Molecular Dynamics Study of Grain Boundary Effects on the Evolution of Irradiation Defects in Austenitic Steels

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Abstract

In this work, we simulate the collision cascade process of 10 keV primary knock-on atoms in austenitic stainless steel alloy systems (Fe-18Cr-10Ni) and grain boundary (GB) systems (Σ3(111), Σ3(112), Σ27(115)) at various temperatures using molecular dynamics. The extent of radiation damage and defect types in alloy systems with and without grain boundaries are analyzed. Statistical analysis reveals that, with the exception of Σ3(111), a large number of defects reside at grain boundaries during the recombination stage and do not participate in bulk recombination, while only a few defects remain in the matrix, indicating that grain boundaries can attract cascade-induced defects and reduce defect concentrations in the matrix. The strength of the grain boundary effect is evaluated by calculating the absorption efficiency. Therefore, from a microscopic perspective, our results reveal that grain boundaries can act as strong absorption traps in materials, providing theoretical guidance for subsequent studies of grain boundary effects.

Full Text

Preamble

Molecular Dynamics of Grain Boundaries on the Evolution Behavior of Irradiation Defects in Austenitic Steels

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This work employs molecular dynamics simulations to investigate the cascade collision process of primary knock-on atoms with an energy of 10 keV in austenitic stainless steel alloy systems (Fe-18Cr-10Ni) and grain boundary systems (Σ3(111), Σ3(112), Σ27(115)) at different temperatures. We analyze

the extent of radiation damage and defect types in alloy systems with and without grain boundaries, and evaluate the strength of the grain boundary effect by calculating absorption efficiency. Our results reveal, from a microscopic perspective, that grain boundaries can act as strong absorption traps in materials, providing theoretical guidance for subsequent studies of grain boundary effects.

Keywords: Austenitic stainless steel, Grain boundaries, Molecular dynamics, Cascade collision process

Introduction

Austenitic stainless steel is a face-centered cubic structured metallic material with high Cr and Ni content and low C content. It exhibits good corrosion resistance, high-temperature oxidation resistance, and excellent processing and welding performance [1], making it commonly used as a material for reactor core cladding. Grain boundaries (GBs) are an important component of crystalline structures, representing incomplete two-dimensional structural defects compared to the perfect crystal structure. The GB structure is much more complex than the internal structure of grains and often possesses properties different from the grain interior. These properties affect many physical, chemical, and mechanical characteristics of crystals, including thermal conductivity, corrosion resistance, and mechanical strength [2–4], ultimately influencing the overall macroscopic properties of the material.

During long-term service in reactors, structural materials suffer varying degrees of radiation damage, with the root cause being the interaction between irradiation defects that leads to changes in material microstructure. The defects generated during irradiation mainly originate from cascade collisions. The molecular dynamics (MD) method is one of the most effective means for studying collision cascade processes and has been widely applied in materials research. In studies of γ-Fe, Wu et al. [5] used 40 keV primary knock-on atoms (PKA) at 300 K to characterize the peak stable stage for the first time. Compared with α-Fe, they found that γ-Fe has fewer defects in the stable stage and produces more aggregated defects. Meanwhile, low-dose neutron irradiation below 350 °C was applied to austenitic stainless steel, revealing that the yield strength increased while ductility decreased. This phenomenon was speculated to be mainly caused by the aggregation of point defects, particularly dislocation loops, which promote material deformation through local interaction between radiation damage structures and dislocation slip. Lin et al. [6] discussed the effects of different PKA energies, PKA incident directions, and temperatures on F-321 austenitic stainless steel. The number of Frenkel pairs increases with PKA energy. When the energy is below 30 keV, the effect of PKA direction on defect formation is relatively small, while at higher energies, the PKA direction effect becomes more significant.

Currently, most research focuses on basic radiation damage in austenitic stain-

less steel, while systems containing GBs are rarely discussed. The existence of GBs plays a crucial role in influencing material plastic deformation and point defect movement. GBs can serve as effective absorption traps for radiation-induced point defects, where vacancies and interstitial atoms tend to diffuse to GBs and be absorbed by them [7]. In GB research, boundaries are divided into high-angle and low-angle GBs based on the orientation difference between adjacent grains. If the misorientation exceeds 15°, it is considered a large-angle grain boundary, typically described using the Coincidence Site Lattice (CSL) model [8–11]. Σ is a symbol representing the density of overlapping sites. Higher Σ values indicate greater lattice mismatch near GBs, providing more sites for solute atoms. Normally, defects in materials originate from collision cascades of high-energy particles, such as vacancies and self-interstitial atoms (SIAs), which initially interact with GBs. Gao et al. [14] used MD simulations to study radiation defect recombination at different temperatures with various GBs. As temperature increased, the interaction between GBs and radiation-induced defects strengthened. Bai et al. [13] found that GBs can serve as effective absorption traps for vacancies and interstitials. After irradiation, interstitial atoms are attracted to grain boundaries and then act as sources, emitting interstitial atoms toward annihilated vacancies in the matrix. This recombination mechanism has a lower energy barrier than traditional vacancy diffusion and can annihilate nearby vacancies in the matrix, leading to self-healing of radiation-induced damage.

In further evolution, the accumulation of vacancies and SIAs can lead to dislocation loops, voids, and stacking fault tetrahedra (SFT) [14, 15]. The existence of GBs can affect the formation, quantity, and distribution of point defects, and the evolution of defects during cascade collisions is also influenced by GBs. Zhu et al. [16] proposed a grain formula that can evolve by coupling GBs and point defects, indicating that the concentration fraction of point defects is related to irradiation dose, laying the foundation for studying the long-term morphological evolution of radiation-induced defects. Experimental studies have measured that grain boundaries with high defect absorption strength can reduce void expansion in austenitic stainless steels by up to 10% [17], and even in nanometals with high grain boundary ratios, the absorption of large-scale dislocation loops by grain boundaries has been observed [18]. Irradiation damage in materials can be attributed to point defects caused by irradiation, and the ability of materials to resist irradiation damage depends on the extent to which the microstructure can eliminate equal amounts of vacancy and interstitial defects.

In this study, we primarily conducted cascade collision simulations of 10 keV primary collision atoms at different temperatures for systems with and without grain boundaries. Based on CSL theory, we selected and constructed three different large-angle GB structures: Σ3(111), Σ3(112), and Σ27(115). First, we briefly analyzed the stability of point defects at different locations relative to the grain boundaries. Subsequently, we simulated the cascade collision process in systems with and without grain boundaries, finding that both systems experienced three cascade processes. The number of defects produced by the grain boundary system was significantly greater than that of the alloy system, but

the number of defects in both systems increased with temperature. In the stabilization stage, for systems without GBs and with Σ3(111), higher temperatures resulted in lower defect numbers, indicating that temperature provides energy that enhances defect recombination. For Σ3(112) and Σ27(115), the number of residual defects increased with temperature, and a large number of residual defects existed primarily within the GBs, suggesting that defects absorbed by GBs do not participate in the recombination stage. To further confirm defect existence, defect cluster analysis shows that most defects in GBs exist as small defect clusters, while large defect clusters are relatively rare, though special SFT structures may form. By comparing defect differences between systems with and without GBs after cascading, analyzing defect forms, and further evaluating absorption effects at GBs, we demonstrate that strong absorption trap GBs can serve as effective absorption traps for irradiation-induced point defects, absorbing defects generated in the matrix during irradiation and thereby changing material properties, providing a theoretical basis for subsequent GB research.

2. Simulation Methods

We conducted static and molecular dynamics simulations using the open-source software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [19]. The models were built using the open-source program Atomsk [20] and visualized and processed through OVITO. In all simulation processes, periodic boundary conditions were applied in all directions [21].

In the constructed model, we use a face-centered cubic lattice constant a0 = 3.553 Å as the basic unit for the austenitic stainless steel system. The lattice sites in the supercell are randomly occupied by Fe, Cr, and Ni atoms with an atomic ratio of Fe-18Cr-10Ni, and the unit cell size is controlled to approximately 175.5 Å × 175.5 Å × 175.5 Å. The main composition is 69.2% Fe, 19.2% Cr, and 11.6% Ni, which is similar to industrial-grade AISI-304 austenitic stainless steel [22].

The three grain boundaries selected in this paper are Σ3(111), Σ3(112), and Σ27(115), all of which are large-angle grain boundaries constructed based on the coincidence site lattice theory for high-angle grain boundaries. This theory focuses on the geometric characteristics of crystal spatial positions, is mathematically rigorous and universal, and is applicable not only to GBs but also generalized to phase interfaces. According to GB energy theory [23], we obtained the GB energies for the three boundaries, with specific models and parameters shown in Fig. 1 [Figure 1: see original paper] and Table 1 .

Table 1. Basic parameters related to the three GBs.

GB type	GB angle (°)	Number of atoms	GB energy (J/m^2)
Σ3(111)			
Σ3(112)			

GB type	GB angle (°)	Number of atoms	GB energy (J/m^2)
Σ27(115)	31.59		

Fig. 1. Schematic diagram of the ion irradiation sample stage.

In classical MD simulations, interatomic interactions are specified primarily by potential functions, and Newton's equations of motion are solved to obtain trajectories of microscopic atoms [24]. The reliability of current MD simulations for predicting and evaluating irradiation properties, mechanical properties, and chemical properties of materials has been widely accepted and applied extensively. In this paper, we describe the interactions between Fe, Cr, and Ni ternary alloys using the Embedded Atom Model (EAM) potential developed by Bonny et al. [25]. The constructed alloys and GB models are subjected to static energy minimization using the Conjugate Gradient (CG) method [24] to obtain the most stable GB system structure. Subsequently, different systems undergo systematic NPT ensemble simulations with pressures (P) and temperatures (T_0 = 300 K, 573 K, and 873 K) set, and thermodynamic treatments are carried out for up to 30 ps until each system reaches a steady state to eliminate temperature-induced errors.

In the cascade simulation, we select the primary knock-on atom in a plane approximately 20 Å away from the GB position [26, 27] and set its kinetic energy to 10 keV. In that study [8], it was clearly shown that when the PKA energy is less than 30 keV, the incident direction has very little effect on defect formation. Therefore, the incident direction in the present study is chosen based on the optimal direction for each system: the <135> direction [28] is used for the grain boundary-free system, while the incident direction for the grain boundary-containing system is perpendicular to the GB. Subsequently, 15 cascade simulations were performed for systems with and without GBs at 300 K, 573 K, and 873 K, respectively, and the resulting number of defects was averaged to reduce statistical errors. After evaluating electronic stopping effects, we found that the electronic stop term mainly influences the number of defects produced in the cascade simulation, while the overall trend remains basically unchanged. Therefore, electronic stopping effects are not considered in this paper. During the collision cascade process, the pre-simulation is carried out for 5 ps with a time step of 0.1 ps, while the subsequent cascade simulation increases the simulation time to 100 ps with a time step of 1 ps. To avoid unwanted interactions during cascade and sub-cascade processes and to ensure temperature control, we define the outer region of the simulation box as a constant-temperature region. During relaxation and incidence, Berendsen and Nose-Hoover temperature control methods are applied to the outer region to control the system temperature, as shown in Fig. 2 [Figure 2: see original paper]. We use the visualization tool OVITO to visualize atoms and employ Wigner-Seitz (WS) Defect Analysis and Common Neighbor Analysis (CNA) [29, 30] to analyze the distribution of point defects and defect clusters.

Fig. 2. Schematic diagram of cascade collision.

Based on the above simulation process, we discuss point defect formation energies in GB-containing systems by performing atom insertion or deletion at different positions. These energies are obtained using molecular static calculations to compute the difference in cohesive energy of the whole system before and after the simulation. To eliminate errors, we consider 15 atoms at random positions for insertion or deletion in both systems and average the calculated energies to obtain the average formation energy. The formulas for the two formation energies can be expressed as:

interstitial = E_{interstitial} - E_0 -
vacancy = E_{vacancy} - E_0 +

where E_{interstitial} and E_{vacancy} denote the energy of the system after interstitial insertion or atom deletion, respectively, and E_0 denotes the total energy of the initial system. Additionally, this work considers segregation energy to study the energy difference of point defects at various distances from the GB. The segregation energy for different point defects can be expressed as:

E_{segregation} = E_f^{bulk} - E_f^{GB}

where E_f^{bulk} represents the formation energy of point defects at positions in the grain interior within the GB-containing system, and E_f^{GB} represents the formation energy of point defects at GB positions within the GB-containing system.

The absorption efficiency (FSE) of internal defects in GB is defined as the number of point defects absorbed by the GB (N_{GB}) divided by the total number of surviving point defects (N_S) after cascading:

FSE = N_{GB} / N_S

3.1. Stability Analysis of Point Defects at Different Positions from the GB

First, we analyzed the defect stability of point defects at different locations relative to the GB, as shown in Fig. 3 [Figure 3: see original paper]. When point defects are near the GB, the formation energy is substantially reduced, particularly for interstitials, while vacancies in the GB show different degrees of reduction that are not as severe as for interstitials. This phenomenon occurs because the atomic arrangement at the GB is less symmetric and more dispersed, with numerous sites inside the GB that can be occupied by interstitial atoms, creating an attractive effect on interstitials.

In different types of GBs, defects in the amorphous region fluctuate around a certain energy value. For the special Σ3(111) boundary, there is no obvious energy reduction phenomenon because the GB width is almost zero, as Σ3(111) belongs to coherent twin boundaries [31]. In the model construction, it is clear

that Σ3(111) exists only as a planar interface with atomic arrangement misalignment between two adjacent layers. From an energy perspective, the grain boundary width can be determined by the formation of an energy change region, which shows that Σ3(111) almost does not produce effective defect absorption wells, as shown in Fig. 3(a). As for Σ3(112) and Σ27(115), both GBs exhibit more obvious grain boundary widths, with Σ3(112) having a width of about 13.91 Å and Σ27(115) about 7.12 Å, as shown in Fig. 3(b) and (c). However, there is no clear relationship between grain boundary width and absorption capacity or grain boundary energy [7, 32]. In the GB, the steepening of interstitials is significantly larger than that of vacancies, and notably, in Σ27(115), the formation energy of some interstitials and vacancies can be reduced to negative values, indicating that Σ27(115) is the strongest defect absorption trap compared to the other two GBs.

Fig. 3. Energy of point defect formation at different positions from different GBs: (a) Σ3(111)-Fe-18Cr-10Ni; (b) Σ3(112)-Fe-18Cr-10Ni; (c) Σ27(115)-Fe-18Cr-10Ni.

Subsequently, we calculated the segregation energy under different GBs using Eq. (3), as shown in Fig. 4 [Figure 4: see original paper]. In Σ27(115), the segregation energies of point defects are generally higher than those of the other two GBs, while the interstitial segregation energies of Σ3(112) are all greater than 1.1 eV, suggesting that Σ3(112) also forms a strong defect absorption trap. In Σ3(111), the segregation energies of point defects are all on a lower energy scale, confirming that there is no significant GB absorption effect in Σ3(111). It is worth noting that for GBs forming strong absorption traps, the segregation energy of interstitials is always higher than that of vacancies. Relevant calculations show that vacancy migration energy is between about 0.7 and 1.7 eV, while interstitial migration energy is between about 0.05 and 0.1 eV [33, 34]. Since interstitial migration energy is much smaller than vacancy migration energy, interstitials migrate faster in the system and are more likely to be attracted by GBs during migration.

Fig. 4. Segregation energy of point defect formation at different positions from different GBs.

3.2. Cascade Analysis of Systems with and without GBs

To further determine the role of GBs, we carried out cascade collision simulations for systems with and without GBs, as shown in Fig. 5 [Figure 5: see original paper]. We found from the simulations that in the system without GBs, the cascade collision process is usually divided into three stages: the initial accumulation stage, the thermal spike stage, and the thermal equilibrium stage. Defects are generated and accumulate rapidly in the initial stage of the cascade, reaching a peak of Frenkel defects (the thermal spike) at about 1.5 ps. Subsequently, most defects recombine and annihilate during the thermal peak annealing stage, leaving only a few defects in the thermal equilibrium stage, as

shown in Fig. 5(a).

As temperature increases, the time for the system to reach the thermal peak is delayed, and the number of Frenkel defects generated during the thermal peak stage increases. In the thermal equilibrium stage, the number of Frenkel defects decreases with increasing temperature, indicating that temperature provides more energy for atomic movement, leading to increased Frenkel defect production at the thermal peak stage and enhanced defect recombination efficiency at the thermal equilibrium stage.

Systems containing GBs underwent the same cascade process. We found that the three different types of GB systems also exhibited the same three cascade processes, with the time to reach the thermal spike delayed as temperature increased, and the number of Frenkel defects increasing significantly during the thermal spike stage. In the thermal equilibrium stage, results obtained for the system containing Σ3(111) are consistent with the lower cascade law in the GB-free system, i.e., the number of Frenkel defects decreases with increasing temperature, as shown in Fig. 5(b). Notably, the number of residual Frenkel defects in systems containing Σ3(112) and Σ27(115) is higher with increasing temperature, as shown in Fig. 5(c-d).

Fig. 5. The number of Frenkel defects over time in different systems. (a) Alloy-Fe-18Cr-10Ni; (b) Σ3(111)-Fe-18Cr-10Ni; (c) Σ3(112)-Fe-18Cr-10Ni; (d) Σ27(115)-Fe-18Cr-10Ni.

In response to this special phenomenon, we counted the number of interstitials and vacancies within the GBs and the overall number of Frenkel defects during the thermal equilibrium stage, taking the cascade process at 873 K in different systems as an example, as shown in Fig. 6 [Figure 6: see original paper] and Table 2. We found that in cascade simulations of the grain-boundary-free system, most defects generated at the thermal spike complete recombination before reaching the thermal equilibrium stage, leaving only a few defects in the system, as shown in Fig. 6(a). However, the presence of strong absorption traps leads to increased defect production during the cascade process. At the thermal equilibrium stage, nearly 90% of defects in systems containing Σ3(112) and Σ27(115) exist inside the boundaries, while only a small number of defects remain in the matrix, as shown in Fig. 6(c)-(d). This indicates that most interstitial and vacancy defects recombine during the transition from thermal spike to thermal equilibrium and also migrate to the GBs, while defects attracted to the interior of GBs no longer recombine, leading to increased defect numbers remaining in the thermal equilibrium phase [35].

In contrast to Σ3(111), a large number of defects are present in the matrix, with only a few or no defects inside the GB, indicating that strong absorption traps are not formed in the system containing Σ3(111), as shown in Fig. 6(b). In all statistical data, the number of interstitial defects in GBs is significantly higher than that of vacancies, indicating that GBs absorb more interstitial defects than vacancies.

Fig. 6. Defect evolution at a temperature of 873 K in different systems: (a) Alloy-Fe-18Cr-10Ni; (b) Σ3(111)-Fe-18Cr-10Ni; (c) Σ3(112)-Fe-18Cr-10Ni; (d) Σ27(115)-Fe-18Cr-10Ni.

To further understand the state of defects after cascading, we statistically analyzed the average number of clusters of different sizes and evaluated the absorption efficiency of internal defects in GBs at a temperature of 873 K. Since vacancies can exist as single defects while interstitials are usually bonded as interstitial pairs, cluster size values are statistically different. All systems containing GBs produced larger numbers of defects than systems without GBs. Notably, for grain-boundary-free and Σ3(111) systems, defects are mostly present in the matrix as small clusters, with large clusters less likely to occur. For Σ3(112) and Σ27(115), the probability of generating large clusters increases considerably due to their overall high defect numbers. These large clusters can form stable arrangements at the GBs, but under certain conditions in the matrix can also form special stacking fault tetrahedra, as shown in Fig. 7 Figure 7: see original paper-(b1). This structure is also possible in simulations of systems without GBs and weak absorption traps. Calculating the GB effect for different GBs, we found that defect absorption efficiency is positively correlated with GB energy, as shown in Fig. 7(c). Σ3(111) has very low grain boundary energy with an absorption efficiency of about 6%, while Σ27(115) has the highest grain boundary energy and an efficiency of 92%, indicating the highest defect absorption capacity. Therefore, Σ27(115) has the strongest efficiency in absorbing defects, while Σ3(111) has the smallest grain boundary energy, indicating weaker defect absorption ability.

Fig. 7. (a)-(b) Average number of different cluster sizes for systems with and without GBs at 873 K. (a1)-(b1) Stacking fault tetrahedra formed by vacancies (a1) and interstitials (b1), respectively. (c) Defect absorption efficiency.

Table 2 . The density and diameter of dislocation loops.

GB type	Type of defect	Σ3(111)	Σ3(112)	Σ27(115)
Vacancy number				
Interstitial number				
All number				
Vacancy number				
Interstitial number				
All number				
Temperature (K)				

4. Conclusion

In summary, to analyze the microscopic influence mechanism of GBs on material properties, we conducted a series of irradiation simulation studies on systems with and without GBs using molecular dynamics. We primarily analyzed the

formation energies of point defects at different positions from GBs, the segregation energies of point defects, the comparison of Frenkel numbers inside and outside GBs during the cascade process, and the state of defect existence in the composite phase. From the results obtained, we can summarize the following conclusions:

(1) For the three types of GBs, Σ3(112) and Σ27(115) belong to GBs with strong absorption traps, while Σ3(111) is a GB with weak absorption trap characteristics. In Σ3(112) and Σ27(115), the formation energy of point defects is significantly reduced when close to the GB, indicating that point defects easily exist in GBs. The formation energy of interstitial atoms is particularly reduced, and interstitials are more likely to exist in GBs than vacancies.

(2) In cascade simulations, all systems undergo three processes: initial accumulation stage, thermal peak stage, and thermal equilibrium stage. During the thermal peak stage, the number of defects increases with temperature. In the thermal equilibrium stage, for systems without GBs and with Σ3(111), increased temperature results in decreased Frenkel defects, mainly due to enhanced defect recombination efficiency with increasing temperature. However, for Σ3(112) and Σ27(115), a large number of defects exist inside the GB while only a few remain outside the GB, indicating that the GB acts as an absorption trap for defects.

(3) Upon comparing the defect absorption efficiencies of the three different GBs, we find that Σ3(111) has very low grain boundary energy and an absorption rate of almost 0, whereas Σ27(115) has the highest grain boundary energy and the highest defect absorption efficiency. Additionally, due to the presence of strong absorption traps, most defects do not participate in the recombination phase but exist in the form of clusters within GBs. Large defect clusters are usually formed in ordered arrangements within GBs, whereas in the matrix they typically appear as stacking fault tetrahedra.

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Note: Figure translations are in progress. See original paper for figures.