

The influence of temperature and energy on defect evolution and clustering during cascade in GaAs

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ABSTRACT

Molecular dynamics (MD) is used to simulate cascade collision in gallium arsenide (GaAs) under different temperatures (300–900 K). During the entire simulation, the primary knock-on atom (PKA) is incident at a special angle, and its energy (E_{PKA}) is within 10 keV. The simulation results are found to be reasonable based on the NRT equation and show that high E_{PKA} causes direct damage, thereby increasing all evolution parameters such as the peak time (t_p), steady time (t_s), peak (N_p) number, and steady (N_s) number of defects. Compared to E_{PKA} , high temperatures reduce N_s of Frenkel pairs and increase the threshold displacement energy (E_d), during which Ga defects occupy the main part. It is also found that the difference between Ga and As vacancy-interstitial pairs on the amount makes t_p of Ga_{As} defects longer than As_{Ga} defects, leading to a significant delay in antisite defects as temperature increases. Regarding clusters, high temperatures can promote the transformation of large clusters to isolated point defects for the vacancies, while only the transformation of large and small clusters is observed in the interstitials.

1. Introduction

As a member of direct-bandgap materials, Gallium arsenide (GaAs) has high carrier mobility and excellent electrical properties. It has gradually replaced silicon (Si) to become one of the important choices for optoelectronic devices [1]. However, in the space environment, particles such as protons and neutrons [2] can cause displacement damage (DD) to these devices. DD is from the stable defects produced by the elastic collision of the primary knock-on atom (PKA) in the cascade. These defects will accumulate regionally under long-term irradiation and influence the electrical properties, thereby hindering normal space tasks [3]. Thus, the investigation of the evolution and clustering of defects in GaAs is meaningful to radiation-resistant work.

In recent decades, some technologies represented by deep-level transitive spectroscopy [4,5] (DLTS) have been used in experiments to obtain defect information. They have advantages of convenience, simplicity, and sensitivity. However, there are some limitations for these technologies to investigate the atomic level process because the primary displacement damage (PDD) process is at the level of picoseconds (ps)

and nanoscale (nm). With the development of computer simulation, molecular dynamics (MD) simulation which is consistent with time and space scales of displacement cascade can overcome these difficulties and accurately describe the cascade processes in semiconductors [6–9,17] and metals [9–11].

For GaAs, a few MD simulations on DD are carried out and are mostly concentrated in the ion beam environment [12–15]. The exact potential function is quite important for MD simulations. Albe et al. [16] developed an analytical bond-order potential that can well describe the physical properties and point defect information of GaAs. Further, based on this analytical bond-order potential, Nordlund et al. [13] investigated the defects within 10 keV cascades and proposed the reasonable assumption that the threshold displacement energy is 15 eV. Subsequently, more research studies on cascade collisions in GaAs are conducted. Regarding defects distribution such as clusters, Björkas et al. [14] reported that heavy ions cause serious damage to large clusters and decrease the attenuation time of the carrier itself. After optimizing the short-range potential called as Ziegler-Biersack-Littmark (ZBL), Gao et al. [3] indicated that the amorphous region has an obvious effect on

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defects at low temperature, and the results show that non-ionizing energy loss (NIEL) is larger than the value by the classical analytical method. Regarding the effect of temperature on semiconductors such as SiC, Farrell et al. concluded that high temperatures influence the evolution of C_{Si} defects and the distribution of vacancies, resulting in decreasing the damage generated during cascade formation.

However, for GaAs, to date, there are very few studies on cascade collisions combined with temperature. In this paper, the MD method is used to simulate cascade processes under different temperatures. By comparing with the energy effect, the effect of temperature on the evolution and various types and clusters of defects (distribution) is determined. Finally, the key parameters such as spatial distribution, complex rate, and cluster rate of defects are helpful to future studies on multiscale simulations.

2. Methodology

This work simulates the cascade collision process in GaAs (\sim ps) by using the open-source software called large-scale atomic/molecular massively parallel simulation (LAMMPS) [18] with Tersoff/ZBL potential developed by Albe et al. [11] and Gao et al. [3], which can accurately represent the sphalerite structure, physical properties, and defect formation energy of GaAs at room temperature. To restore the actual environment, the entire system relaxes under the isothermal-isobaric (NPT) ensemble, and the lattice constant corresponding to different temperatures at normal pressure is shown in Table 1. We can assume that Ga and As have very little differences in causing damage due to the same mass. Thus, a Ga atom with kinetic energy from the top-center of the entire system is selected as PKA, whose incidence angle deviates approximately 7° from the Z-axis to avoid the channel effect [19].

To better investigate the effect of temperature on PDD, the PKA energy (E_{PKA}) from 1 keV to 10 keV is simulated at five different temperatures from 300 K to 900 K to ensure the universality of results. The entire process consists of two steps. First, the entire system is relaxed for 15 ~ 20 ps under the isothermal-isochoric (NVT) ensemble to arrive at a thermal stability structure. Then, we describe the cascade collision process from PKA excitation to terminal by using a multiple-phase timestep procedure successfully applied to simulate PDD of semiconductor materials [6,8], and the total time is 20.4 ps. It is necessary to build a reasonable model size to prevent PKA from crossing the boundary. For instance, Fig. 1 shows that the displacement cascade of 1 keV PKA is simulated by $20 \times 20 \times 20$ unit cells including 64,000 atoms. The thermostat region can release heat to maintain the temperature [20] during this reaction, and the periodic boundary conditions are used in all three directions. Each event is simulated 20 times to obtain meaningful average statistics, among which the error bar is the standard error of average as shown in Table 2 and Figs. 5, 6, and 11.

Because of the plurality of GaAs, different types of defects are produced, which have an obvious impact on the properties. The Wigner-Seitz cell method in Ovito [21] is adopted to analyze the defects in the cascade process. These defects are divided into vacancies, interstitials, and antisite defects. Vacancy defects imply that one atom leaves the original lattice position to form an empty site such as V_{Ga} and V_{As}. In contrast, if a cell contains two or more atoms, the atom farther away from the center site will be identified as the interstitial (I_{Ga} and I_{As}). The antisite defect (G_{As} and As_{Ga}) is that there is one atom in the site, but different from the original atom type. The defect distribution is usually analyzed in light of clusters and isolated defects [21]. A group of defects is defined as a cluster within the cutoff distance of one lattice constant (5.653 Å) and the size of the cluster relates to the number of defects

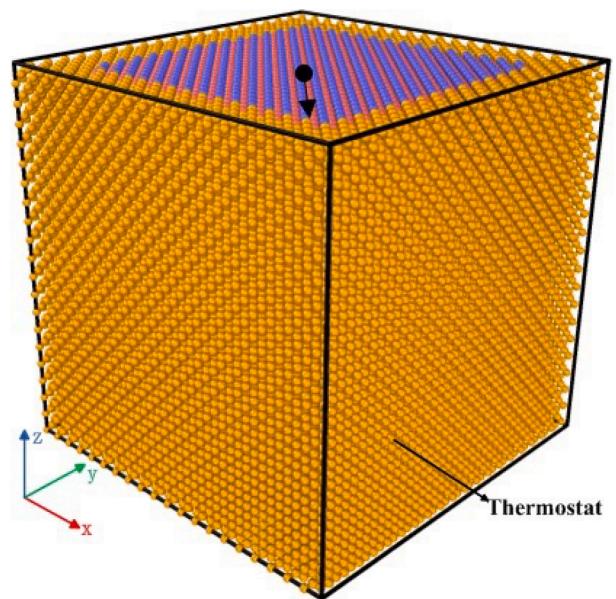


Fig. 1. Diagram of the simulation model; the black atom is PKA and yellow atoms are in the thermostat region.

contained: between 2 and 5 represents a little cluster, while over 6 represents a large cluster [13]. If the cutoff distance is more than 5.653 Å, these defects are isolated point defects.

3. Results and discussion

3.1. Evolution of the cascade defects

As shown in Fig. 2, in a short period of elastic collision, different point defects rapidly generate and extend around the trajectory of PKA, which tend to congregate to form some amorphous regions and reach the maximum in \sim 0.4 ps. This moment when defects arrive at the thermal peak is t_p , and their number is N_p . However, most defects in the ballistic phase are thermal instability and will decrease through spontaneous recombination within vacancies and interstitial defects. Then, when the standard deviation of the number is less than 1, the distribution and number of defects are defined as basically stable at the ps level, which is based on the criterion of the Wigner-Seitz method. Simultaneously, the time and number for defects are defined as t_s and N_s respectively. This stable phase continues for 15 ps and to the end.

Previous studies [22–24] on material PDD show that E_{PKA} and temperature are the main influencing factors. In Figs. 3 and 4, the number of antisite defects shows a similar trend of “rise, fall, and stability” to Frenkel pairs. Fig. 3(a) and (b) show that high E_{PKA} can easily move atoms through elastic collision, thus increasing both t_p and N_p for Frenkel pairs and antisite defects. From 1 keV to 10 keV, N_p of Frenkel pairs and antisite defects increase by approximately 629.9 and 175.8, respectively. The high peak value implies a violent collision between the dislocated atoms, resulting in a long time of recombination. Therefore, this behavior prolongs t_s of Frenkel pairs and antisite defects by approximately 4.2 and 8.7 ps respectively. Beyond this, the stable defects are also influenced, and there is an increasing trend for N_s , which is more obvious in Frenkel pairs. The result indicates that increasing E_{PKA} directly affects the evolution parameters of cascade defects and will aggravate PDD.

Fig. 4 shows that the dynamic evolution of defects under different temperatures, among which N_p and t_p also become larger for Frenkel pairs and antisite defects with increasing temperature. There is a direct relationship between temperature and atomic kinetic energy. The high temperature will accelerate the atomic motion and weaken the bond

Table 1

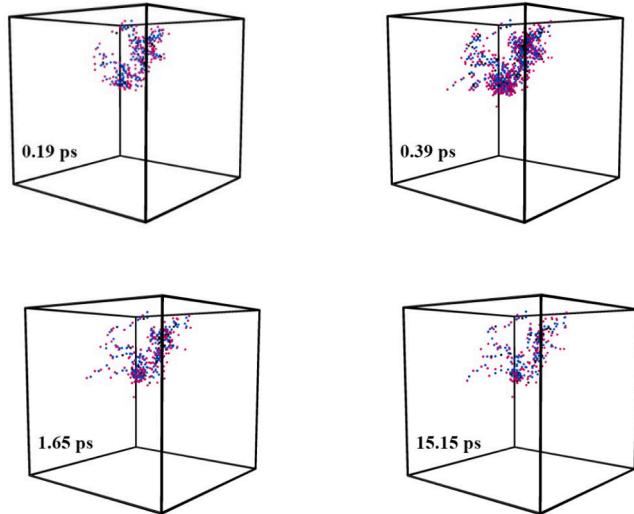
The balanced lattice parameter of GaAs at different temperatures.

Temperature (K)	300	450	600	750	900
Lattice parameter (Å)	5.667	5.675	5.682	5.689	5.696

Table 2

Cascade parameters of Ga and As vacancy defects at different temperatures.

Temperature (K)	Peak number		Stable number		Stable time (ps)		Recombine efficiency (%)	
	Ga	As	Ga	As	Ga	As	Ga	As
300	213.4 ± 32.1	148.4 ± 20.9	104.8 ± 8.6	28.6 ± 5.3	6.2 ± 0.3	5.0 ± 0.2	50.1 ± 0.9	80.6 ± 1.3
450	222.8 ± 33.2	147.7 ± 18.7	101.9 ± 9.3	26.1 ± 3.1	8.3 ± 0.3	7.2 ± 0.2	53.3 ± 0.7	81.4 ± 1.2
600	232.4 ± 29.7	163.4 ± 23.4	97.2 ± 7.2	27.0 ± 5.6	10.3 ± 0.3	8.1 ± 0.2	57.2 ± 1.0	82.4 ± 0.9
750	244.7 ± 34.0	167.1 ± 25.2	93.9 ± 7.7	25.3 ± 4.1	12.1 ± 0.4	8.9 ± 0.2	60.6 ± 1.1	83.8 ± 0.7
900	262.6 ± 35.6	188.3 ± 29.7	90.2 ± 6.1	24.6 ± 3.9	15.0 ± 0.5	10.3 ± 0.2	64.9 ± 1.2	85.5 ± 1.3

**Fig. 2.** The defect distributions of 5 keV cascade at different times under 300 K. Blue, red, and black spheres represent vacancy, interstitial, and antisite atoms, respectively.

energy, thus increasing the possibility of the atoms being knocked out and leading to larger N_p and t_p . Hence, in Fig. 4(a) and (b), N_p increases by 89.7 and 40.5, respectively, at 900 K relative to 300 K, similar to that for E_{PKA} . The phenomenon related to t_p is interesting, and it can be seen that high temperature has an obvious delay capability in antisite defects particularly, where the extension of t_p is approximately 0.4 ps. It will be discussed later. The aspect of N_s is different from that shown in Fig. 3. There is an effective decline in N_s with increasing temperature, which is from 132 to 116.1. Thus, it can be concluded that the temperature will affect N_s and effectively reduce PDD. Because of the variation of N_s , the long-time recombination is needed here, and t_s increases in Fig. 4(a) and (b). The validation of the simulation results is concentrated in the

following discussion.

On the basis of continuous summarization and improvement, some theoretical models [25,26] for predicting the number of steady Frenkel pairs are proposed, in which the Norgett-Robinson-Torrens (NRT) equation [25] is the standard model based on the relationship of threshold displacement energy and E_{PKA} . It can be written as follows:

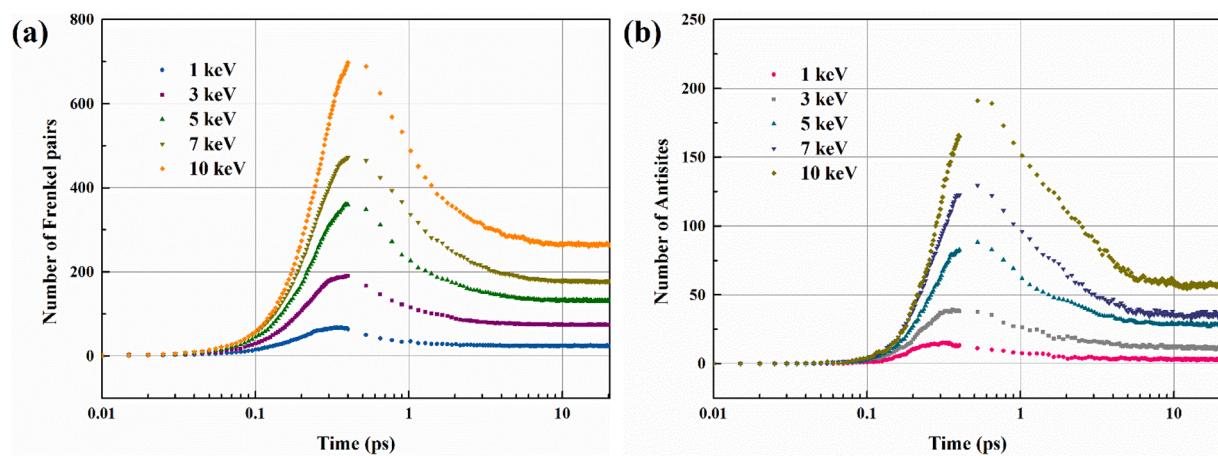
$$N_{Fs} = 0.4 \frac{E_{PKA}}{E_d} \quad (1)$$

where N_{Fs} is the number of steady Frenkel pairs and E_d is the threshold displacement energy of the material itself. Theoretical studies on E_d of GaAs have been performed for several decades [13,27], and the reasonable value was reported to be approximately 15 eV [13]. In Fig. 5, the errors between the values estimated by the NRT equation and N_{Fs} at 300 K are small, thus showing N_{Fs} is in good agreement with the NRT equation. It can be found that when E_{PKA} is less than 5 keV, the stable numbers of Frenkel pairs under different temperatures are similar. With E_{PKA} increasing steadily and exceeding 5 keV, it is clear that the differences between N_{Fs} of all temperatures become more obvious. And N_{Fs} also exhibits a downward trend with increasing temperature, resulting in a larger E_d , which is similar to GaN and Zr [8,11]. To some extent, Fig. 5 indicates that temperature has a direct effect on E_d .

As a specific property of the material, the recombine efficiency φ is closely related to temperature and reflects the radiation-resistant level. This is defined as follows:

$$\varphi = 1 - \frac{N_{Fs}}{N_{Fp}} \quad (2)$$

where N_{Fp} represents the maximum number of Frenkel pairs. As shown in Fig. 6, there is a nonlinear relationship between φ and E_{PKA} , and the declining trend tends to be smooth, which implies that the damage will be limited at high E_{PKA} . For instance, although the reduction of φ at 300 K was 2.4% from 1 keV to 5 keV, it was 1.4% from 5 keV to 10 keV. Moreover, high temperatures can promote the recombination of additional defects in particular in the range from 750 K to 900 K. From the

**Fig. 3.** The number of (a) Frenkel pairs and (b) antisites at 300 K varies with E_{PKA} .

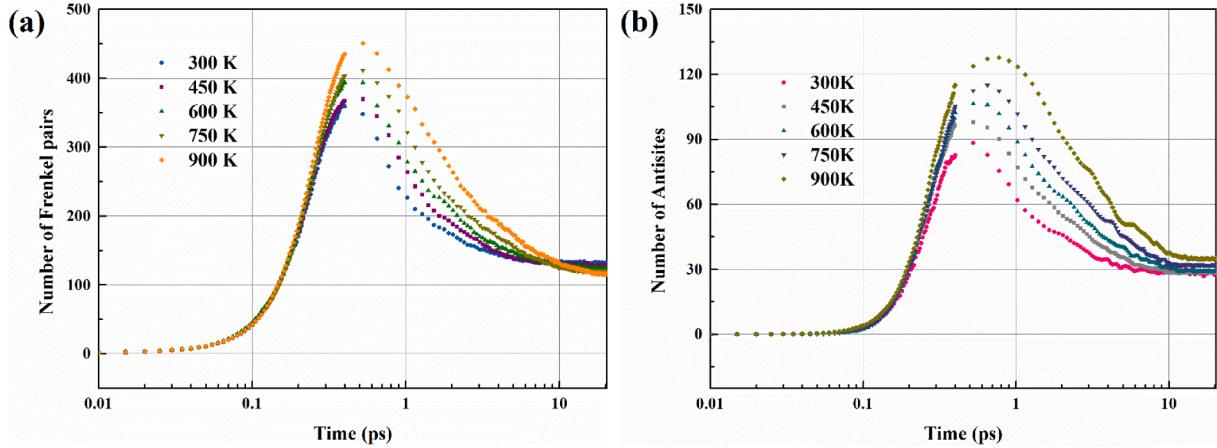


Fig. 4. The time evolution of (a) Frenkel pairs and (b) antisites varies with temperature when $E_{\text{PKA}} = 5 \text{ keV}$.

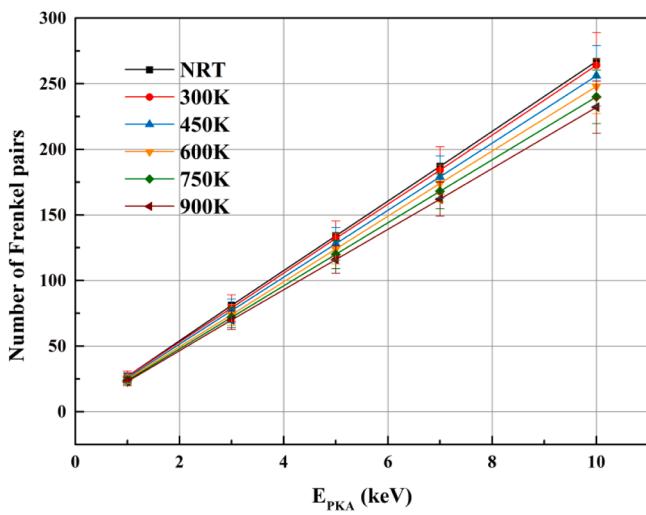


Fig. 5. Comparison between simulation and NRT values of steady Frenkel pairs at different temperatures and E_{PKA} .

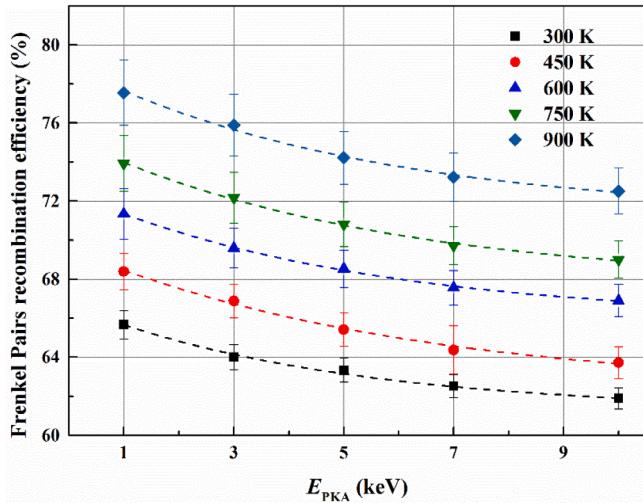


Fig. 6. The recombination efficiency at different temperatures and E_{PKA} .

comparison of 300 K with 900 K, it is clearly seen that the more significant increase is approximately 11.9% at 1 keV, which implies that the damage under low energy can easily recover.

3.2. Point defects of various types under different temperatures

To analyze in detail the reason for the variation in N_s and t_p under different temperatures, the dynamic evolution of defects is examined in terms of various defects. Unlike the total ionizing dose (TID), DD is dominated by vacancy-interstitial pairs which are the most common type of defects in materials. It is observed clearly from Fig. 7(a) and (b) that the number of Ga defects is greater than that of As defects, which may be the reason for E_d . As previously reported [28], it was proved that E_d for Ga is less than that for As at room temperature (300 K). This implies that Ga atoms are more likely to move to form defects during the cascade than As atoms. In addition, Fig. 7 highlights that although Ga and As defects have a similar trend of t_p and N_p from 300 K to 900 K, they differ greatly in the recombination phase. For instance, by combining Fig. 7(a) and Table 2, it is found that N_s of V_{Ga} reduces by approximately an average number of 14.6, and t_p of V_{Ga} increases by approximately 8.8 ps, which is more obvious than V_{As} . The recombine efficiency of V_{Ga} increases from 50.1% to 64.9%. The same is true for interstitials. These results show that Ga defects play an important role under change in temperature.

In addition to vacancies and interstitials, the dynamic evolution of antisite defects (Ga_{As} and As_{Ga}) is also studied. As shown in Fig. 8, both Ga_{As} and As_{Ga} have similar trends, but the number and variation range of As_{Ga} defects is more than Ga_{As} defects during the entire cascade. This may be the reason for the existence of vacancy-interstitial pairs. Because of the larger number of Ga vacancy-interstitial pairs, there are more possibilities for As atoms to enter the empty lattice position to form As_{Ga} defects. Equally, the rapid reduction of As_{Ga} defects is due to nearly Ga atoms that kick out As atoms to restore the original position, which is similar to Si_C defects in SiC [6]. Then, the kicked As atoms will travel in the crystal structure and recombine with As vacancies, which may result in the high recombining efficiency of As vacancies in Table 2. In contrast, the number of Ga_{As} defects is smaller, and it takes a longer time to reach the maximum, which causes a delay in t_p of antisite defects above. And this delay phenomenon in t_p is more obvious at 900 K.

3.3. Defect clusters

For the radiation damage of semiconductors, many point defects usually accumulate in the region and exist in terms of defect clusters [6] and dislocation rings [29]. In the environment of low-energy irradiated particles, the defect cluster is the main displacement defect, which hinders point defect migration and recovery at the atomic scale. Finally,

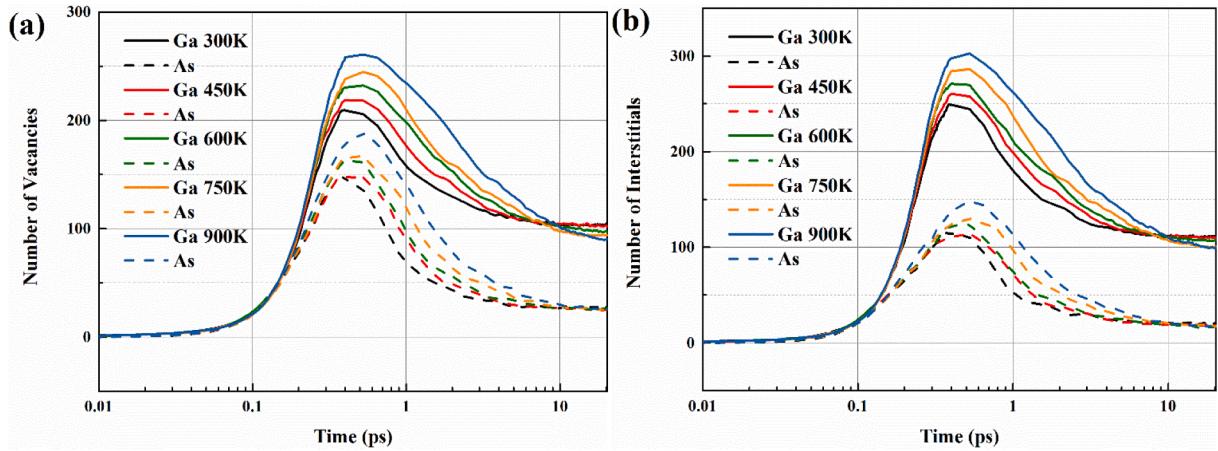


Fig. 7. The time evolution of (a) vacancies and (b) interstitials in the 5 keV cascade process under different temperatures; solid and dotted lines represent Ga and As, respectively.

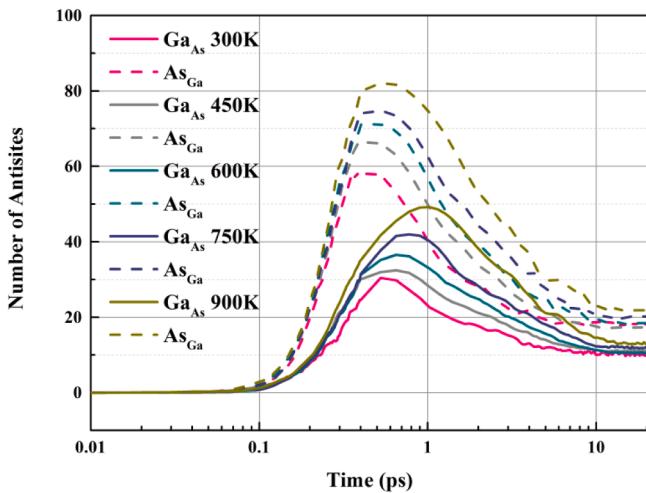


Fig. 8. The evolution of antisites in the 5 keV cascade process at different temperatures. Solid and dotted lines represent Ga_{As} and As_{Ga} respectively.

this leads to different forms of defect distribution and affects the mechanical and electrical properties of GaAs.

In terms of defect clusters, high E_{PKA} will enlarge the distribution range of defects and cause more serious PDD, as shown in Fig. 9(a) and (b). It is also found that the proportion of large vacancy clusters is

approximately 22.8% to 49.2% with increasing E_{PKA} and is greater than that of large interstitial clusters. Moreover, from 3 keV to 10 keV, the number of the larger size (larger than 10) of vacancy clusters increases quickly, suggesting that high E_{PKA} is more likely to produce large vacancy clusters. In contrast, interstitial defects are concentrated in small clusters and isolated point defects, which occupy a larger proportion than the vacancy. This is similar to GaN [8] and can be explained by the observation that the vacancy transfer energy is lower relative to the interstitial, thereby making it easy for vacancies to form clusters.

Temperature shows different trends from E_{PKA} . As shown in Fig. 10 (a) and 11(a), although there are still more large vacancy clusters at different temperatures, the proportion of large vacancy clusters continues to decrease from 48.6% of 300 K to 36.6% of 900 K. Because of the recombination of large clusters of vacancies, more isolated point defects generate, the proportion of which increases from 24.9% of 300 K to 30.1% of 900 K. However, in Fig. 10 (b) and 11(b), the number of interstitial point defects has little change, thus showing more thermal stability in temperature change; the large interstitial clusters are mainly transformed into small clusters. Therefore, regardless of whether it is the vacancy cluster or the interstitial cluster, from the cluster point of view, it is concluded that high temperature can promote the recovery of the damage, but the mode of transformation for vacancy and interstitial cluster is completely different.

4. Conclusions

In this paper, MD is used to simulate the cascade collisions of bulk

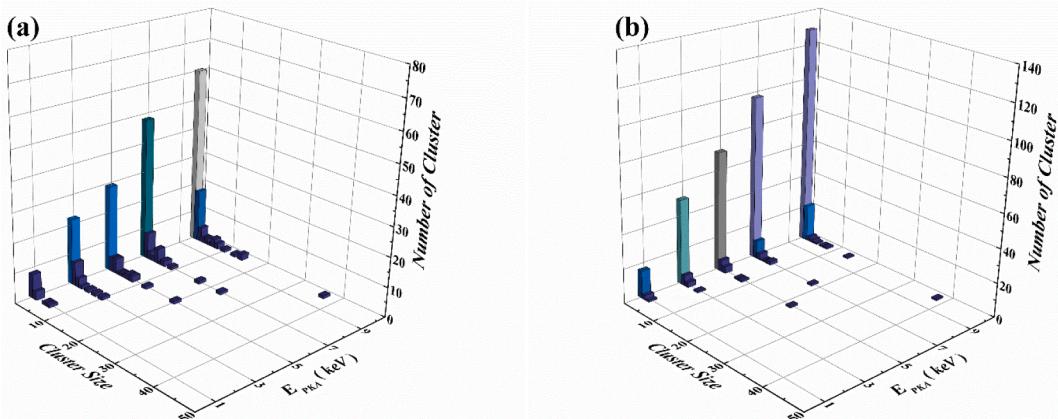


Fig. 9. The size and number of (a) vacancy and (b) interstitial clusters under different E_{PKA} at 300 K.

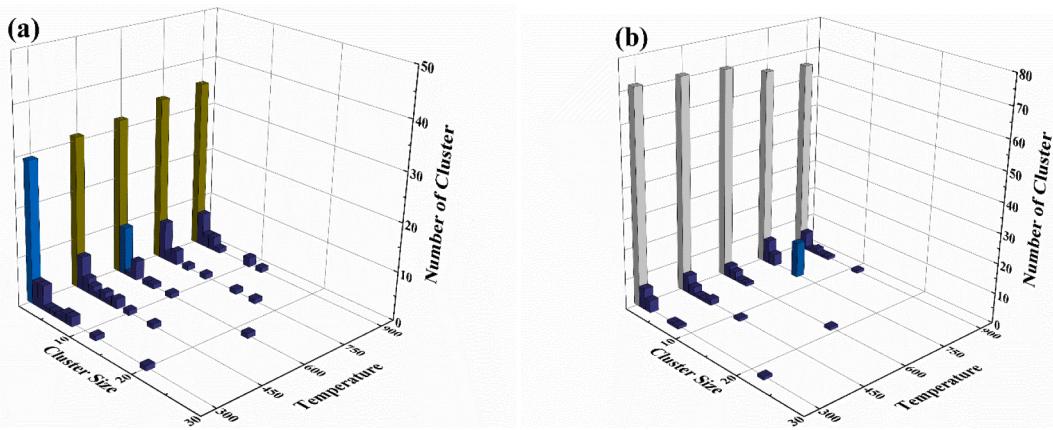


Fig. 10. The size and number of (a) vacancy and (b) interstitial clusters under different temperatures when E_{PKA} is 5 keV.

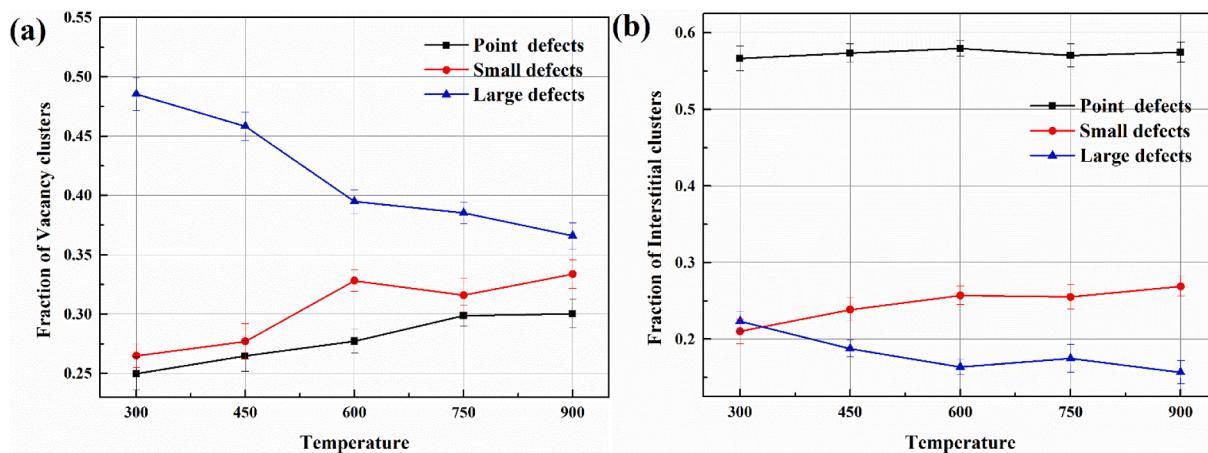


Fig. 11. The fraction of (a) vacancy and (b) interstitial clusters under different temperatures when E_{PKA} is 5 keV.

GaAs, with simulation temperature from 300 K to 900 K and E_{PKA} (Ga PKA) within 10 keV. By comparing it with E_{PKA} , the effect of temperature on the evolution and distribution of cascade defects is investigated.

The results show that E_{PKA} will effectively increase all cascade parameters (t_p , t_s , N_p , and N_s), resulting in a direct expansion of PDD. As temperature increases, the trend of some cascade parameters (t_p , t_s and N_p) of Frenkel pairs is similar to that under high E_{PKA} , while N_{FS} decreases (E_d increases), suggesting that high temperatures can directly affect E_d and reduce the degree of PDD, which is more obvious at low E_{PKA} . In addition, when N_s of defects changes with temperature, Ga defects (vacancies and interstitials) are mainly affected, while As defects remain stable.

Because of different E_d for Ga and As, there is a difference between Ga and As vacancy-interstitial pairs on the amount, thereby making the generation and recombination of Ga_{As} defects always slower than that of As_{Ga} defects. The difference in antisites also affects the recombination of As vacancies and interstitials.

Regarding clusters, the proportion of large vacancy clusters is greater than interstitials under high E_{PKA} . Different from the expansion effect of E_{PKA} on clusters, high temperatures can affect the distribution of defects in another way to reduce PDD. Larger vacancy clusters are mainly transformed into isolated point defects, which are responsible for the thermal instability of vacancies. However, only the transformation from large clusters to small clusters is observed in the interstitials.

CRediT authorship contribution statement

Tongxuan Jia: Investigation, Data curation, Visualization, Writing -

original draft. **Zujun Wang:** Conceptualization, Formal analysis, Funding acquisition, Writing - review & editing. **Yuanyuan Xue:** Conceptualization, Formal analysis, Writing - review & editing. **Qianli Jiao:** Supervision, Writing - review & editing. **Xie Yang:** Supervision, Writing - review & editing. **Xu Nie:** Supervision, Writing - review & editing. **Shankun Lai:** Supervision, Writing - review & editing. **Wuying Ma:** Supervision, Writing - review & editing. **Baoping He:** Supervision, Writing - review & editing. **Minbo Liu:** Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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