Damage Cascade Simulation in Zirconium Nitride: A Molecular Dynamics Study

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Article

Damage Cascade Simulation in Zirconium Nitride: A Molecular Dynamics Study

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Abstract: Zirconium nitride (Zr-N) is a candidate material for inert matric fuel elements in breeder reactors. They have shown exceptional resistance to radiative corrosive environments. They have shown excellent resistance to radiation stability at operational conditions in current generation reactors. But being a candidate nuclear fuel material in generation reactors, their radiation stability at higher temperature conditions observed has not been reported. We have employed molecular dynamics simulations to study the damage cascades and radiation stability of ZrN at 600K. The process of primary damage evolution by considering varying overlapping cascades with 10, 20 keV incident PKA's reported here. The defects interface interaction and diffusion mechanism at the interface are reported.

Keywords: Molecular dynamics; LAMMPS; displacement cascade; defects

1. Introduction

Nuclear energy is considered a reliable source of energy free from CO_2 emissions [1–21]. But it has some critical concerns about waste fuel by-products and their storage [22]. Another major concern involves the recycling of transuranic waste. This can be reduced by reprocessing it into the reactor core to obtain complete transmutation of transuranic products. This technique involves placing the waste into the fuel matrix which acts as inert or neutron transparent [23]. This inert matrix nuclear fuel contains a single or mixed element [24]. Zirconium nitride (ZrN) exhibits FCC structure being one of the potential candidates for inert matrix materials because it has low neutron absorption cross-section, high thermal conductivity, and low solubility. They display excellent radiation resistance to various types of nuclear byproducts and fission fragments. Additionally, nitride nuclear fuels are reported as a surrogate for actinide nitride for advanced generation reactors [25]. Moreover, Zr is mainly used as nuclear fuel cladding pallets for UO_2 in LWR due to its corrosion resistance at elevated temperatures [26].

Nanostructured alloys have shown radiation resistance at higher temperature materials due to the existence of high-density nano-oxide and interfaces that act as a sink for radiation defects [27]. Such resistive nature can be the reason for defects sink efficiency in these materials [28]. The initiated process starts from the damage cascade and the propagation of defects near the interfaces exhibit defect sink efficiency. The process responsible for displacement cascades in ZrN can be well understood through atomic-scale simulations. Molecular dynamics simulations are considered a viable tool to understand the process of defect evolution at the atomic scale but the main concern in MD simulations is reliable potentials. In this study, we have reproduced MEAM potential for ZrN developed by Narayanan et al [29]. Two model cases are considered one is containing damage cascade in ZrN and the other containing one portion of the model as Zr and the other parts as ZrN to observe defect trapping and diffusion mechanism for constituents on either side. The incident PKA were nitride initially and later Zr to compare the damage cascade evolution due to mass effect.

This study will provide atomic insight into the effect of displacement cascades in ZrN and the effect of mass and energy of PKA on the diffusion mechanism in ZrN. The effect of mass on the density of radiation defects was analyzed.

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2. Computational details

The computational model of ZrN containing Zr right side and ZrN on the left side of the simulation box is developed in this study. Initially, we considered Zr matrix with (60x30x30) lattice units, where lattice parameter 4.529Å. Later N atoms were 50% substituted on the other half creating $Zr_{0.75}N_{0.25}$. The relaxed system size ensures that the collision cascades initiated by E_{PKA}~ 10, 20 keV PKA's do not interact with the boundaries simulating displacement cascades computationally expensive and traceable. We have conducted MD simulations using large-scale atomic/molecular massively parallel simulator (LAMMPS) code. Periodic boundary conditions (PBC) were applied to all axes to ensure replicating desirable computations. The interatomic interactions between the atoms have been described by the modified Embedded Atom Model (EAM) potential developed by Narayanan et al [29]. This potential was tested for energy minimization and a stable structure was obtained at 600K. The model was thermally relaxed using NPT ensemble for 50ps at time step 1fs for 50000 steps. The cascade simulation was performed by NVT ensemble for 25ps keeping the same time steps. The postprocessing of the computational model was done using open visualization tool (OVITO) developed by Stukowski et al [30].

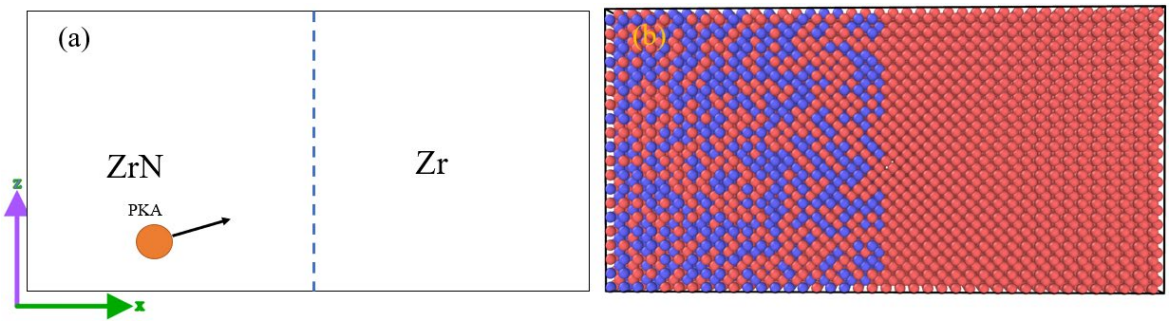

Figure 1. Illustration of the computational model. a) Schematic representation b) Lateral 2D MD snapshot of the computational model where red color represents Zr and blue is N.

Figure 1 represents an illustration of the relaxed ZrN model at 600K. The incident PKA is selected on the ZrN side with incident energies 1,10,20 KeV closer to the interface by selecting a spherical region containing N atoms having a unique group id for each simulation. The same method was adapted for Zr. The velocity of each incident is selected equivalent to each energy in such a way that the maximum magnitude of the velocity vector is velocity along the X-axis. The displacement atom DPA for each type of PKA is calculated through SRIM code and later conversion of energy to DPA for calculations. The number of cascade simulations for each PKA was used through DPA calculations and found 0.002DPA/PKA energy.

3. Results and discussion

3.1. Displacement cascade vs Mass of the incident particle

Incident particles were imparted energy to initiate the displacement cascades. The PKA was selected from the ZrN .

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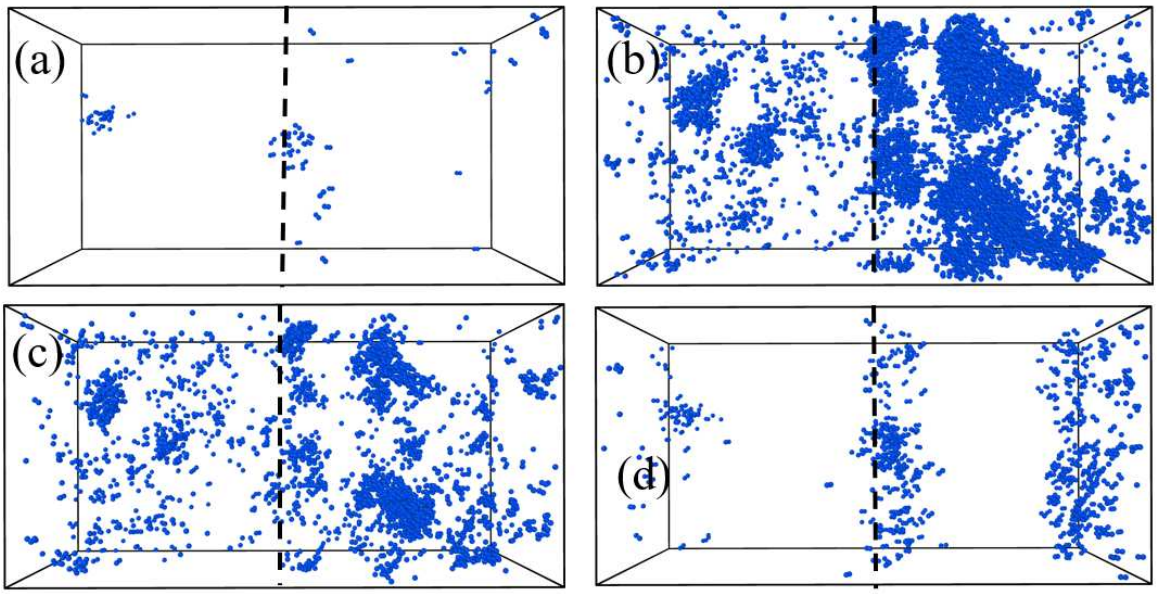

Figure 2. Displacement cascade initiated by Zr atoms 10keV PKA at 600K. where (a-d) displays evolution of defects at 0.01, 0.1, 0.2 and 25ps.

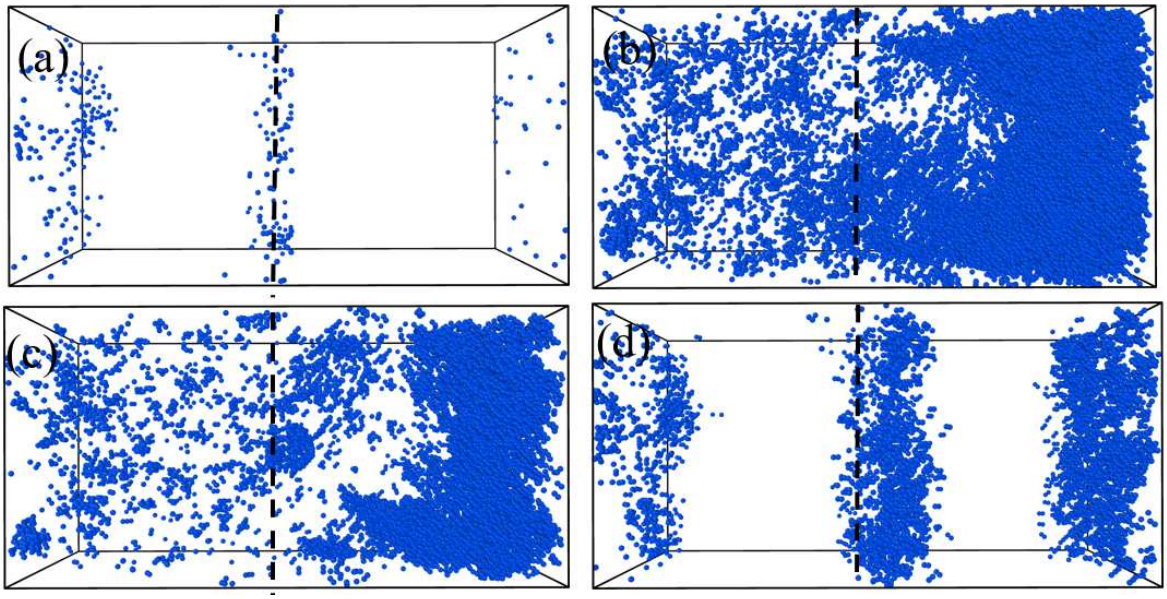

Figure 3. Displacement cascade initiated by Zr atoms 20keV PKA at 600K, where (a-d) displays evolution of defects at 0.01, 0.1, 0.2 and 25ps.

3.2. Defect analysis

During radiation damage, incident PKA having $E_{pka} > E_{threshold}$ displaces the original particles from the lattice sites and generates a displacement cascade during its interaction with other atoms in the vicinity of PKA [31]. These collision cascades interact generating overlapping cascades and potentially shock waves and high energy subcascade that multiply creating a larger number of defects after the cascade cools down [32]. Our simulation used a successive cascade algorithm to select PKA, considering a single atom for the bombardment every time [33]. The incident PKA's were selected through a spherical region in such a way that one PKA is bombarded at a time for each cascade. It is very challenging to determine an exact number of defects when there is a large number

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of defects and clusters present due to displacement cascades. The density of defects (r_d) and interstitials are determined using the Wigner-Seitz cell analysis and the OVITO software [34].

The defects concentrations as a function of time are displayed in Figure 4 for Zr PKA. The number of surviving defects (in terms of density) is proportional to the energy of the incident PKA. Moreover, the lower energy incident particle has lesser surviving defects as seen in Figure 5 for NPKA

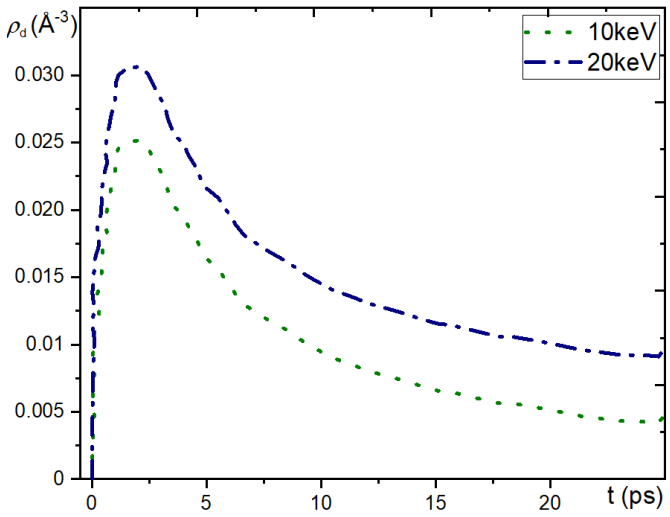

Figure 4. Defect density as a function of time over EPKA. The number of surviving defects is proportional to the energy.

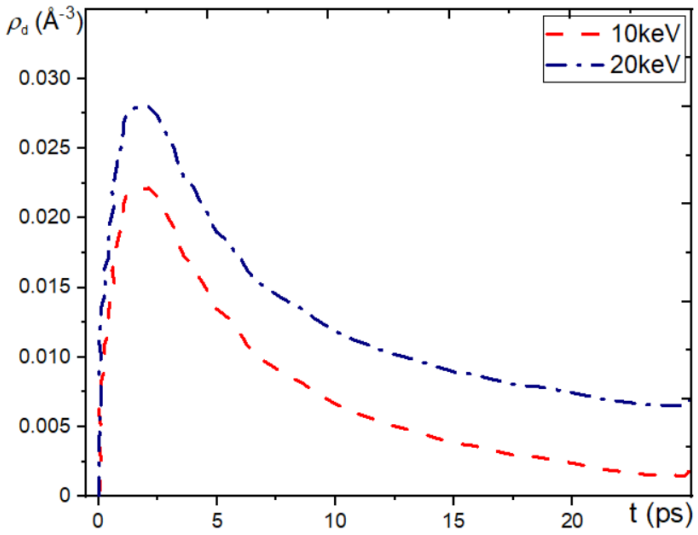

Figure 5. Defect density as a function of time over EPKA. The number of surviving defects are proportional to the incident energy.

4. Conclusions

In this study , molecualr dynamics simuation were performed to observed the displacement cascades in ZrN using many body potential. The defects evolution as a fucntion of cascade energy was observed and it was seen that higher incident energies were more scattered cascades and higher deffect trapping near the interface. The interface act as defect sink for higher energy incident PKA's.

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