Proceedings of ICONE14
International Conference on Nuclear Engineering
July 17-20, Miami, Florida, USA

ICONE14-89685

MODELLING OF IRRADIATED MATERIALS

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ABSTRACT

Irradiation of materials by energetic particles causes significant degradation of the mechanical properties, most notably an increased yield stress and decrease ductility, thus limiting lifetime of materials used in nuclear reactors. The microstructure of irradiated materials evolves over a wide range of length and time scales, making radiation damage and inherently multi-scale phenomenon. At atomic length scale, the principal sources of radiation damage are the primary knock-on atoms that recoil under collision from energetic particles such as neutrons or ions. These knock-on atoms in turn produce vacancies and self-interstitial atoms, and stacking fault tetrahedra. At higher length scale, these defect clusters form loops around existing dislocations, leading to their decoration and immobilization, which ultimately leads to radiation hardening in most of the materials. All these defects finally effect the macroscopic mechanical and other properties. An attempt is made to understand these phenomena using molecular dynamics studies and discrete dislocation dynamics modelling.

INTRODUCTION

The microstructure of irradiated materials evolves over a wide range of length and time scales, making radiation damage and inherently multi-scale phenomenon. The primary source of damage in the irradiated material is the displacement cascades generated by the primary knock-on atom (PKA) recoiled under the collision with the energetic particle. The spectrum of energy acquired by recoiled PKA is very wide ranging from few hundred electronvolts to tens of kiloelectronvolts. The number of atoms perturbed by primary and secondary collisions depends upon recoil energy of the PKA and can reach up to few thousands. The recoiled energy of the PKA is dissipated in the lattice and if the KE of PKA is sufficiently higher it results in the formation of heated core and hundreds of atoms displaced from their equilibrium lattice position. Temperature of this heated core dissipated gradually in surroundings and overall temperature of the system is raised. Most of the displaced atoms regain some equilibrium position in the lattice but some of them failed to return on equilibrium position and thus form self-interstitial atoms (SIA) and vacancy pair. Local stress concentration in the lattice is resulted due to formation of SIA-vacancy pair. The movement of the dislocations is also affected by creation of SIA-vacancy formation. The deformed lattice evolves over prolonged periods of time and affects several physical and mechanical properties.

For irradiated materials, interaction of dislocations with irradiation-induced defects entirely controls the plastic yield. Over macroscopic length scale, these defects can alter the microstructure causing significant degradation of mechanical and other properties. The main notable features of irradiation-induced mechanical behavior are: an increased yield strength with irradiation dose, and an instability that results in plastic flow localization within dislocation channels leading to loss of ductility and premature failure. Because of present computer simulation techniques, it has become possible to model these irradiation phenomena and their corresponding effect on macroscopic deformation behavior. We used the atomistic modelling using molecular dynamics studies and the discrete dislocation dynamics studies for determining the irradiation effects on material behavior.

ATOMISTIC MODELLING

The process of irradiation involves extremely small time and length scales, which makes experimental study of the phenomenon impractical. With the ever-increasing computational power associated with advance techniques to simulate the material at atomistic level it is possible to simulate the process of irradiation and displacement cascading. Molecular Dynamics (MD) provides a suitable tool to simulate the process of irradiation with high degree of accuracy. A typical MD system for irradiation simulation consists of model

of crystal with thousands of atoms, which interacts with each other with many body potential (MBP). Embedded Atom Method (EAM) potential is a MBP and is used to simulate the metals successfully.

One of the atoms in the domain is selected as PKA and it is provided with some kinetic energy. The kinetic energy of PKA is dissipated in the lattice with time and in this process displacement cascades is produced if KE of PKA is sufficiently high. A region of highly perturbed atoms is formed in the core of the system and in this core region temperature reaches extremely high values. The temperature of the core is gradually dissipated into the system. The simulation is continued till the system reaches uniform temeprature. MD simulation is performed in NVE ensemble (Constant volume and energy) and no attempt has been made to control the temperature. The output of the simulation is in the form of trajectory of atoms displaced due to cascade, number of SIA-vacancy pairs proudced N_F and their distribution in the lattice [1].

SEMI-EMPIRICAL RELATIONS

NRT model by Norgett et. al [2] provides theoretical assessment of defect production in displacement cascades by deriving simple relationship between the number of SIA-vacancy pairs (N_{NRT}) created by cascade and kinetic energy E_P of PKA:

$$N_{NRT} = 0.8\,E_{dam}/(2\bar{E}_d) \tag{1}$$

where N_{NRT} is the value of N_F in the Norgett, Robinson and Torrens (NRT) formulation, E_d is the value of the threshold displacement energy over all crystallographic directions and E_{dam} is the damage energy available for elastic collision i.e. E_P with inelastic losses subtracted (since losses have not been included in most MD simulations the replacement of Edam by E_P in eqn. (1) is appropriate for comparing its prediction with N_F obtained from MD).The binary collision model on which the NRT formula is based does not accurately describe atomic interactions take place in the heated core due to cascade and is not suitable modeling the actual configuration of defects. MD simulation on the other hand, use inter-atomic potential fitted to many of the equilibrium and defect properties of metals and do offer more realistic description of cascade process [3].

NRT model does not predict the accurate number of defects, in fact, N_F us typically only 20% to 40% of N_{NRT} for a given cascade energy when E_P is larger then about 1-2 Kev. By considering MD generated N_F data for several metals, it was shown in [4] that a empirical relationship between N_F and E_P gives a good fit to the simulation data for E_P up to 10 Kev:

$$N_F = A\left(E_p\right)^m \tag{2}$$

where, A and m are constants which are weakly dependent on the material and temperature.

MD SIMULATION DETAILS

In this paper we have estimated the number of SIA-vacancy pairs (N_F) produced in displacement cascade using our in-house MD simulation code for Nickel with different recoil energy of PKA. Cubical and parallelepiped domain has been taken for the analysis and the size of computational domain is taken proportional to the recoil energy of the PKA so that the final temperature of the domain should remain in desired limits. A typical size of domain taken for 5 Kev recoil energy of PKA run is 20 unit cells in each direction with 32000 atoms in the computational domain. The system is equilibrated until the temperature of the domain becomes uniform (approximately 5 pico-second). In the cascading process a number of collisions take place and atoms come very close to each other. This reduced atomic distance associated with the high kinetic energy of the atoms poses stringent requirement on the size of time step. This makes the run of typical MD run for irradiation very slow. However, we don't need the smallest time step at all inter-atomic distances. A lower value of time-step is needed when the inter-atomic distance is small and vice-versa. Similarly, when the speed or kinetic energy of the atoms is high we need small time step. By using adaptive time step size according to the above requirement, we can speed up the MD run and use the computational resources optimally. The force of repulsion between two atoms is exponential in nature such that the gradients are steeper at smaller separations. Similar to the exponential nature of repulsive force we can choose time step, which exponentially depends on the minimum value of separation in the domain and inversely proportional to the maximum value of speed in the domain.

$$\Delta t = A\exp(-B\,r_{\min})/v_{\max} \tag{3}$$

where A is the parameter controls the minimum value of the time step and B controls the rate of decrement of time step, v_{max} is the maximum speed in the domain. The size of time step in a typical MD run varies from 10^{-16} to 10^{-18} seconds. We have used this adaptive time step in our MD run to simulate the cascading process optimally.

RESULTS OF ATOMISITC SIMULATIONS

We have performed MD simulation for three different recoil energies of PKA i.e. 2 Kev, 3 Kev and 5 Kev. Domain size for 2 Kev and 3 Kev MD run is 20x16x16 unit cells with number of atoms in the domain are 20480. Cubical domain has been taken for the 5 Kev run with 20 unit cells in each direction and the total number of atoms in the domain is 32000. Initial temperature of the domain for each run is taken 50 K. Final temperature after the irradiation process for 2, 3 and 5 Kev run is found out to be 464 K, 594 K and 667 K respectively. The trajectory of the perturbed atoms in displacement cascade are depicted in Fig. 1. Figure 2 shows the distribution of SIA-vacancy defects (N_F) in the domain in typical displacement cascade. Snapshots at different time steps after the energetic particle collides with PKA are shown in Fig.3. The values of N_F generated by our in-house code for Nickel with different recoil energy of PKA are shown in Table. 1. The N_F values generated are in close agreement with the values predicted by eqn.(2). Values of A and m in equation 2 are taken from [3] as 4.37 and 0.74 respectively.

Table 1: Vacancy-interstitial pairs for different PKA energies

Recoil energy of PKA (in Kev)	No. of vacancy/ interstitials pairs N_F	
	By simulation	By eqn. (2)
2.0	9	7
3.0	10	10
5.0	12	14

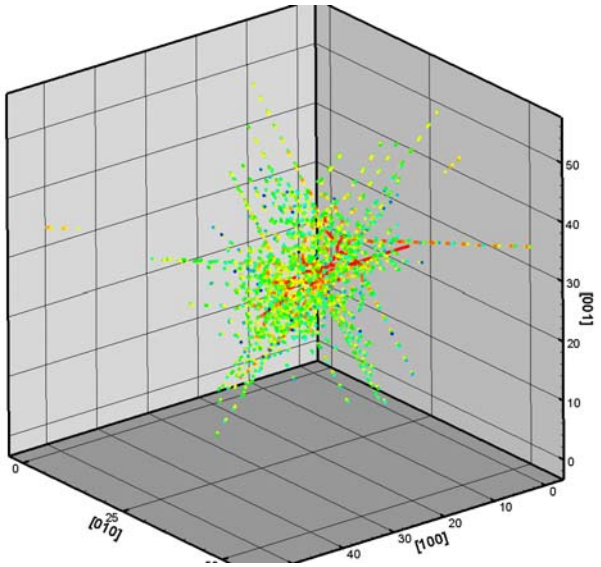


Fig. 1: Trajectory of atoms which acquire at least 1 ev KE

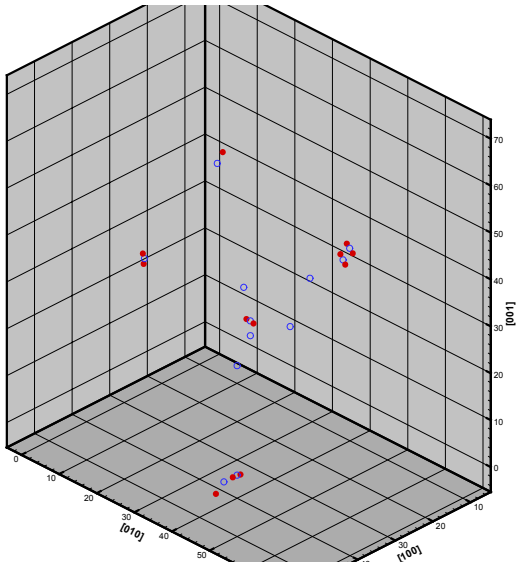


Fig. 2: Vacancy (open circles) and interstitial(filled circles) pairs generated as result of displacement cascade.

DISCRETE DISLOCATION DYNAMICS MODELLING

In a second kind of study dealing with higher length scale, we used the two dimensional discrete dislocation dynamics (DD) modelling to study the irradiation effects on material stress-strain response. An in-house code for DD analysis is developed based on formulation given in [5]. The plastic flow is represented by collective motion of a large number of edge dislocations. The dislocation fields are specified by continuum elastic theory. Since the elastic fields act infinite in medium, corrections for boundaries are specified by a complimentary problem which consists of solving a linear elastic boundary value problem through finite element method. The dislocation phenomenon like annihilation, generation and pinning of dislocations by obstacles are incorporated in the model through some constitutive rules. Irradiation effects are numerically modeled by locking all the dislocations with irradiation induced defects thus characterizing the fluence. These dislocations get unlocked when the stress on them exceeds a critical stress due to irradiation defects. The stress-strain response of an irradiated Copper as a function of total fluence is studied.

FORMULATION FOR 2D- DD ANALYSIS

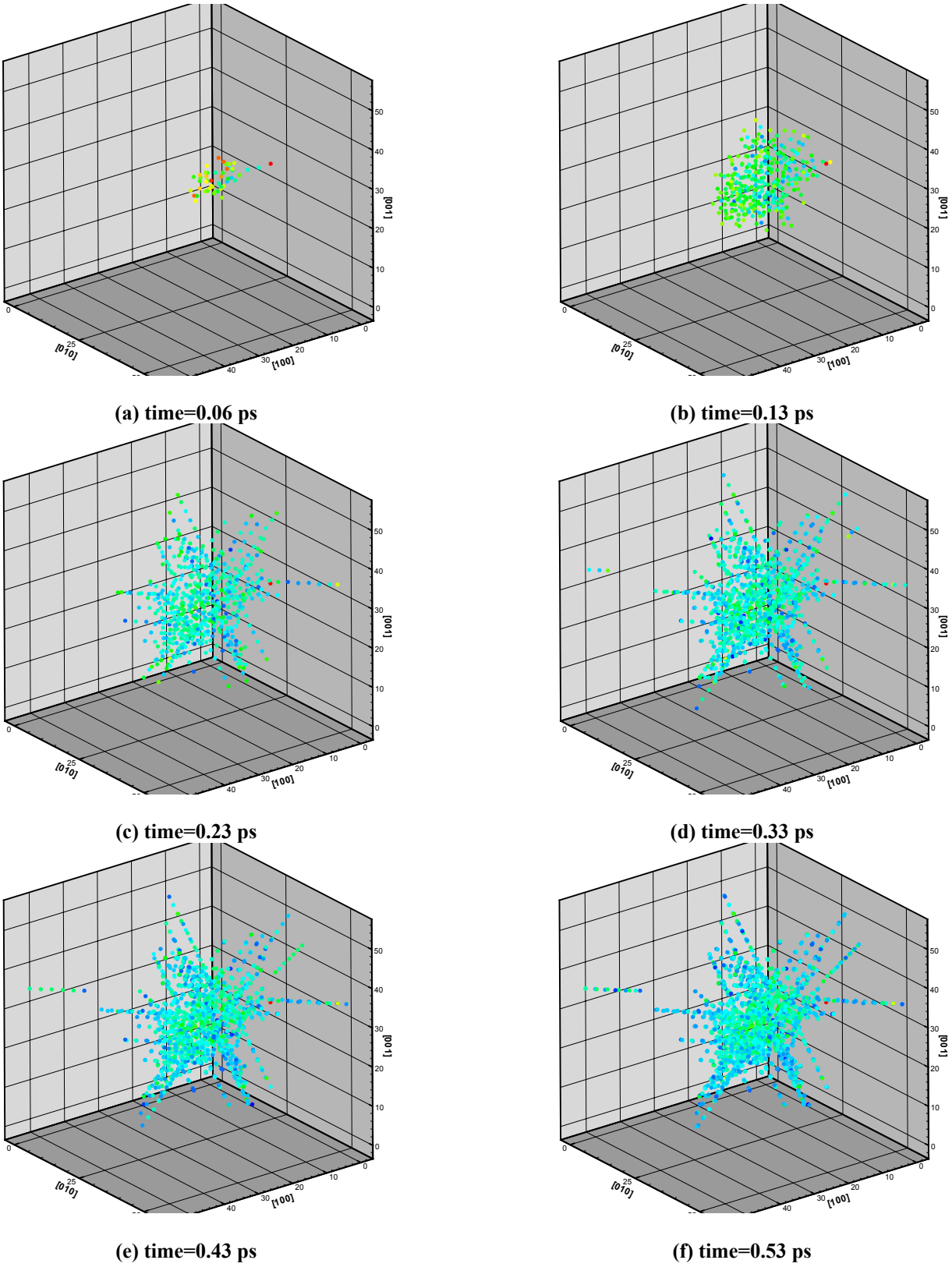
The problem is formulated as follows: Consider a linear elastic body of volume V which contains a distribution of dislocations. The dislocations are treated as line defects in the elastic continuum. Each dislocation is characterized by its Burger's vector bi and its slip plane. The body is subjected to time dependent traction and displacement boundary conditions $T=T_o(t)$ on S_f and $u=u_o(t)$ on S_u. The deformation process will lead to the motion of dislocations, mutual annihilation and generation of new dislocations and their pinning at point obstacles. The obstacles may be second phase particles, defects generated due to irradiation etc. The analysis of deformation process is performed in an incremental manner in time, where the incremental step at any instant t involves three main computational stages: (i) determining the current stress and strain state of for the current dislocation arrangement; (ii) determination of the so-called Peach-Koehler force, i.e., the driving force for changes in dislocation structure; and (iii) determination of the instantaneous rate of change of dislocation structure on the basis of a set of constitutive equations of motion, annihilation and generation of dislocations. All the three stages of computation are described below.

The current state of body in terms of the displacement, strain and stress fields is written as the superposition of two fields,

$$u = \tilde{u} + \hat{u} \quad \varepsilon = \tilde{\varepsilon} + \hat{\varepsilon} \quad \sigma = \tilde{\sigma} + \hat{\sigma} \ \ in \ \ V \tag{4}$$

respectively, as illustrated in Fig. 4. The (~) fields are associated with the n dislocations in the current configuration but in infinitely large medium of material. These fields are obtained by superposition of the fields associated with each individual dislocation,

$$\tilde{u} = \sum_{i=1}^{n} u^i \quad \tilde{\varepsilon} = \sum_{i=1}^{n} \varepsilon^i \quad \tilde{\sigma} = \sum_{i=1}^{n} \sigma^i .$$



(a) time=0.06 ps **(b) time=0.13 ps**

(c) time=0.23 ps **(d) time=0.33 ps**

(e) time=0.43 ps **(f) time=0.53 ps**

Fig. 3: Snapshots of perturbed atoms which acquired at least 1ev of KE in cascade process at intermediate time steps.

The corresponding displacement ($\tilde{u}$) and stress ($\tilde{\sigma}$) fields of a dislocation i are given by:

$$u_1^i = \frac{b^i}{2\pi(1-\nu)}\left\{\frac{1}{4}\frac{\pi\Delta\xi_2 \sin\pi\Delta\xi_1}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1}-(1-\nu)\tan^{-1}\left(\frac{\tan\pi\Delta\xi_1/2}{\tanh\pi\Delta\xi_2/2}\right)\right\} - \frac{b^i}{2}\delta^i sign(\Delta\xi_2)$$

$$u_2^i = \frac{b^i}{2\pi(1-\nu)}\left\{\frac{1}{4}\frac{\pi\Delta\xi_2 \sinh\pi\Delta\xi_2}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1} - \frac{1}{4}(1-2\nu)\ln(\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1)\right\}$$

$$\sigma_{11}^i(x_\alpha) = -\frac{\mu}{2\pi(1-\nu)}\frac{\pi b^i}{2w}\frac{1}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1} \times\left\{2\sinh\pi\Delta\xi_2+\pi\Delta\xi_2\frac{1-\cos\pi\Delta\xi_1\cosh\pi\Delta\xi_2}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1}\right\}$$

$$\sigma_{12}^i(x_\alpha) = \frac{\mu}{2\pi(1-\nu)}\frac{\pi b^i}{2w}\frac{\sin\pi\Delta\xi_1}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1} \times\left\{1-\pi\Delta\xi_2\frac{\sinh\pi\Delta\xi_2}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1}\right\}$$

$$\sigma_{22}^i(x_\alpha) = \frac{\mu}{2\pi(1-\nu)}\frac{\pi b^i}{2w}\left\{\pi\Delta\xi_2\frac{1-\cos\pi\Delta\xi_1\cosh\pi\Delta\xi_2}{\cosh\pi\Delta\xi_2-\cos\pi\Delta\xi_1}\right\}$$

where, $\Delta\xi_\alpha = (x_\alpha - X_\alpha^i)/w \quad (\alpha = 1,2)$, $u_\alpha^i(\alpha = 1,2)$ are the displacements due to dislocation *i* at (x,y). The term δ^i in displacements fields ensures that the solution is valid for $\Delta\xi_1 \in (-1,1)$, by letting

$$\delta^i = \begin{cases} -1 & if\ \Delta\xi_1 \in (-3/2,-1/2) \\ +1 & if\ \Delta\xi_1 \in (1/2,3/2). \end{cases}$$

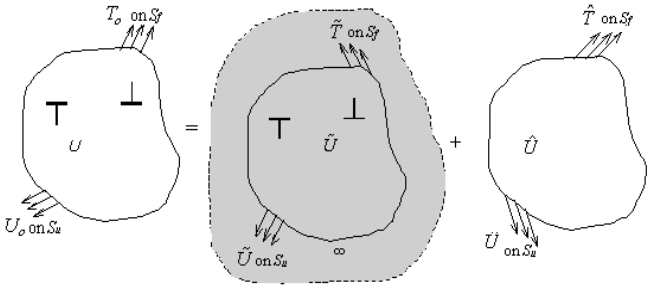


Fig. 4: Decomposition of problem into problem of dislocations in infinite solid (~fields) and complementary problem without dislocation fields (^ fields)

Because of periodic boundary conditions, dislocation leaving the cell at $x_1 = \pm w$ will re-enter at the opposite side $x_1 = \mp w$. Only the displacement fields of the dislocation need to be corrected for that by adding the contribution,

$$u_1^i(x_\alpha) = \frac{b^i}{2}\delta^i sign(\Delta\xi_2).$$

As the solution for (~) fields is facilitated by virtue of absence of boundaries, the (^) fields are added to correct the actual boundary conditions on S. This leads to a linear elastic complementary boundary value problem, the governing equations of which are given by,

$$\left.\begin{aligned}\nabla.\hat{\sigma} = 0 \\ \hat{\varepsilon} = \nabla\hat{u}\end{aligned}\right\} in\ V$$

$$\left.\begin{aligned}\hat{T} = T_o - \tilde{T}\ \ on\ S_f \\ \hat{u} = u_o - \tilde{u}\ \ on\ S_u\end{aligned}\right\} b.c's$$

Solution to this complementary boundary value problem is obtained using finite element method. The motion of the dislocations is governed by constitutive equations according to liner drag relation given by,

$$\tau^i b^i = Bv^i \tag{5}$$

where, $\tau^i b^i = f^i$ is the Peach-Koeheler force, B is the drag coefficient and v is the velocity of a dislocation. The result of the above formulation is a set of non-linear first order differential equations governing the motion of the dislocations, which are solved using Euler forward time integration method.

The motion of dislocations along a slip plane can be hindered in real crystals by obstacles such as dislocations on intersecting slip planes, small precipitates etc. We model this by means of point obstacles at which moving dislocations get pinned down. Such pinned dislocations will be released when the resolved shear strength on them exceeds the obstacle's strength (τ_{obs}). Two edge dislocations with opposite Burger's vector will annihilate each other when they are brought closer together within a critical annihilation distance Le. New dislocations are being generated through the operation of Frank-Read sources. We assume that sources are point sources on the slip plane, which generate a dislocation dipole when the magnitude of the shear stress exceeds the critical stress (τ_{nuc}) during a period of time t_{nuc}. The distance L_{nuc} (see [5]) between the two dislocations is determined by the critical stress according to

$$L_{nuc} = \frac{\mu}{2\pi(1-\nu)}\frac{b}{\tau_{nuc}}.$$

STRESS-STRAIN RESPONSE FOR IRRADIATED COPPER UNDER SIMPLE SHEAR USING DD

Here, we consider the problem of irradiation-induced hardening in Copper. Plastic deformation and hardening in irradiated materials is controlled primarily by the defects due to irradiation (vacancies, self-interstitial atoms and SFT's) and their interaction with dislocations. These defect clusters will tend to form loops around existing dislocations, leading to their decoration and immobilization. In order to understand the effect of this phenomenon on deformation behavior, we

consider irradiated copper under simple shear using two-dimensional DD model described above. An attempt is made to find the relationship between the irradiation fluence and yield stress of Copper using DD modelling. In spite of the fact that this phenomenon is fully three dimensional in nature, first order prediction can be made of yield stress as a function of fluence level using the two-dimensional model.

The irradiation induced hardening may be understood in terms of cascade induced source hardening in which the dislocations are considered to be locked by the loops decorating them[6,7]. The density and strength of these defect loops depend on the fluence level. To mimic these irradiation effects, we assume that all the dislocations are locked by the defect loops thus characterizing the fluence. When the total stress on the dislocations exceeds a critical value σ_{cr}, they get unlocked and become free to move on their glide planes. The motion of the dislocations is governed by eqn.(5). During gliding, any dislocation may get pinned down by the point obstacles or may get annihilated by an opposite dislocation. New dislocations will be generated by Frank-Read mechanism, which is mimicked here by point sources. These sources will nucleate a dislocation dipole when stress on a source exceeds a critical value. The effect of irradiation on stress-strain behavior is then obtained by subjecting the copper unit cell to simple shear.

The simulated copper cell is assumed to be of dimensions 2μm × 2μm. The shear modulus μ =55 Gpa and the Poisson's ratio is ν = 0.3. The drag coefficient B in eqn. (5) is taken as 10^{-4} Pa.s. The plastic flow is represented by a collection of large number of edge dislocations. We assume that the material consists of randomly distributed defect structure, such as point obstacles, Frank-read dislocation nucleation sources. The material is assumed to have an initial dislocation density of $\rho_{disinit}$= 200/hw, which is then relaxed. During relaxation, the dislocations will interact with each other and try to attain equilibrium position. In the relaxed configuration, obstacles and nucleation sources are randomly generated. All the obstacles are assumed to have same strength $\tau_{obs}=5.7\times10^{-3}\ \mu$. The strength of sources is selected randomly from a Gaussian distribution with a mean strength of $\bar{\tau}_{nuc}=1.9\times10^{-3}\ \mu$ corresponding to a mean nucleation distance of L_{nuc}= 125b and the nucleation time is taken as $t_{nuc}=2.6\times10^{6}\ B/\mu$.. The strength distribution is assumed to have a standard deviation of $0.2\,\bar{\tau}_{nuc}$. The critical annihilation length is taken as L_e=6b. The unit cell is subjected to simple shear along top and bottom edges in time incremental manner, with a strain rate of $\dot{\Gamma}$,

$$\left.\begin{aligned} u_1(t) &= \pm h\dot{\Gamma}t \\ u_2(t) &= 0 \end{aligned}\right\} \quad \text{along } x_2 = \pm h.$$

Typical predicted stress-strain curves for various critical values of σ_{cr} are shown in Fig.5 which reveals the effect of dislocation loops on increased yield stress. In order to eliminate any numerical fluctuations, averaging over 5-6 samples is done to obtain the observed stress-strain behavior. Any fluctuation thus seen in Fig.5 is because of the physics of dislocation motion rather than numerical computation.

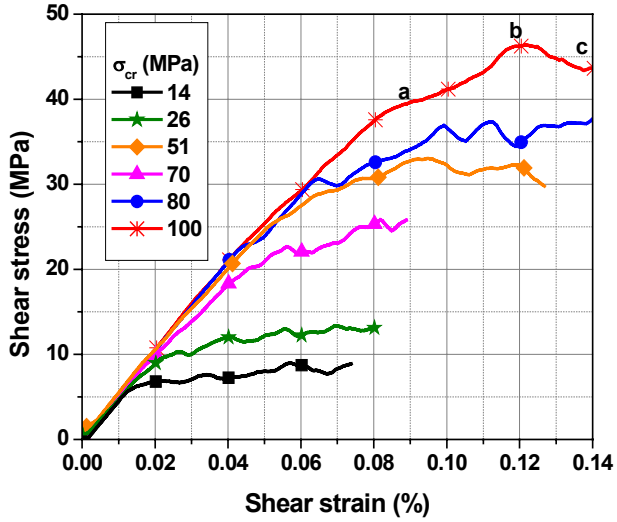


Fig. 5: Stress-strain response of irradiated Copper as a function of critical locking stress σ_{cr}.

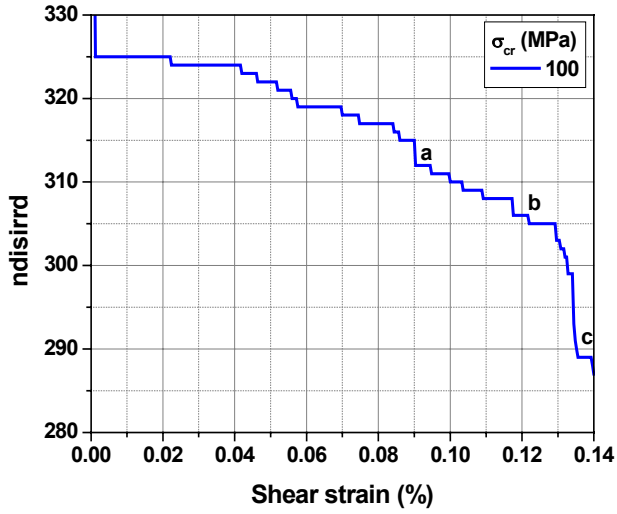


Fig. 6: Variation of no.of dislocation locked by irradiation defects (ndisirrd) Vs. shear strain for σ_{cr}=100 MPa .

When σ_{cr} is increased from 14 MPa to 100 MPa, the corresponding yield stress σ_y increases from 6 MPa to 40 MPa. Without irradiation, the single Copper crystal yields at 2-4 MPa[8]. When irradiation induced-defects are present, the yield point rises drastically which can be attributed to the locking of dislocations by these defects. Moreover at very high values of fluence, the experimentally observed instability can also be reproduced by DD modelling as shown in Fig. 5 for high values of σ_{cr}. At larger values of fluence, two characteristics are seen. First, the system yields at very high stress and second, a sudden instability occurs after reaching a maximum stress value. This can be attributed to a sudden unlocking of a large chunk of dislocations from the irradiation-induced defects. This

is clearly seen by points *a,b&c* in Fig. 5 corresponding to σ_{cr}=100 MPa. The system yields at point *a*; there is strain hardening upto point *b* and then a sudden drop in stress value occurs (point *c*).

This effect can be clearly seen again at point *a,b &c* in Fig. 6, where the variation of number of dislocations being locked by irradiation-induced defects is shown as a function of shear strain. As seen from point *b* to *c*, a large number of dislocations are unlocked from irradiation induced defects and hence the instability in stress-strain response occurs. These results show that such instabilities can be reproduced by numerical DD modelling. Fig. 7 shows the dislocation configurations corresponding to σ_{cr}=80 MPa at: a) zero strain and b) after shearing upto 0.14%; the Frank-Read dislocation nucleation sources and the point obstacles are also shown in the figure.

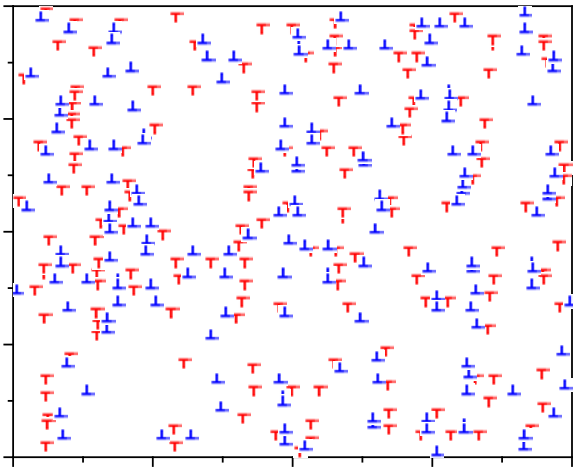


Fig. 7 a: Initial dislocation configuration in the cell

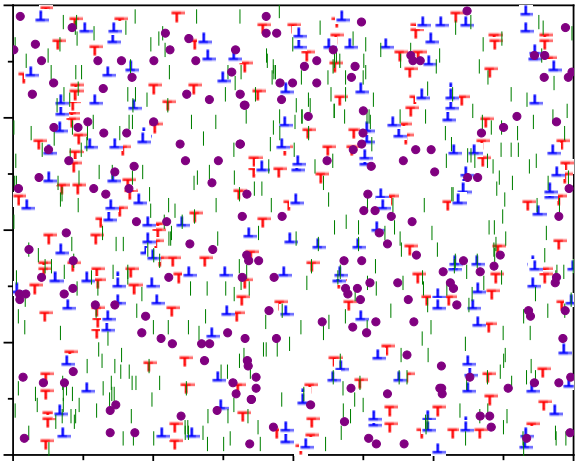


Fig. 7 b: The dislocation configuration in the cell at shear strain of 0.14% and σ_{cr}=80 MPa. ⊥ indicates a +ve dislocation, ⊤ indicates a –ve dislocation. Frank-Read sources (•) and obstacles (|) are also shown.

Finally, to correlate the irradiation fluence to critical stress σ_{cr}, we made use of experimental yield stress values (at 77 ^{o}K) of single crystals of Copper [8] irradiated at different fluence levels. Table.2 gives these experimental upper yield points as a function of irradiation fluence ϕ. From the results of our DD model (*see* Fig.5), the critical stress values σ_{cr} corresponding to the experimental yield stress values are obtained. In Fig.8, these critical stress values (σ_{cr} -exptal) are plotted as function of irradiation fluence ϕ. We also tried to make a possible curve fit of these experimental critical stress values in terms of ϕ as given below:

$$\sigma_{cr} = 5+9\times\phi\times10^{-20}; \quad for\ \phi\times10^{-20}<5$$

$$= 46+\frac{\sqrt{3}}{2}\phi\times10^{-20}; \quad for\ \phi\times10^{-20}>5$$

Such expressions can then be used to find out critical locking stress σ_{cr} at any other fluence ϕ. Now, to find out the yield stress σ_y at any fluence ϕ, first using this expressions, the corresponding σ_{cr} is determined. Then the DD model is run with this σ_{cr} to find out the yield stress of the crystal at that fluence level. Even though current model is two-dimensional and considers only edge dislocations, the results illustrate the use of DD simulations for first order prediction of σ_y as a function of fluence.

Table 2: Experimental yield stress values of irradiated Copper single crystal at 77 ^{o}K [8]

Irradiation fluence ϕ (n m^{-2})	Upper yield stress (MPa)
0	3
4.7x10^{20}	18.75
1.0x10^{21}	21.7
5.0x10^{21}	35.38

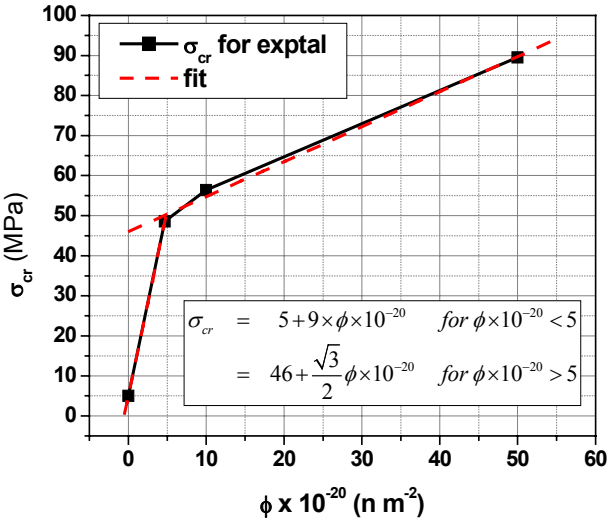


Fig. 8: Variation of critical locking stress σ_{cr} as a function of fluence ϕ. Possible two linear fit expressions for the same are also shown.

CONCLUSION

The irradiation effects on metals are studied using the atomistic molecular dynamics simulations and two-dimensional discrete dislocation dynamics modelling. At atomic length scale, cascading effects of irradiation on Nickel single crystal have been studied using the MD simulation technique with EAM potential. An adaptive time step scheme has been used to speed-up the MD simulation. Number of SIA-vacancy pair ($N_{F)}$ is determined for different recoil energies of PKA. At a higher length scale, two dimensional discrete dislocation modelling is used to determine irradiation induced hardening of Copper single crystal. Dislocations get pinned down due to irradiation induced defects. This is modeled by locking all the dislocations by critical stress σ_{cr}, thus characterizing the irradiation fluence phenomenologically. The dislocations are required to overcome this σ_{cr} to get unlocked before they can move on their glide planes under external stress. The dislocation phenomena like annihilation, nucleation, pinning down by obstacles are also incorporated. Parametric study with respect to the critical locking stress and its effect on stress-strain response is studied. An expression for this critical locking stress in terms of irradiation fluence is proposed. The yield stress of irradiated copper crystal can then be determined by the DD model by taking the critical locking stress corresponding to that fluence level.

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