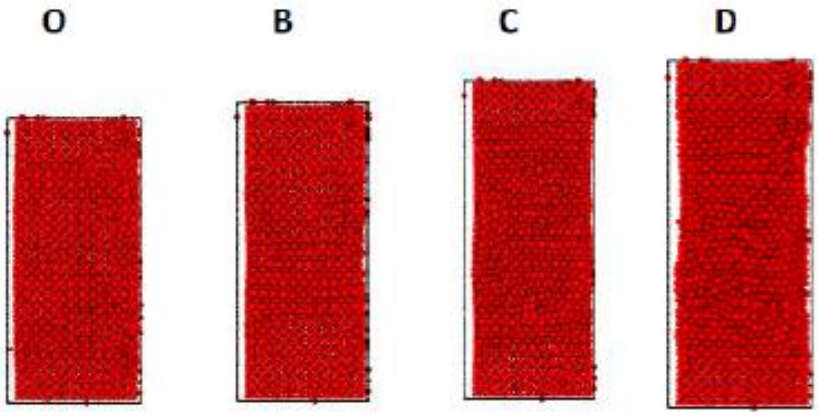


Fig.4.1.2.8.1(b)

Fig.4.1.2.8.1(a) Stress-Strain curve of 3KeV Irradiated Nano copper single crystal. Points O,A,B,C,D,E and F represents different strian points during tension.Fig.4.1.2.8.1(b) Atomic configuration of Nano copper correponding to stress-strain curve at points O,B,C, D.

Incident radiation	Vacancy No.	Young's Modulus(E_t) (GPa)	Maximum Tensile strength (σ_t) (MPa)
3KeV	84	105.916	2050

Table.4.1.2.8.1 No. of vacancies, the young moduli(GPa), and Maximum tensile strength(MPa) of the 3KeV Irradiated Nano copper single crystal.

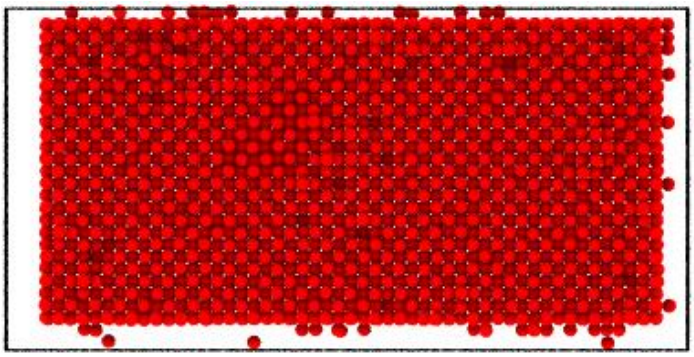


Fig.4.1.2.8.2 3KeV Irradiated Nano copper single crystal of size 5*10*5 nm^3.

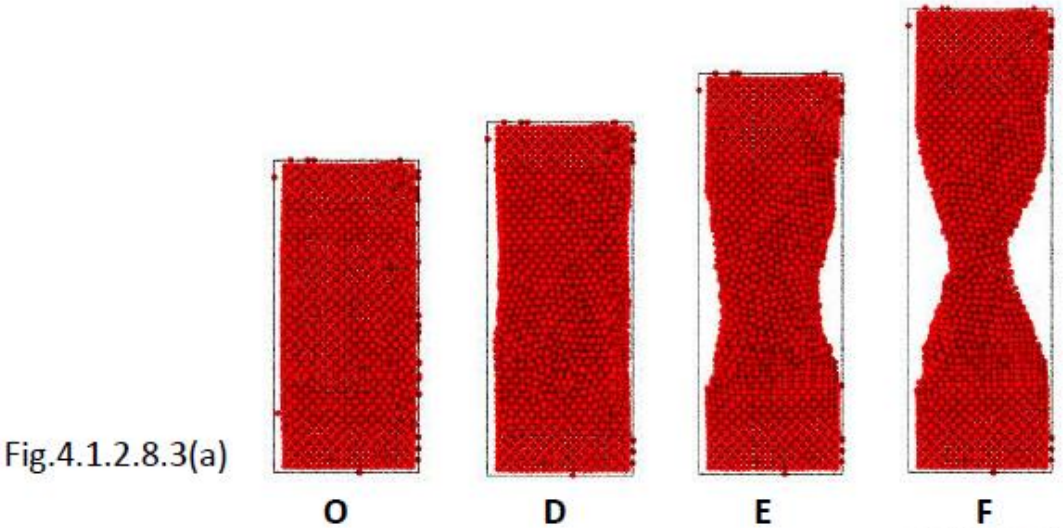


Fig.4.1.2.8.3(a)

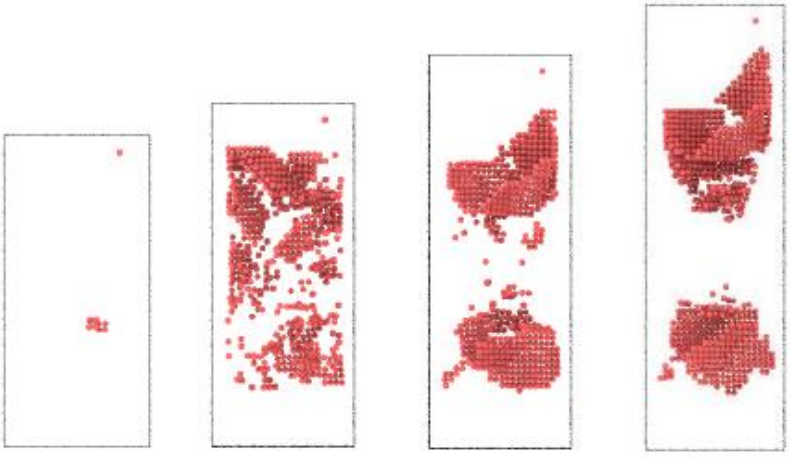


Fig.4.1.2.8.3(b)

Fig.4.1.2.8.3(a) Atomic configuration of Nano-copper at points O, D, E, F corresponding to the stress-strain curve of Fig.4.1.2.8.1(a). Fig.4.1.2.8.3(b) The perfect fcc atoms and surface atoms are removed to show the stacking fault generated by the {1 1 1}/{1 1 2} partial slip.

The No. of vacancies generated due to 3KeV irradiation in the Nano copper sample is 84. The major cause for the fall of tensile strength and Young modulus is creation of point defects(vacancies) and displacement of atoms. Fig.4.1.2.8.2 clearly shows the defects creation in copper sample due to 3KeV irradiation.

Stacking fault has generated during the tensile deformation of 3KeV irradiated Nano copper sample and this can be observed in the below fig.4.1.2.8.3(b). The creation of stacking faults has been taken place only at 0.2, 0.3, 0.5, 2 and 3KeV irradiated Nano copper single crystal samples only. From this we come to know that the generation of stacking faults will not take place in all irradiated samples.

4.2 Variation of Mechanical properties with Incident energies and Vacancies.

We irradiated the simulated single crystal Nano copper with eight different incident energies and we observed two different kind of defects, i.e., the point defect (vacancies and interstitials) and stacking faults are generated. The defect types will generally influence the mechanical properties of the copper. It is seen that for most of the irradiated samples, No. of point defects produced are more when compared to the stacking faults. The stacking faults produced in 2 and 3KeV irradiation Nano copper are more. Due to irradiation, defects appear in Nano copper and the defects distributions increased with the incident energy. From 0.2KeV to 0.75KeV the No of defects produced are 30 to 45 and for 1KeV irradiation, there is a sudden rise in No of defects, almost 90.

The point defects(vacancies) are induced by the collision between the PKA and the target atoms, in which some of the target atoms can get enough kinetic energy to get displaced from its original lattice. As the interstitials are not stable inside the irradiated copper sample, so they start migrating to the surface to form adatoms during the relaxing process. Therefore, we haven't concentrated on this interstitials and adatom defects. In this work we concentrated only on the vacancies, stacking faults and explained the mechanical properties of irradiated copper sample.

In order to analyze the effect of incident energy on the mechanical properties of the irradiated Nano copper, we plot the maximum tensile strength versus incident energy in Fig.4.2.1(a) and Young moduli(MPa) versus Incident energy(KeV) in Fig.4.2.1(b). Note that the zero incident energy denotes the case of un-irradiated Nano copper. It is observed that the maximum tensile strength decrease dramatically with Incident energy. At zero incident energy the maximum tensile strength is 2442MPa and when irradiation started with 0.2KeV the tensile strength fallen to almost 2000MPa, and as the incident energy increases from 0.2 to 0.5KeV the strength increases to 2200MPA and again falls down with increase in incident energy. There is a variation in tensile strength during irradiation is because of atomic displacement in different incident energies. The Young moduli also follows the same criteria as that of tensile strength that it also falls down with increase in the incident energy. If we observe Fig.4.2.1(b) the young moduli at zero incident energy is 136GPa and at 0.2KeV it is 108.26. Again with increase in incident energy there is a slight increase of young moduli to 114.185GPa at 0.5KeV following a drastic fall of young moduli with incident energy. From this we conclude that, with irradiation the tensile strength and young moduli gradually falls down with increase of incident energy.

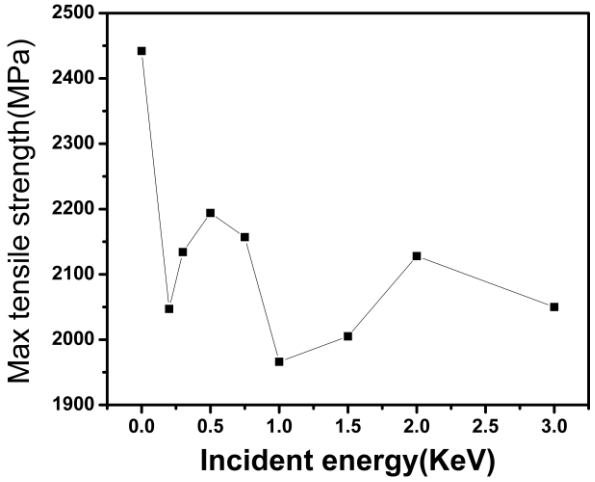


Fig.4.2.1(a)

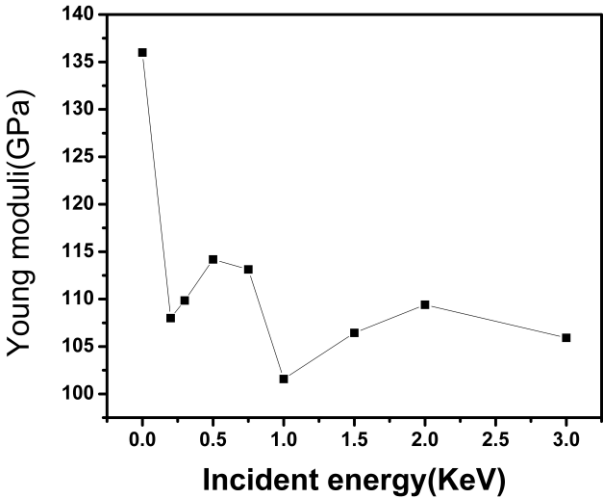


Fig.4.2.1(b)

Fig.4.2.1(a) Variation of the maximum tensile strength(MPa) with incident energy(KeV) (zero incident energy denotes the case of un-irradiated Nano copper sample). Fig.4.2.1(b) Variation of Young moduli(GPa) for tension(E_t) with incident energies(KeV).

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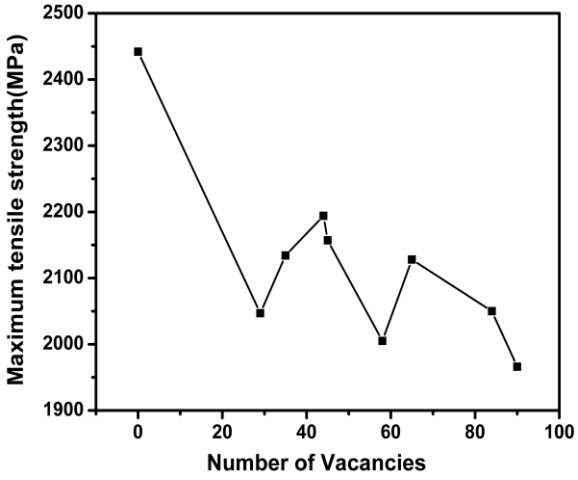

Fig.4.2.2(a)

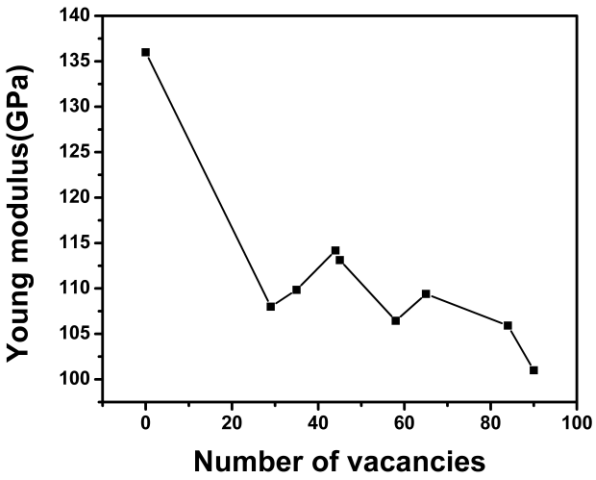

Fig.4.2.2(b)

Fig.4.2.2(a) Variation of maximum tensile strength in tension with number of vacancies. Fig.4.2.2(b) Variation of Young moduli(GPa) for tension (E_t) with number of vacancies.

In Fig.4.2.2 we plot the tensile strength and young moduli with No. of vacancies. Irradiation induced vacancies reduce the young modulus, and the reduction extent is proportional to number of vacancies. In comparison of tensile strength, the young modulus variation with number of vacancies is less and finally there is a decrease of young modulus with increase of incident energy. Hence the young modulus and tensile strength of un-irradiated Nano copper is more when

compared to the irradiated Nano copper. Irradiation induces point defects (including vacancies, interstitials and adatoms) in Nano copper, and these point defects soften the Nano copper. When strain is applied on an irradiated Nano copper, defects (i.e., vacancies) offer room for the atomic relaxation, which relieves the stress. Therefore, compared with un-irradiated Nano copper, a small stress is experienced by the irradiated Nano copper under the same strain, and results in a small young modulus. The yield stress of the Nano copper also decreases with irradiation.

5 Conclusion

1. Defects like stacking fault, vacancies and interstitials are formed due to irradiation.
2. Young's modulus is decreased in the irradiated Nano copper samples due to point defects and that is because of the relief of applied stresses by atomic relaxation near the defects.
3. Due to smaller Young's modulus and yield strain, significant fall of yield stress takes place due to irradiation.
4. Surface defects at the surface edge, advance the nucleation of partial dislocations, that results in the yield of the irradiated Nano copper at a smaller strain.
5. Generating of stacking faults will not takes place in all irradiation conditions.

Future Work

In our research work we have Irradiated the Nano copper samples from 0.2KeV to 3KeV and calculated the mechanical properties and analyzed the defects formation process with radiation. The structural analysis of the irradiated Nano copper has not analyzed in this research work and that can be considered as future work.

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