Effect of irradiation in different velocity vectors on the mechanical properties of Nickel single crystal using Molecular dynamic simulation

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Abstract: In this work, molecular dynamics (MD) based simulation were performed to study the effect of radiation induced defects on the mechanical properties and deformation mechanism of nickel single crystal. Nickel single crystal is created by filling nickel atoms (FCC crystal structure, a = 3.50 Å) under periodic boundary conditions in simulation box of 100 $Å^3$. EAM potential is used to model the interactions between Ni-Ni atoms. The simulation was carried out in two phases and in the first phase, the modeled single crystal is irradiated with 1 keV and 3 keV incident energies using primary knock on atom (PKA) method in three different velocity vectors [1 1 1], [1 1 2] and [5 3 1]. Due to this irradiation effect the sample has undergone abrupt changes, and a large number of defects like vacancies and interstitials have formed. The impact of the velocity vector is different with different incident energies, and there is a minimum number of vacancies generation with [1 1 1] velocity vector. The amorphization at PKA region can be observed in the irradiated sample using radial distribution function (RDF). In the second phase of simulation, the irradiated samples were tensile tested at a temperature of 300 K at a strain rate of 10^{10} s^{-1}. There is a substantial decrease of yield strength and Young's modulus in the irradiated nickel samples (due to the formation of defects) when compared with that of the unirradiated nickel sample. Due to different velocity vectors within the incident energy, there was a slight variation in the mechanical properties as observed from the stress-strain graphs. Deformation mechanism features such as dislocations, partial dislocations and surface defects such as stacking faults are observed in the deforemd samples.

Keywords: Molecular dynamics, irradiation, vacancies, deformation.

Indian Institute of Metals, NMD-ATM

71st Annual Technical Meeting

November 11-14, 2017

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Abstract number: 8

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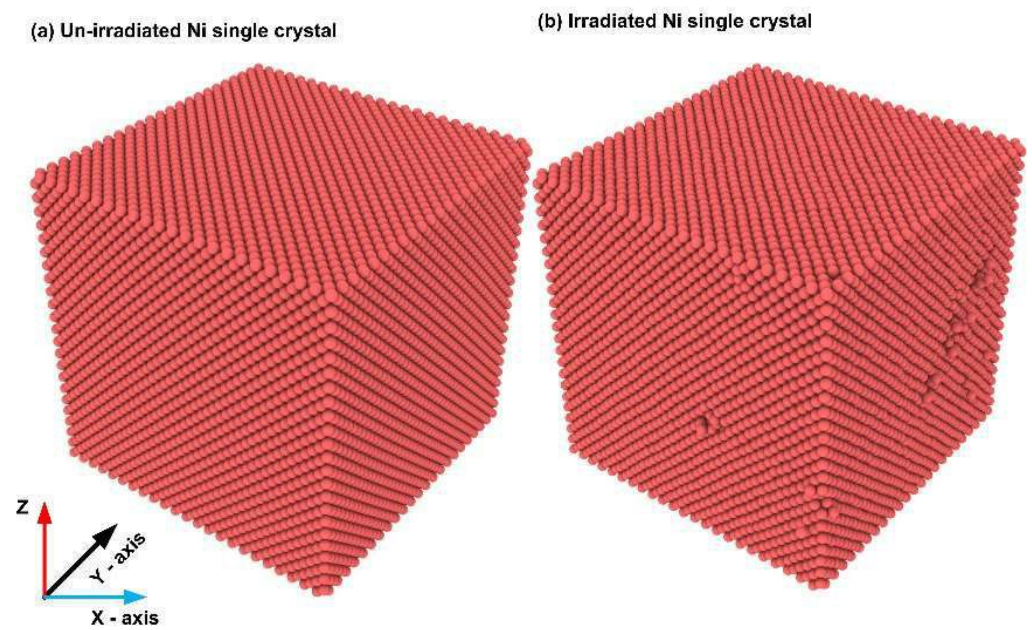
Introduction

- Defect generated in nuclear materials due to irradiation, significantly affects the microstructure of such materials [1,2].
- Although the period required to induce micro structural changes in nuclear materials spans from weeks to years, the primary irradiation damage events leading to such micro structural changes last only for couple of picoseconds.
- There are limitations associated with experimental techniques to study these irradiation effects at such spatial and time scales.

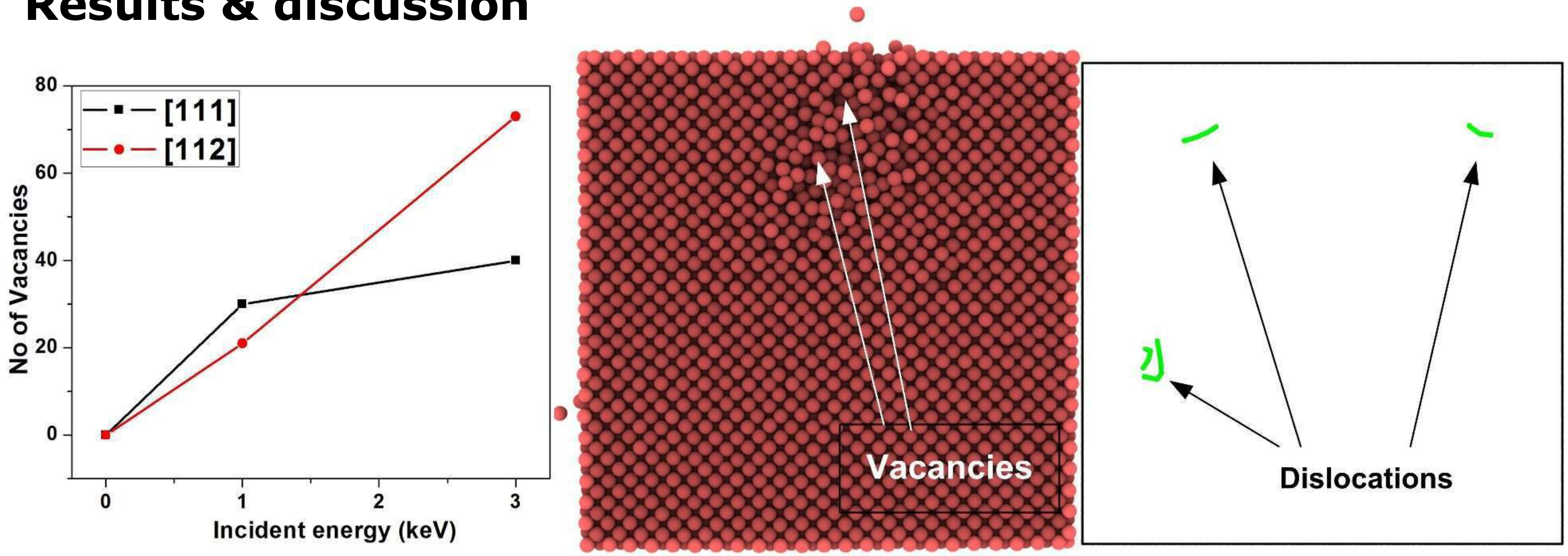
Modelling and Simulation

- Radiation damage in Nickel single crystal with different velocity vectors and subsequent uniaxial tensile have been carried out using LAMMPS.

Box dimension: 80 Å(x) * 80 Å(y) * 80 Å(z)
No of atoms: 48668 (FCC, a = 3.51Å)
Boundary conditions: P P P
Ensemble: nve (Irradiation)
nvt (Tensile deformation)
Potential: Embedded atomic method
Irradiation: PKA method
Incident energies : 1keV, 3keV
Velocity vectors : [111]; [112]; [531]



Results & discussion



(a) (b) (c)

- The numbers of defects are analyzed with Wigner–Seitz cell method [3] which is implemented in OVITO [4]
- No of vacancies increases with increase of Incident energy (1 and 3keV)
- No of vacancies generated are different with different velocity vectors with same incident energy can be observed.
- Defects like dislocations (Shockley partial) stacking faults and voids that are generated during irradiation can be observed.
- From stress-strain graphs, mechanical properties like Young’s modulus and yield strength of un-irradiated sample is higher than irradiated samples and this is due to the defects generated during irradiations.

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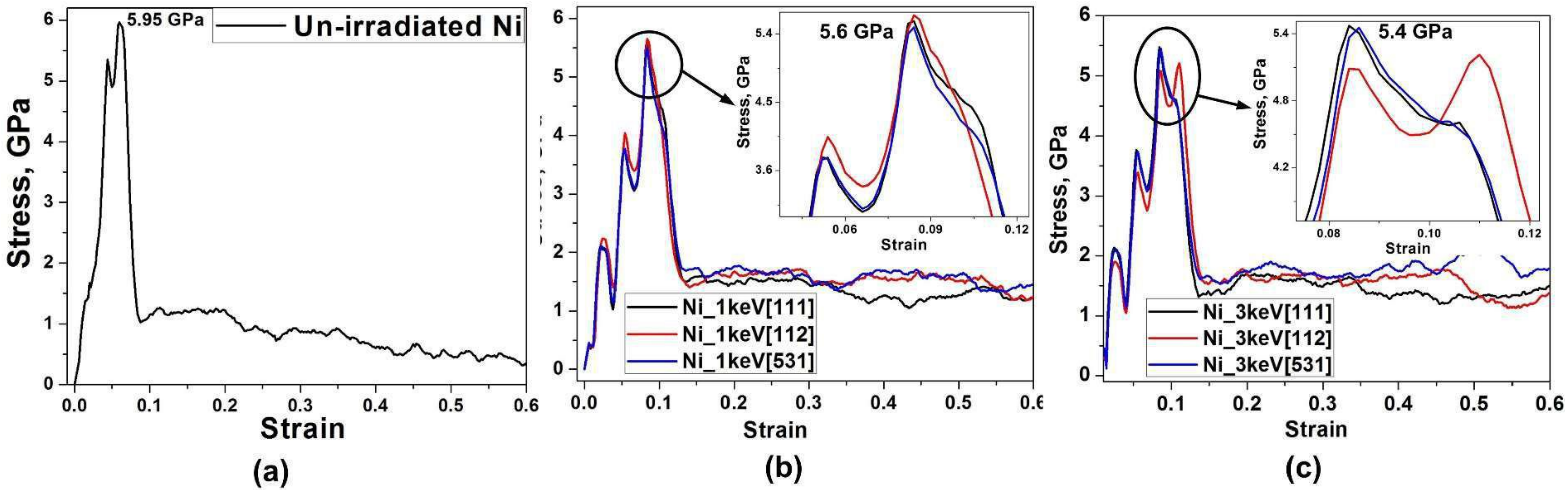
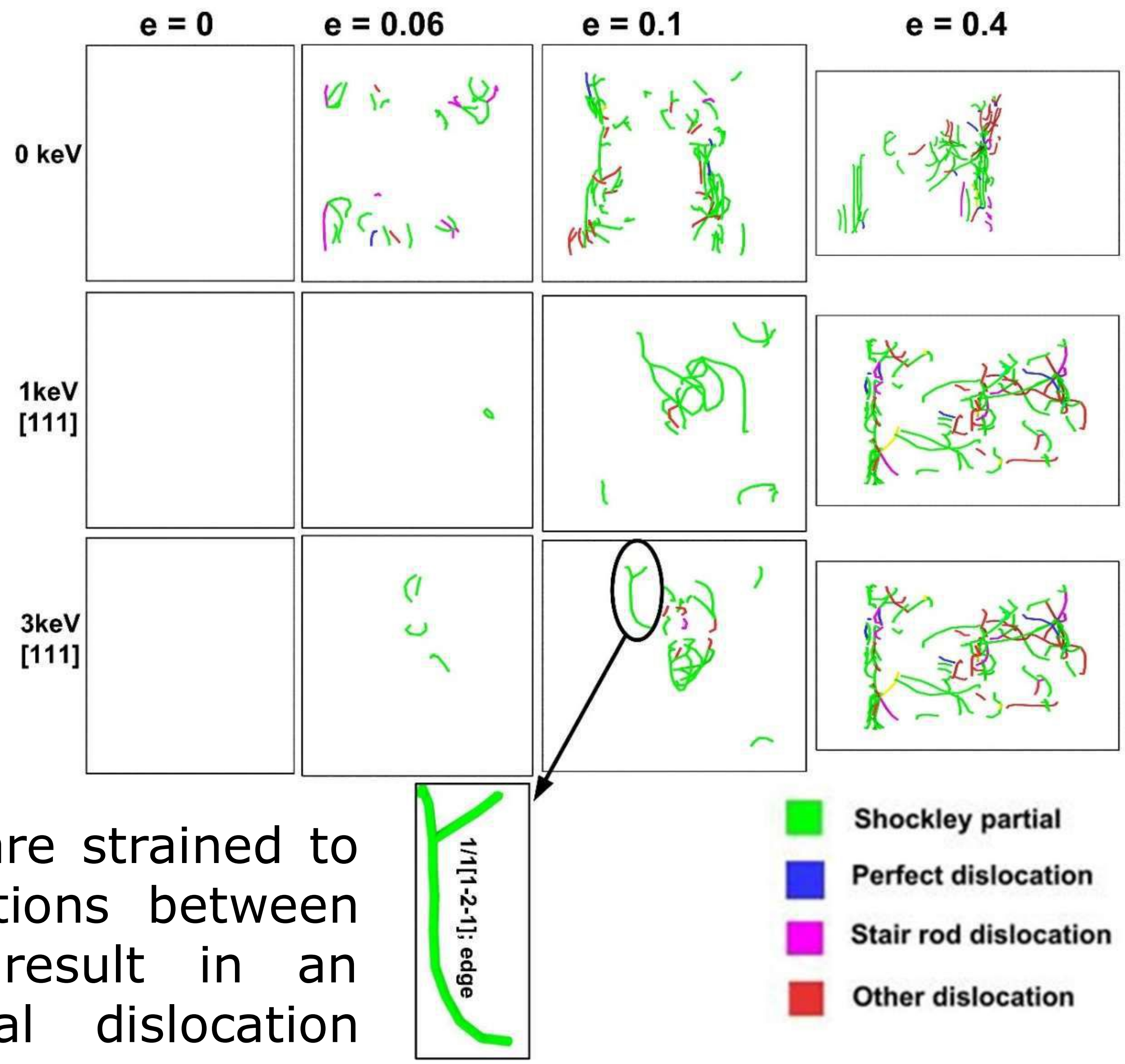
Stress-strain graphs of un-irradiated & irradiated Nickel samples



	Young's mod (GPa)	Yield strength (GPa)	Yield strain (%)
Ni Un-irradiation	107 (81.6[5])	5.95	6
Ni_1keV[111]	53.5	5.57	8.4
Ni_3keV[111]	53.2	5.47	8.4
Ni_1keV[112]	56.4	5.64	8.4
Ni_3keV[112]	47.71	5.21	11
Ni_1keV[531]	52.93	5.48	8.4
Ni_3keV[531]	52.23	5.45	8.6

Dislocation analysis

- Dislocation analysis is vital to understand the underlying deformation mechanism.
- Ni single crystal is free from dislocations in the elastic region under un-irradiated condition.
- For irradiated samples we can observe the dislocations before the sample reaches yield at strain e= 0.06.



- As the Nickel single crystals are strained to the elastic limit, the interactions between vacancies and dislocations result in an increase in Shockley partial dislocation density which is clearly seen at strains e = 0.06 and e = 0.1.

Conclusions

- It can be concluded from the simulations that radiation induced defects, even at low PKA energies (1 & 3keV) have significant impact on the mechanical behavior of single crystal of Nickel.
- The strength of radiated Nickel single crystal reduces significantly as compared to Nickel crystal without any defect (Un-irradiated sample).
- Radiation induced defects increases with the increase in PKA energy.
- Irradiation in [112] velocity vector have more impact on Nickel, when compared with that of radiation energies on other velocity vectors.
- Finally, irradiation deteriorates stiffness and yield strength of the Nickel.

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