Molecular dynamics study on single particle displacement damage of ZB InN

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Abstract. To evaluate single-particle initial displacement damage of InN, the MD method is used to simulate the cascades, where the energy of PKA ($E_{PKA}$) ranges from 1 to 5 keV. From these results, we can find that high $E_{PKA}$ will increase $N_p$ and $N_i$ of defects, and aggravate the damage of InN, which is more obvious in Frenkel pairs. The formation efficiency of vacancy and interstitial is influenced by antisite defects, thereby causing the difference between vacancies and interstitials for the same atomic type. About the distribution of InN defects, it is mainly caused by vacancy defects, indicating that vacancy damage occupies the main position in displacement damage.

1. Introduction
With the advantages of high optical absorption coefficient and small electron effective mass, Indium nitride (InN) has great potential in applications such as broad-band photo detectors, near-infrared emitting LEDs and solar cells [1]. However, under a strong irradiation background, the performance parameters of these optoelectronic devices will be seriously damaged. Similar to another III-nitride semiconductor GaN, InN shows higher radiation resistance than that of GaAs. High tolerance for proton irradiation of InN was studied by photoluminescence spectroscopy and performing Hall and resistivity measurements in InGaN with different In content, including InN. At present, few studies have been done on the radiation effect of InN, and mostly focus on the ionizing radiation effect. In contrast to some semiconductors (GaN or GaAs), the formation of vacancy under total ionizing dose (TID) radiation promotes the increase of electron density. As one of the spatial radiation effects, the single particle displacement damage (SPDD) will form micro defects through the elastic collision of primary knock-on atom (PKA) in cascade and finally form a stable distribution of defects. The existence of these steady-state defects leads to the carrier non-radiative complex process in semiconductor, which affects the carrier mobility and lifetime, and finally changes the device performance parameters [2,3]. Therefore, the multi-scale simulation of semiconductor displacement damage defects has been an important issue in the field of radiation. About SPDD in InN has not been studied much, especially in theory.
Multi-scale simulation provides an effective method to study the production and evolution of micro defects. It is important to understand the initial stage of displacement damage. Molecular dynamics (MD) simulation is an effective mean to reproduce the atomic trajectory at picosecond and nanoscale based on the first principle fitting potential function. Compared with experiments, MD simulation has the advantages of lower cost, larger operating space and less risk. In recent decades, MD simulation has been used to describe the initial evolution stage of defects in semiconductors and metals [3-6].

In this paper, MD simulation is used to study the initial evolution stage of defects in InN. In this simulation, PKA energy ($E_{PKA}$) ranges from 1 to 5 keV at the temperature of 300 K. The evolution of cascade defects, various type point defects and defect clusters are discussed. And the key parameters obtained from this paper are helpful for future work on SPDD of InN.

2. Methodology

2.1. Inter-atomic potentials

In this work, we use the open-source software called as LAMMPS [7] to simulate this cascade in InN. The choice of inter-atomic potential is a key part, where we adopt the MEAM potential [8] to describe the primary damage process. The MEAM is created based on changes made on the EAM. With the development of MEAM potential, it can consider partially interactions and overcome some key shortcomings. The parameters between In-In, N-N and In-N are obtained from cheol et al. [9] The MEAM potential can describe various physical structural properties of zinc-blende (ZB) InN, such as elastic and defect properties, which agree well with experimental data.

2.2 Simulation details

The simulation procedure is divided into model specification and cascade simulation. First, the system is large enough to avoid cascading overlap, so the system size varies according to the kinetic energy of the PKA. The ZB structure is generated for InN with various sizes from 20a x 20a x 20a to 30a x 30a x 30a as shown in Table 1, where a is the lattice constant and is initialized to 4.98 Å. Before cascade simulation starts, the ZB InN structure should be initialized in the constant pressure and temperature (NPT) ensemble to arrive one equilibrium state, where the target pressure is zero pascals (Pa) and the preset temperature is 300 K. The total simulation time is approximately 30 picoseconds (ps). Periodic boundary conditions are used along all axes.

| $E_{PKA}$ (keV) | Box size (a) | Number of simulations | Simulation time (ps) |
|----------------|-------------|----------------------|---------------------|
| 1              | 20×20×20    | 10                   | 20.4                |
| 2              | 20×20×20    | 10                   | 20.4                |
| 3              | 25×25×25    | 10                   | 20.4                |
| 5              | 30×30×30    | 10                   | 20.4                |

Next, the collision cascade event is initiated by injecting kinetic energy into the selected In PKA located near the center of the system. Then, as shown in Fig.1, collision cascades are triggered within an internal region defined as the micro-canonical (NVE) ensemble. At the same time, the isothermal-isochoric (NVT) ensemble will be applied to the outermost atomic layer to release the cascade heat and keep the temperature constant. The outermost atomic layer has a thickness of approximately two to three atomic lattice constants. In addition, the multiphase time step method is used to accurately describe the atomic motion according to the different collision intensities between atoms. The range of time step is between $10^{-5}$ and $10^{-3}$ ps. The total time is 20.4ps, and the simulation times in Table 1 are 10 times to obtain meaningful statistical data.
2.3. Defect analysis
To analyze the output cascade data from MD simulation, the Open Visualization Tool (OVITO) is used for defect configuration analysis in this work. We use the Wigner-Seitz (W-S) method to identify the various point defects. In addition, the analysis method of defect clusters for these point defects is the linked-group method. The analytical principles of various point defects (\(V_{\text{In}}, V_{\text{N}}, I_{\text{In}}, I_{\text{N}}, I_{\text{InN}}\) and \(N_{\text{In}}\)) and clusters is the same as work what we did before [10]. The number of defects in a cluster represents the size: if the number is more than 6, it is a large cluster; meanwhile, smaller cluster is the number range from 2 to 6. The other cases are considered into isolated point defects.

3. Results and discussion
3.1. Evolution of the cascade defects
From Figs. 2(a) and (b), whether it's Frenkel pair or antisite, the evolution process of defects in the cascade shows a normal "rise, fall and stability" trend, which is the same as previous studies. In the cascade initial process, PKAs will quickly hit these atoms in original site to form plenty of defects. The kinetic energy of PKAs decrease gradually during this process, and the number of defects will reach the maximum. After this point, the number of defects will decrease to a stable value because of self-recombination in the region called as thermal spike. When defects arrive at the thermal peak or stable stage, the number of defects is \(N_p\) or \(N_s\). With the increase of energy, \(N_p\) or \(N_s\) of Frenkel pairs and antisite defects has been improved. These results point out that high \(E_{\text{PKA}}\) will aggravate the damage of InN and make it difficult to recover, which is more obvious in Frenkel pairs.
As a specific property of the material, to some extent, the recombine efficiency $\varphi$ reflects the radiation-resistant level. This is defined as follows:

$$\varphi = 1 - \frac{N_{FS}}{N_{FP}}$$

where $N_{FS}$ and $N_{FP}$ represent the stable and maximum number of Frenkel pairs. As shown in Fig. 3, there is a fitting relationship between $\varphi$ and $E_{PKA}$. In addition to 1keV, $\varphi$ decreases with the increase of $E_{PKA}$, also indicating that high energy causes severe irreversible damage.

### 3.2. various type defects

The point defects of InN generated during the whole displacement cascade process mainly focus on vacancies and interstitials. For different atomic types, the effect of defect energy level on the properties of the material itself are different. To investigate various types of defects in InN comprehensively, various defects including $V_{In}$, $I_{In}$, $V_N$, $I_N$, $In$ and $N_{In}$ are all introduced. Due to the existence of Frenkel pairs, the number of vacancies and interstitials is also same in InN ($V_{In} + V_N = I_{In} + I_N$). However, it can be seen from Fig. 4(a) that the amounts of vacancy and interstitial are not the equal for the same atomic types such as In, and N atoms. For instance, for In type, the number of interstitials is less than vacancies. The reason can be found from Fig. 4(b) because of antisite defects. And it shows the quantitative relation among these parameters that $I_{In} + I_N = V_{In} + N_{In}$ by analysing. It may be that moving In interstitials can occupy the N vacancies to form $In_N$. Similarly, there is also a possibility that In vacancies may be
occupied by N to form N\(_{\text{In}}\). So, it can point out that antisite defects influence the formation efficiency of vacancy and interstitial.

![Figure 4](image)

**Figure 4.** The number of stable defects in InN as a function of \(E_{\text{PKA}}\), (a) Frenkel pairs and (b) antisite defects.

### 3.3 Defect clusters

In the environment of low energy SPDD, defect cluster is the main distribution of displacement defect, hindering point defects migration and recovery at atomic scale. As shown in Fig. 5(a), the stable defect distribution characteristics of InN are very concentrated, which is different from other types of semiconductors. In order to analyze the reasons, the defect cluster types are divided into two types: vacancy and interstitial.

![Figure 5](image)

**Figure 5.** The stable defect distribution in InN. (a) total defects (green and blue spheres represent vacancies and interstitials, respectively), (b) vacancy clusters and (c) interstitial clusters (pink, yellow and black spheres represent larger clusters, smaller clusters and point defects, respectively).

It is found from Figs. 5(b) and 6(a), the vacancy cluster is mainly concentrated on the super-large cluster (size > 60), which shows that the damage space characteristic of the vacancy is especially concentrated, and it is more likely to affect the change of the property of InN material, resulting in the failure of the device parameters. As shown in Figs. 5(c) and 6(b), unlike the vacancy, the interstitial clusters showed certain dispersion, and the large clusters are relatively small. As \(E_{\text{PKA}}\) increases, cluster size decreases and cluster number increases. In general, it can be concluded that the distribution of InN defects is mainly caused by vacancy defects, which indicates to some extent that vacancy damage occupies the main position in displacement damage.
4. Conclusions
In this paper, MD method is conducted to simulate the displacement cascades of InN. Here $E_{PKA}$ is range from 1 to 5 keV. The defect behaviors including evolution, various types, and clusters are investigated, respectively. It can be found that high $E_{PKA}$ will increase $N_p$ and $N_s$ of defects and aggravate the damage of InN, more obvious in Frenkel pairs. The formation efficiency of vacancy and interstitial is influenced by antisite defects. About the distribution of InN defects, it is mainly caused by vacancy defects, indicating that vacancy damage occupies the main position in displacement damage.

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