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Molecular dynamics based study of an irradiated single crystal of niobium

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ABSTRACT

In this article, molecular dynamics based simulations were performed to study the effect of radiation induced defects on the mechanical properties and deformation mechanism of a single crystal of niobium. Niobium is an important constituent of zirconium based alloys employed as fuel cladding and pressure tubes in nuclear reactors. Overall, simulations were divided in two broad sections, initially, displacement cascade was generated with varying PKA parameters to study defect formation in single crystal of niobium. Later, the same defected crystal was subjected to tensile loading to study deformation mechanism of niobium containing these radiation induced defects.

1. Introduction

Defect generated in nuclear materials due to irradiation, significantly affects the microstructure of such materials [1,2]. Radiation induced defects have extensively been studied by many researchers [3–7]. 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. Molecular dynamics (M.D.) based atomistic modeling is emerging as a viable tool to model and investigate irradiation induced micro structural changes at such short spatial and time scales. Molecular dynamics based simulations has extensively been employed by the researchers to study displacement cascades in metals such as α-Fe [8], copper [9], tungsten [10] and hcp-zirconium [1–3].

Superior mechanical properties of zirconium (Zr), such as low thermal neutron absorption cross section, high hardness, ductility, and corrosion resistance make it a perfect material for nuclear industries. Significant improvement has been observed in the mechanical properties of Zr, when it is alloyed with a small content of niobium (Nb) [11]. Due to the superior mechanical properties and low neutron absorption of Zr-2.5Nb alloys, are widely employed for the cladding of fuel rods and pressure tubes in nuclear reactors. Because of the importance of niobium as an alloying element in Zr-2.5Nb for nuclear applications, it is of interest to investigate the effects of radiation on niobium. Despite significant efforts made by researchers to understand the effect of radiation on zirconium [1–3], literature is very limited for the same effect on niobium. To date the most significant contribution on niobium was in 1969, when Tucker et al. [12] performed studies on the formation of dislocation channelling in irradiated niobium crystals.

In this article, author has tried to develop an understanding of the effect of radiation on the deformation mechanism of a body centered single crystal of niobium. Focus in the paper is given to development of a methodology to characterise slip planes in irradiated single crystal of niobium. The molecular dynamics based investigations were divided in two phases, initially, radiation induced defects were generated in a single crystal of niobium as a function of primary knock on atom (PKA) energy, direction, and overall simulation temperature. Later, atomic configurations with generated defects were then subjected to uni-axial tensile loading to observe the deformation behaviour of single crystal niobium.

2. Embedded atom method potential

The accuracy of any molecular dynamics based simulation entirely depends on the potential employed to represent atomistic interactions. The force matched embedded atom method (EAM) potential proposed by Fellinger et al. [13] has been used in this work. The EAM potential has been well-established for use in atomistic simulations of metals and alloys, and a variety of interatomic potentials based on EAM have been devised and validated against either experimental or higher fidelity modeling

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data [14–17]. The EAM potential consists of two terms: a many body term that represents the interaction between the atom and electron cloud of the surrounding atoms, and a pair wise interaction term that represents the interaction between the atom and its neighbours. Mathematically, EAM potential can be represented as mentioned in Eq. (1).

$$E = \sum_i F_i(n_i) + \sum_{i<j} \varnothing_{ij}(r_{ij}) \quad (1)$$

Here, E is the overall potential energy of an atom, n_i is the electron density, F_i is the embedding energy and $\varnothing_{ij}$ is the component representing the pair wise interaction. In the EAM potential proposed in the paper [13], the three functional forms (F_i, n_i and $\varnothing_{ij}$) were determined by optimising parameters to a well converged set of energies, forces, and stresses by employing density functional theory.

For the present research application, it is desired that the potential accurately reproduces the elastic constants, cohesive energy and stacking fault energy. To investigate the effects of radiation on the mechanical properties of a single crystal of niobium, simulations were initiated by imparting low kinetic energy ($\leqslant$2 keV) values to one of the atoms for generating displacement cascade or point defects. As lower energy PKA ($\leqslant$2 keV) has been used in all the simulations, no modification has been performed in the equation of EAM potential to account for the strong repulsive interaction not represented by EAM that would occur because of close approach between atoms. The strong short-range repulsive term is not included with the EAM potential because at low values of PKA energies ($\leqslant$2 keV), the interatomic repulsion due to the embedding term in the EAM is sufficient to shield the nucleuses of two atoms from the short-range repulsion experienced by higher energy atoms. Position of vacancy and interstitials in single crystal of niobium generated with PKA were identified with the help of Wigner –Seitz cell.

3. Description of molecular dynamics models

Simulations were performed in two stages. In first stage, radiation induced defects such as vacancy and interstitials were generated in single crystals of niobium with respect to simulation box temperature, PKA energy and PKA direction. In the next stage, effect of these defects on the mechanical behaviour of niobium was investigated. All the molecular dynamics based calculations were carried out in parallel Large Scale Atomic/Molecular Massively Parallel Simulator or LAMMPS [18] and post processing of dump files generated from LAMMPS was performed in OVITO [19]. A schematic of the simulation box along with its dimensions is shown in Fig. 1. In order to avoid edge effects, periodic boundary conditions were imposed on all the sides of the simulation box. Size of the simulation box was kept large enough to avoid any image interactions between the defects generated even with the highest energy PKA ($\approx$2 keV). In order to fix the size of simulation box, the atoms displaced from the lattice position was checked at the time of thermal spike with 2 keV PKA. It can be seen in Fig. 1c that the size of the simulation box was good enough to hold all the displaced atoms away from the boundaries of the simulation box. A NPT ensemble (constant atoms, pressure, and temperature) consisting of 128,000 atoms, at 10°K and zero pressure were simulated to depict the effect of radiation induced defects on the deformation mechanism of a single crystal of niobium. In order to avoid the thermal disturbance from statistical distribution of temperature over the atoms, simulations were performed at a low temperature of 10 K. Atoms were generated in the simulation box in such a way that [1 0 0], [0 1 0] and [0 0 1] crystal orientations were aligned with the x, y and z directions, respectively.

The atomic placement was followed by an equilibration process for a total time of 50 ps with a time step of 0.001 ps ($\approx$1 fs). After achieving a minimum potential energy configuration for the single crystal of niobium, a PKA atom was selected and a velocity vector

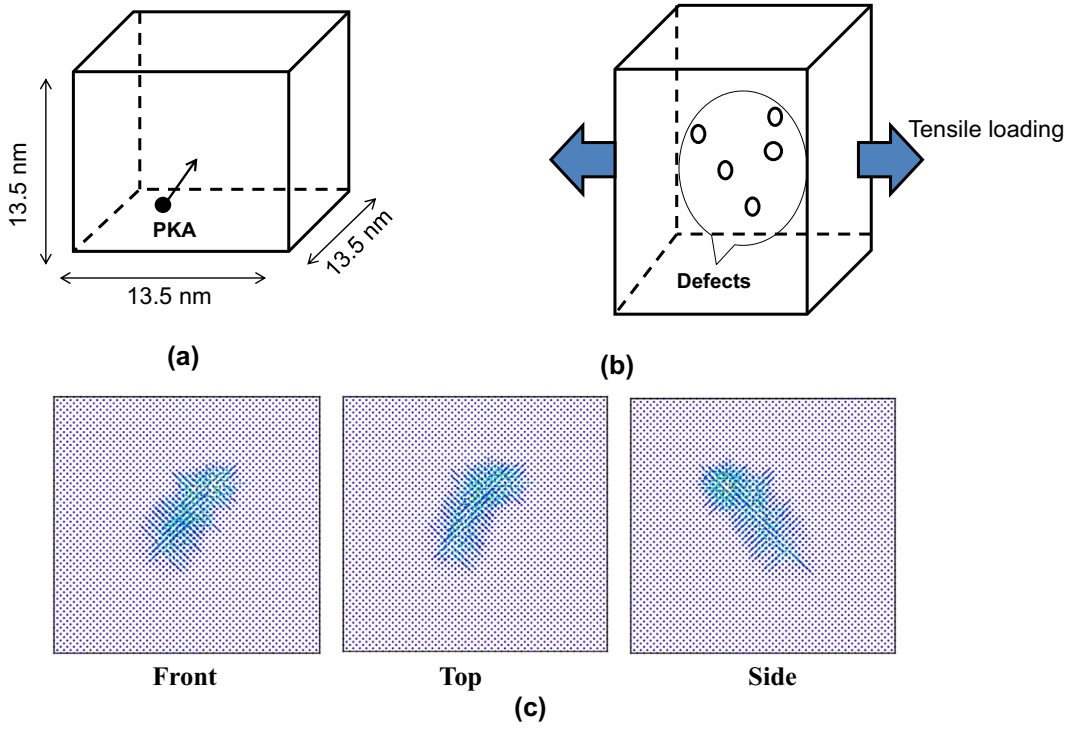

Fig. 1. Schematic of simulation box (a) PKA with a predefined velocity vector in a simulation box for generating defects, (b) second phase of simulation with tensile loading in conjunction with radiation induced defects, and (c) three views of simulation box at the time of thermal spike for simulations performed with 2 keV PKA.