

Article

Atomic-Scale Dislocation Structure Evolution and Crystal Ordering Analysis of Melting and Crystallization Microprocesses in Laser Powder Bed Melting of γ -TiAl Alloys

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Abstract: Laser Powder Bed Fusion (LPBF) technology exhibits significant advantages in the manufacturing of components with high dimensional accuracy and intricate internal cavities. However, due to the inherent room-temperature brittleness and high-temperature gradient induced by the laser forming process, the LPBF fabrication of γ -TiAl alloy is often accompanied by the initiation and propagation of defects. The aim of this study is to investigate the forming process of γ -TiAl alloy by the LPBF method through molecular dynamics simulation, and to explain the microparticle arrangement and displacement evolution of the melting and crystallization processes, thus elucidating the link between the variations in the laser process parameters and defect generation during microscopic laser heating. The results show that during the melting process, the peaks of the radial distribution function (RDF) decrease rapidly or even disappear due to laser heating, and the atomic disorder is increased. Although subsequent cooling crystallization reorders the atomic arrangement, the peak value of the RDF after crystallization is still 19.3% lower than that of the original structure. By setting different laser powers (200–800 eV/ps) and scanning speeds (0.2–0.8 Å/ps), the effects of various process parameters on microforming and defect evolution are clarified. When the laser power increases from 200 to 400 eV/ps, the stable value of atomic displacement rises from 6.66 to 320.87, while it rises from 300.54 to 550.14 when the scanning speed is attenuated from 0.8 to 0.4 Å/ps, which indicates that, compared with the scanning speed, the atomic mean-square displacements are relatively more sensitive to the fluctuation of laser power. Dislocation analysis reveals that a higher laser power significantly increases the cooling rate during the forming process, which further aggravates the generation and expansion of dislocation defects.

Keywords: laser powder bed fusion; molecular dynamics simulation; γ -TiAl alloys; dislocations; crystallization



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1. Introduction

The aerospace field has become one of the most active and influential scientific and technological fields in the 21st century [1]. As the heart of aerospace equipment, engines are known as the “jewel on the crown of modern industry”. Turbine blades, as key components of aero-engines, are subject to thermal-mechanical coupling damage at high temperatures and pressures [2–4], which can have a significant impact on their service life [5,6]. γ -TiAl alloy has attracted great attention due to its low density, high specific strength, and outstanding corrosion and oxidation resistance. It has emerged as one of the most promising advanced lightweight high-temperature structural materials for the aerospace, automotive, and other industries [7].

Currently, the forming methods for γ -TiAl alloys primarily include casting [8], ingot metallurgy [9], and powder metallurgy [10,11]. Casting, despite its lower cost and simpler process, is prone to the creation of defects such as segregation, coarse grain structures, and shrinkage of porosity. Additionally, γ -TiAl alloys exhibit high reactivity in the molten state, making them susceptible to reactions with casting mold materials, resulting in the formation of brittle layers that significantly impact their durability [12]. Ingot metallurgy, on the other hand, has the capability of producing large, homogeneous γ -TiAl alloy components with outstanding performance. However, its high-temperature heating requirements above 1000 °C impose strict demands on equipment, and the process is complex, leading to a high cost and low raw-material utilization [13]. Powder metallurgy, while effective in reducing casting defects and enabling precise control of the alloy composition, faces limitations in the low flowability of powders, restricting the fabrication of components with complex shapes. Moreover, it cannot completely eliminate porosity, leading to mechanical properties that are inferior to those of cast alloys [14,15].

Widely applied in industries such as the marine, defense, and aerospace industries, the advancement of 3D printing technology has brought about significant transformation in the traditional manufacturing industry, emerging as a focal point in the field of advanced manufacturing [16,17]. Particularly, Laser Powder Bed Fusion (LPBF) technology, based on powder bed melting, has emerged as a cutting-edge technique. It is capable of achieving smooth surfaces while reducing machining, increasing material utilization, and significantly shortening production cycles [18–20]. In addition, the rapid solidification process of alloys during the LPBF process refines grain structures, enhancing the overall mechanical properties, thus making it highly suitable for the near-net shaping of high-strength refractory metals and complex components [21,22]. Therefore, it is of far-reaching significance to research the process-parameter regulation mechanism of laser powder bed fusion technology in the manufacturing of high-performance, complex structural γ -TiAl alloy components, and to optimize the forming process in order to enhance the forming quality and mechanical properties of γ -TiAl alloys.

However, residual stresses are easily introduced during the laser heating and forming process, which may couple with internal initial residual stresses [23,24], resulting in coupled stresses that lead to structural defects such as cracks [25–27] and, thus, significantly affecting the stiffness, stability, fatigue strength, and lifespan of components. Based on this, numerous scholars have carried out extensive research on approaches to suppress defects in γ -TiAl alloys. Gao et al. [28] explored the crack generation and inhibition mechanism of γ -TiAl alloy and clarified the impact of laser process parameters on the macroscopic sensitivity of cracks. The results indicated that crack initiation and propagation are largely attributed to the formation of coarse grains and brittle B2 phases under the high melt-pool cooling rate during laser processing. Effective crack suppression could be achieved by reducing the cooling rate to refine the grain structure. However, instead of achieving the goal of crack eradication, the process-optimization strategy for the LPBF of γ -TiAl alloys can only reduce the crack generation. In this regard, Polozov and Caprio [29–31] investigated the effect of the substrate temperature on the formation of cracks, and the results showed that the preheating of the substrate during the laser heating and forming process can significantly reduce the high temperature gradient brought about by the rapid cooling and heating characteristics of the laser, thus making the microstructure of the material more homogeneous, and finally improving the quality of the crack formation. This approach successfully achieved the crack-free forming of γ -TiAl alloy when the substrate preheating temperature was raised to 900 °C. Yet, the high equipment cost associated with substrate preheating has seriously hindered its widespread industrial application. In light of this, scholars have turned their attention to the introduction of rare-earth reinforcing phases for crack inhibition research. Based on numerical simulation methods and LPBF experimental analysis, Zhuo et al. [32] investigated the mechanism of crack inhibition in laser powder bed-fused γ -TiAl alloys with the addition of LaB6 inoculant and successfully reduced the

crack density of the formed components, thus significantly enhancing the forming quality of γ -TiAl alloys through the grain refinement and purification effect of LaB6 inoculant.

The aforementioned study meticulously expounds on the origins of defects and strategies for their inhibition during the laser powder fusion process of γ -TiAl alloys. However, the macroscopic mechanical properties of materials are dictated by their atomic arrangement. At the atomic scale, there is still a lack of investigation into the evolution process and defect analysis of the γ -TiAl alloy system during the LPBF process. Also, the experimental study of LPBF struggles to capture the complete particle migration and motion during both the melting and crystallization processes at the nanoscale. Additionally, the high cost associated with nanoscale characterization poses a significant challenge. Utilizing molecular dynamics simulation, however, offers a perfect solution to meet these demands. Therefore, through molecular dynamics simulations, this study investigates the structural evolution of the melting and crystallization process of γ -TiAl alloy in the Laser Powder Bed Fusion process. Through analysis of atomic displacement, ordering, and dislocations, the atomic evolution and mechanisms of defect initiation and propagation during laser processing are elucidated, which provides a crucial theoretical foundation for enhancing the forming quality and inhibiting cracks in components.

2. Materials and Methods

2.1. Atomic Structure Details

Based on the open-source molecular dynamics software LAMMPS (<https://lammmps.sandia.gov>) [33] and microscopic particle evolution algorithm, the microscopic evolution process for the melting and crystallization of γ -TiAl alloy in LPBF process was constructed. Differing from the regular FCC lattice structure, γ -TiAl alloy exhibits the ordered L_{10} face-centered tetragonal (FCT) structure, where the (002) plane is alternately occupied by Ti and Al atoms [34–37]. The initial configuration of the laser powder bed fusion experiment is outlined in Table 1. Based on the above-mentioned microscopic crystal structure of γ -TiAl alloy, initial nanoscale particles with a diameter of 5.2 nm were established through crystal modeling software atomsk (<https://atomsk.univ-lille.fr>). These particles were subsequently replicated in the x and y directions to obtain a prefabricated powder bed consisting of 20 nanoscale particles. Finally, the ordered arrangement of powder bed particles was placed on a pre-constructed substrate in order to complete the initial simulation model for LPBF process. The ultimate model is illustrated in Figure 1. Figure 1d presents the initial atomic stacking arrangement of the γ -TiAl alloy powder bed. In the initial model, at distances of 2.87 Å, 4.07 Å, 4.98 Å, and 5.75 Å, distinct peaks were observed which corresponded to atomic distributions with lattice constants of $\sqrt{2}/2$, 1, $\sqrt{3}/2$, and $\sqrt{2}$ times, respectively. The first peak was the highest, representing the minimum spacing of the γ -TiAl alloy particle distribution. The narrowness of the peaks suggested the initial perfect crystal configuration of the γ -TiAl alloy [38].

Table 1. Experimental parameter diagram of laser powder bed fusion.

Parameter	Quantity
Radius of each nanoparticle	2.6 nm
Elements in each nanoparticle	Ti:2567 Al:2611
Dimensions of the substrate	$22.80 \times 31.01 \times 2.00 \text{ nm}^3$
Atoms in the substrate	96,600
Total atoms	200,160

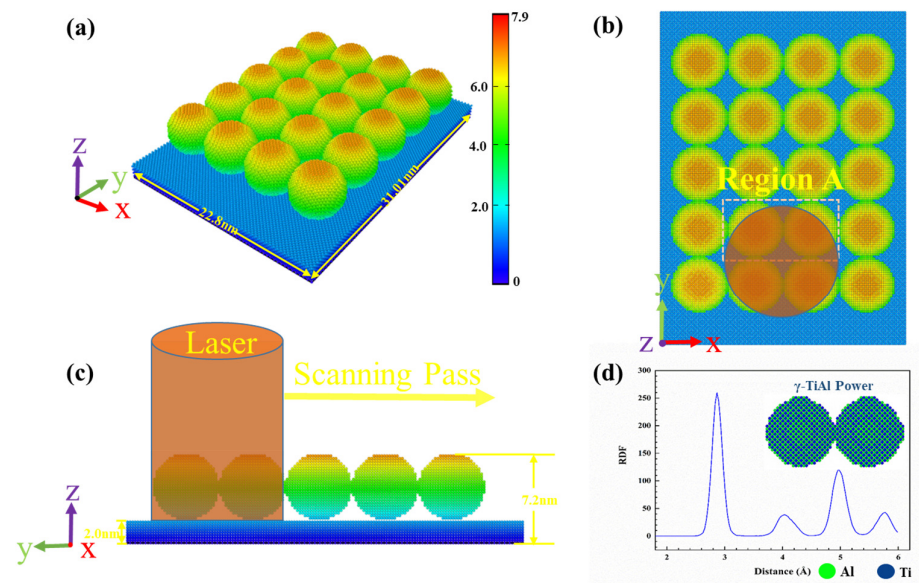


Figure 1. Laser powder bed fusion model configuration: (a) perspective view; (b) top view; (c) front view; (d) radial distribution function of original γ -TiAl powder.

The simulation region was oriented along the X, Y, and Z directions as [100], [010], and [001], respectively. To mitigate the impact of model size effects, periodic boundary conditions were employed in the X and Y directions, while shrink-wrapped boundary conditions were set in the Z direction. In order to reduce simulation errors and enhance the reliability of numerical simulations, the substrate was subdivided along the positive z-axis into three distinct layers. A fixed layer (0–0.4 nm) was employed to immobilize the model, minimizing adverse effects caused by model displacement resulting from stress during LPBF process; the thermostat layer (0.4–0.8 nm) was based on the Langevin temperature-control algorithm to continuously absorb the energy introduced by the laser, maintaining the substrate temperature consistently at 300 K, and thus providing a means to control and dissipate the input laser energy. In order to facilitate the smooth transfer of thermal energy from the powder bed to the constant temperature layer, a Newtonian layer (0.8–2.0 nm) was introduced as a conductive medium.

2.2. Interatomic Potential

Under the microscale simulation environment, the choice of the potential function served as a key parameter for the calculation of interatomic interactions, which plays a crucial role in the accuracy and reliability of the simulation. Based on this, this study adopted the embedded atomic potential function (EAM) developed by Zope and Mishin [39], which accurately reproduced the crystal structure of γ -TiAl alloy and successfully reproduced the fundamental lattice properties of the alloy. Furthermore, on the basis of the previous studies of the EAM potential function of TiAl alloys, high-temperature conditions and lattice thermal expansion theory were introduced into the potential system and proved to be authentic and reliable. The total potential energy of this potential function system can be expressed as follows:

$$E_{total} = \sum_i F_i(D_i) + \frac{1}{2} \sum_{i \neq j} \varphi_{ij}(r_{ij}) \quad (1)$$

where F_i denotes the embedding energy; D_i describes the electron density at atom i , attributed to atom j and separated by r_{ij} ; and $1/2 \sum_{i \neq j} \varphi_{ij}(r_{ij})$ denotes the pair potential energy.

The magnitude of the value of D_i is determined by the following equation:

$$D_i = \sum_{j \neq i} \rho_j(r_{ij}) \quad (2)$$

where ρ_j is the electron density on another atom j , which is isolated from the nucleus of atom i by a distance of r_{ij} [40].

2.3. Simulation Procedures

The microscopic model of laser powder fusion for γ -TiAl alloy was equilibrated for 100 ps under the microcanonical ensemble (NVE) with the timestep of 0.001 ps to eliminate the initial stress effects on the model. Continuous non-translational kinetic energy was applied to a cylindrical region with a diameter of 10.4 nm using the “fixing heat” command to simulate the laser heat source during the laser heating and shaping process of the powder bed. The cylindrical laser region was initially positioned at $(x, y) = (10.3, 5)$, with a height consistent with the powder bed. At the beginning of the experiment, the laser was set to move along the positive y -axis at a given speed to accomplish the melting and shaping process of the powder bed. When a scanning path was completed, the laser was removed and a cooling treatment was applied to the entire simulation system to obtain better crystalline and forming organization. The cooling process lasted for 200 ps. The energy density of the laser processing was determined by the following formula:

$$E_p = \frac{P}{vht} \quad (3)$$

where v represents the laser scanning speed, h is the hatch space, t denotes the powder bed layer thickness, and P characterizes the laser power. At the end of the experiment, further numerical analysis of the microscopic evolution in melting and crystallization were carried out based on the common neighbor analysis (CNA) [41] and dislocation analysis (DXA) modules in the visualization software ovito (<https://www.ovito.org>) [42].

3. Results and Discussion

3.1. Temperature and Structural Evolution

To clarify the microscopic evolution process of the LPBF of γ -TiAl alloy, this study investigated the alloy's atomic structure evolution at different time points during the laser heating and forming process based on the ovito numerical analysis algorithm. The results, as depicted in Figure 2a, reveal that, with the continuous energy input from the laser-heated region dynamically moving along the y -axis onto the powder bed, the temperature of the powder particles steadily rises to the melting point. Consequently, the particles melt into an amorphous state. The high-temperature environment induced by the energy input also accelerates the migration of atoms, rapidly filling the gaps between the powder particles. At the end of the heating process, the energy introduced by the laser is swiftly absorbed by the substrate, resulting in a cooling effect. As the height of the powder particles decreases, the density of the powder bed system is increased.

Figure 2b shows the microscopic evolution of the powder spherical particles in region A during the laser processing. Throughout the laser process, due to the continuous input of laser energy, the γ -TiAl alloy powders gradually melt from their initially intact spherical state to an amorphous state, and ultimately re-transform to the ordered crystalline structure due to the cooling crystallization process.

Varieties of laser process parameters were selected to investigate the effect of the laser power and scanning speed on the temperature of the forming system of the laser powder bed fusion process, and the results are shown in Figure 3. Figure 3a illustrates the influence of different laser powers on the temperature throughout the entire laser forming process. The results indicate that the peak temperature of the molten pool increases significantly with the rise in the laser power, and the peak width also witnesses a gradual increase, which means that the alloy has more time to maintain the molten state, thus promoting the particle displacement and diffusion strength. In addition, the rapidity with which the temperature profile rises and falls is indicative of the rate of heating and cooling during the laser process, as can be seen in Figure 3a, which shows that the heating and cooling of the powder bed is accelerated as the laser power rises.

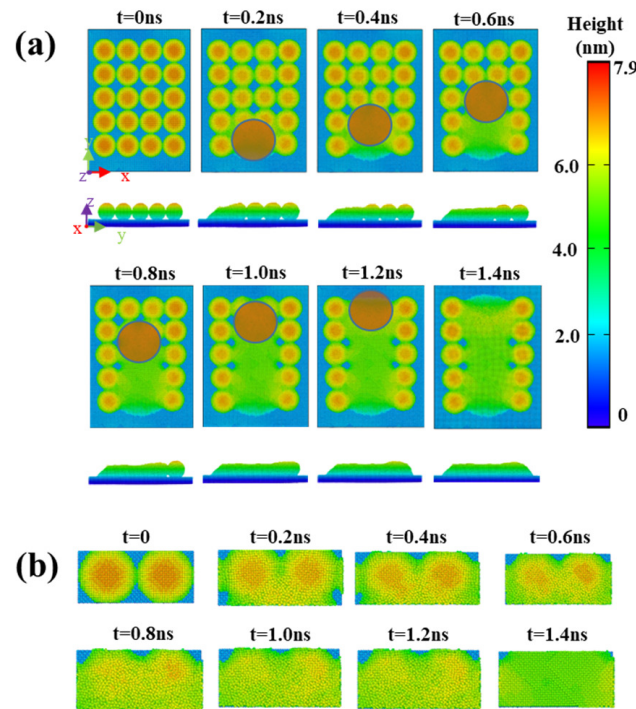


Figure 2. Structural evolution of laser powder bed fusion process when laser power is 400 eV/ps and scanning speed is 0.2 Å/ps: (a) Structural evolution with top view above and cross-section view; (b) structural evolution of region A.

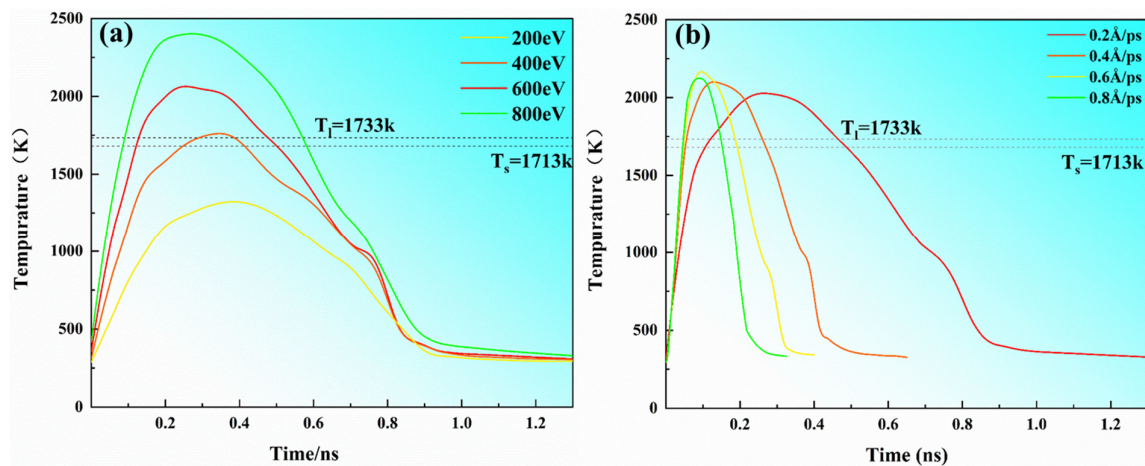


Figure 3. Laser powder bed fusion temperature evolution: (a) Effect of laser power with the scanning speed of 0.2 Å/ps; (b) effect of scanning speed with the laser power of 600 eV/ps.

Figure 3b demonstrates the impact of the scanning speed on the temperature. The results reveal that, compared to the laser power, the scanning speed has a more significant effect on the heating and cooling rate of powder bed formation. Increasing the scanning speed intensifies the rise and fall rates of the powder bed temperature, leading to a reduction in the peak width of the temperature curve. This results in a rapid decrease in the exposure time, which is not conducive to the improvement of the final forming quality. Moreover, in the case of different scanning speeds, the final $T_{\max}$ remains nearly constant, indicating that variations in the scanning speed have a minor influence on the peak temperature of the LPBF process.

Furthermore, the temperature distribution of the laser powder bed fusion of γ -TiAl alloy was obtained by atomic velocity calculations, as shown in Figure 4. The application of a cylindrical moving laser area contributes to a significant increase in the molten pool

temperature, accompanied by an elevation in the temperature gradient [43]. Also, the response time of the melting and crystallization is notably shortened. However, localized temperature distribution irregularities still exist at the edge of the heat-affected zone. The mismatch in the temperature field will greatly affect the stress distribution, which can disrupt the equilibrium of the stress field and lead to the phenomenon of local stress concentration, resulting in the sprouting of cracks and other microscopic defects. Additionally, just as demonstrated by Sharma et al.'s thermos-mechanical coupling experiment in LPBF, the laser processing is a result of multi-physics field coupling [44–46]; the mismatch in the stress field can also induce changes in the temperature within the region, thus further altering the system's temperature field, causing an overall imbalance, and ultimately triggering the expansion of defects.

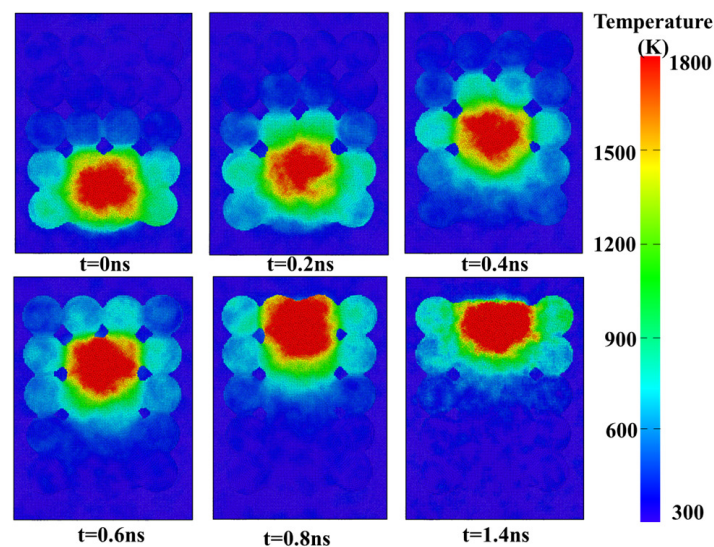


Figure 4. Temperature distribution of laser powder bed fusion process with the laser power of 400 eV/ps and scanning speed of 0.2 Å/ps.

Based on this, employing the CNA algorithm, this study investigated the evolution of the phase structure composition during the laser powder bed fusion process over time. Figure 5 illustrates the specific process of melting and crystallization of a γ -TiAl alloy powder bed under the influence of laser heating. The particles in the molten pool of the powder bed are thermally melted, followed by rapid recrystallization through the cooling process, resulting in their subsequent reformation. Due to the continuous heat exchange process between the substrate and the powder bed, the temperature at the bottom of the powder bed decreases, causing the generation of a temperature gradient along the z-axis direction in the γ -TiAl alloy powder bed system, which in turn propels the formation of the melting and solidification front, the steepness of which reveals the high heating and cooling rate of the laser processing [47]. However, due to the localized uneven distribution of the temperature field during the forming process, coupled with the stress generated by the rapid heating and cooling effects of laser processing, inevitable micro-defects such as vacancies and dislocations are introduced during the melt and crystallization process, severely impacting the final forming quality of the alloy. Therefore, it is imperative to elucidate the atomic-scale arrangement and migration-diffusion behavior during the laser powder bed fusion of γ -TiAl alloys, thus further clarifying the atomic-scale connections between the laser forming parameters and the mismatch in the temperature and stress fields, as well as structural defects in formation.

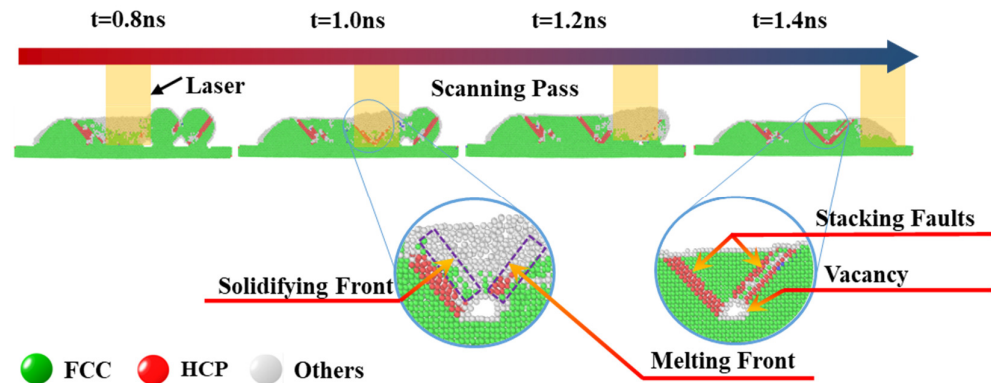


Figure 5. Evolution of phase structure in laser powder bed fusion process with the laser power of 400 eV/ps and scanning speed of 0.2 Å/ps.

3.2. Atomic Ordering Analysis of Melting and Crystallization Evolution

The analysis of atomic snapshots at key time points in the first part of this study provides a clear understanding of the structural transformation of nanoparticles during the melting and forming process. However, it lacks quantitative analysis and validation. The Radial Distribution Function (RDF) is a crucial tool for quantitatively revealing the crystalline, non-crystalline, and liquid characteristics of particles. In addition to the structural evolution analysis of laser forming, this study introduced RDF analysis to further investigate the evolution of particles throughout the entire process. A rectangular region A with dimensions of $10.4 \times 10.4 \times 5.2 \text{ nm}^3$ was selected for investigation. The radial distribution functions of region A at various stages during the melting and crystallization evolution are plotted, as shown in Figure 6. Initially, the entire model remains in an ordered crystalline state. When it comes to 200 ps, the powder bed gradually begins to melt, and the heights of peaks in the RDF rapidly decrease. Simultaneously, the peak widths significantly increase, reflecting the drastic changes in the original lattice structure under the influence of laser processing. The arrangement of the powder bed particles shows a trend towards non-crystalline transformation. At 400 ps, the height of the main peak continues to decrease, while those at greater distances gradually converge and normalize, with the peak width continuing to expand, indicating that the particles have completely melted into a liquid state. As the laser heat source gradually moves away, accompanied by the cooling effect of the substrate, the atomic order of the γ -TiAl powder enhances and the peak values and sharpness steadily rise with the cooling process, which also indicates that, although the atomic order is disrupted and rearranged during the melting and crystallization process of powder particles under laser heating, the crystal characteristics of the γ -TiAl alloy do not undergo significant changes [48]. However, due to the thermal-stress coupling introduced by the laser forming process, the peaks after crystallization are still somewhat (19%) lower than those of the original crystal.

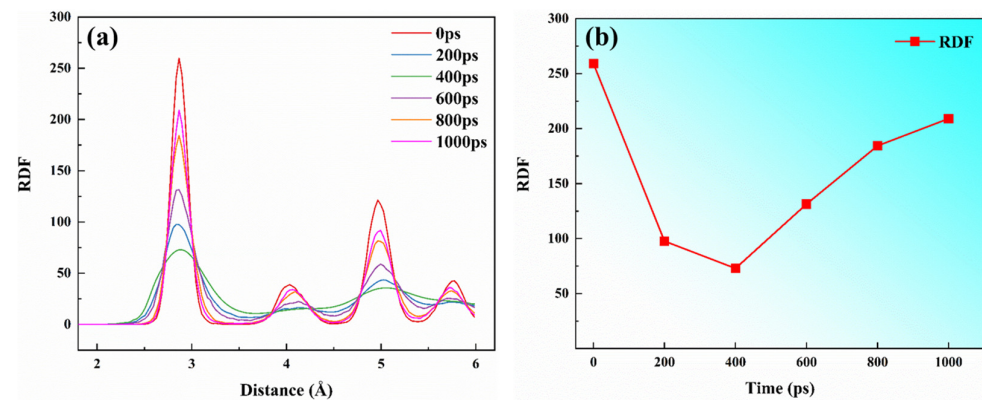


Figure 6. Radial distribution function of laser powder bed fusion when laser power is 400 eV/ps and scanning speed is 0.3 Å/ps: (a) Radial distribution function of region A; (b) evolution of the main peak value.

3.3. Atomic Displacement Analysis of Melting and Crystallization Evolution

In the powder bed system, the diffusion process of particles is extremely complex and differs significantly from the ideal parameters obtained through empirical methods such as diffusion couple and self-diffusion studies. Early studies suggested that the diffusion in the powder bed is primarily driven by surface contact between the particles. As a crucial approach for microscopic characterization, molecular dynamics methods excel in observing the diffusion behavior of each atom rather than relying solely on empirical methods for evaluation. This study, using the mean squared displacement (MSD) algorithm, detected the displacement changes in particles in region A relative to their initial positions during the laser forming process. The calculation method for the MSD can be expressed as:

$$MSD = \langle r^2(t) \rangle = \left\langle \frac{1}{N} \sum_{i=0}^N (r_i(t) - r_i(0))^2 \right\rangle \quad (4)$$

where N represents the total number of particles in the region, $r_i(t) - r_i(0)$ symbolizes the change in the vector distance travelled by the particles throughout the process, and t corresponds to the laser processing time node at different time step [49].

The evolution of atomic displacements in the LPBF process was studied according to Farias et al.'s method [49], and region A was selected for investigation. As is revealed in Figure 7a, in scenarios where the laser power is below 400 eV, the insufficient input laser energy fails to propel powder bed particles to their melting point, resulting in only a slight upward trend in the MSD. However, as the laser power increases to 400 eV, the diffusion behavior of the particles significantly improves. Simultaneously, due to the existence of the inter-particle voids in the powder bed, at the early stage of the particle diffusion, particles detach from the local lattice and move towards the voids in the powder bed, which leads to a non-linear characteristic in the MSD curve during the initial stages of the process. As the filling of gaps between the powder bed particles is completed, the MSD curve steadily increases, and ultimately stabilizes after the final cooling and crystallization process. With the continuous increase in laser power, the final results of the MSD after crystallization show a significant upward trend. Figure 7a,b indicates that a higher laser power and lower scanning speed effectively enhance the input energy during laser forming, thus further accelerating the temperature response of the powder bed, promoting the melting and diffusion of particles, and ultimately achieving higher MSD values. However, an excessively low scanning speed can also lead to particle splattering, posing a risk of burnout. Figure 7c presents the distribution of the final MSD values after crystallization under different laser powers (200–500 eV/ps) and scanning speeds (0.2–0.8 Å/ps). Four samples from Figure 7c were selected to investigate the significance of the effect of the laser power and scanning speed on the final MSD result. The results show that, when the

laser power increases from 200 to 400 eV/ps, the stable value of the MSD rises from 6.66 to 320.87, while the value rises from 300.54 to 550.14 when the scanning speed is attenuated from 0.8 to 0.4 Å/ps. In comparison with the scanning speed, the MSD is more sensitive to fluctuations in the laser power. And from Equation (3), it can be concluded that, in the process of laser forming, increasing the laser power or decreasing the scanning speed can significantly improve the energy density. This also implies that the MSD of particles does not necessarily increase with the rise in laser input energy density but depends on the proportional changes in key input parameters.

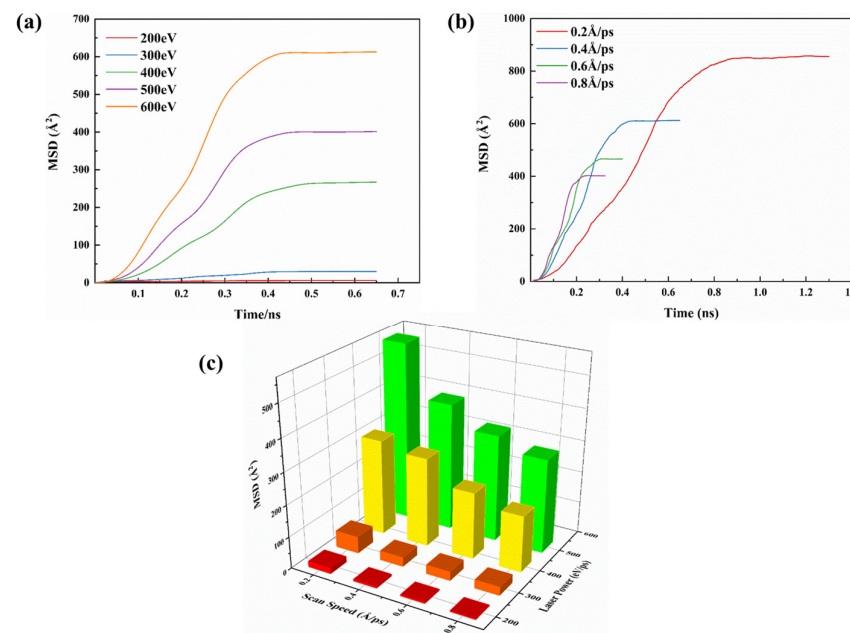


Figure 7. Mean square displacements of selected atoms during laser powder bed fusion when laser power ranges from 200 to 600 with the step of 100 eV/ps and scanning speed ranges from 0.2 to 0.8 with the step of 0.2 Å/ps: (a) Effect of laser power with the scanning speed of 0.2 Å/ps; (b) effect of scanning speed with the laser power of 600 eV/ps; (c) contribution of different parameters to ultimate MSD result.

3.4. Defect Evolution during Melting and Crystallisation Evolution

In order to illuminate the influence of the laser power and scanning speed on the final forming quality, various laser process parameters were selected and their effects on the defects were investigated based on the DXA algorithm. Figure 8a depicts the evolutionary process of powder bed crystal composition with variations in the laser power, and the results reveal that an increase in laser power expedites the cooling rate in the powder bed's molten state, resulting in a higher proportion of the amorphous phase in the final forming part, which is detrimental to overall forming quality. The results are consistent with the molecular dynamics numerical simulation of the rapid cooling process conducted by Farzadi et al. [40]. Conversely, as observed in Figure 8b, under certain laser power conditions, a higher scanning speed significantly reduces the exposure time of the laser powder fusion, impeding the migration and diffusion of powder bed particles, which also leads to an increase in the amorphous phase content in the final forming component. Therefore, lowering the scanning speed during laser processing is advantageous for improving the final forming effect of the powder bed. However, when the laser scanning speed is too low, the increase in exposure time can lead to the splattering of molten pool particles, and the coupling of the temperature and stress field in a mismatched environment also increases the proportion of the amorphous phase in the final forming components of the powder bed, which is also detrimental to the ultimate forming quality. Based on this, within a reasonable range of laser process parameters, it is advisable to

choose a lower laser power if possible and carefully consider the influence of the scanning speed, aiming to further optimize the laser forming process and obtain higher crystallinity in the formed components of γ -TiAl alloys.

Figure 9 illustrates the results of the defect analysis at the end of the laser powder bed fusion process under different laser powers. It is evident that HCP dislocations emanate from multiple planes, initiating from one endpoint of the dislocation line and eventually converging at the termination of the line. Simultaneously, during the extension of Shockley dislocations, the dislocations intersect and interact pairwise, giving rise to the formation of sessile stair-rod dislocation. The formation of Hirth locks is a consequence of the combination of two glissile perfect dislocations whose Burgers vector summation is of type $\langle 100 \rangle$ at their junction [50]. Throughout the powder bed track, dislocation defects tend to accumulate at the edges of the melting track due to the atomic tension between the molten powder particles and the solid-phase particles at the boundary of the molten pool during laser processing. The interatomic tension further intensifies the mismatch stress due to the uneven temperature distribution between the solid and liquid phases, leading to the emergence and expansion of dislocation defects. As the laser power increases, the number of dislocations in the melting track also witnesses a significant rise. This is attributed to the elevation of the peak temperature in the melting pool along with the steepness of the solidification front and the increase in the cooling rate. However, a higher cooling rate magnifies the concentrated stress in the melting pool, thus inducing the initiation and extension of central dislocations.

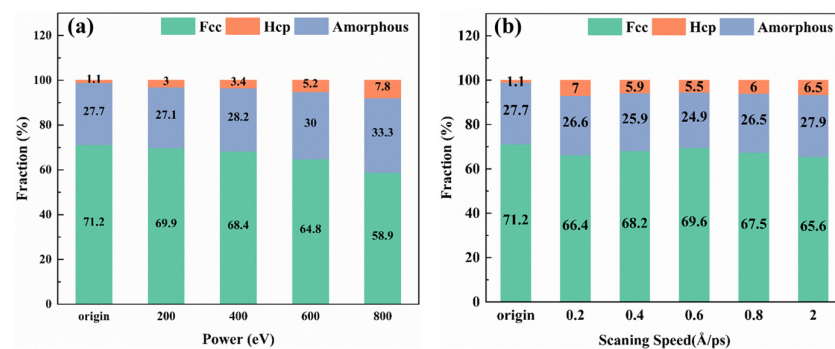


Figure 8. Evolution of powder bed crystal composition: (a) Effect of laser power with the scanning speed of 0.4 Å/ps; (b) effect of scanning speed with the laser power of 600 eV/ps.

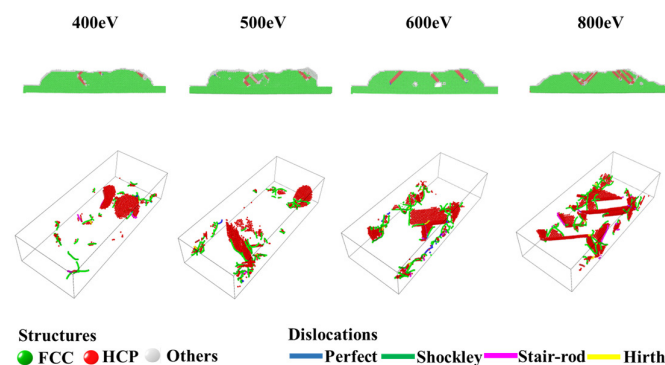


Figure 9. Defect analysis at the end of LPBF process under different laser powers with the scanning speed of 0.4 Å/ps.

Figure 10 reveals that, as the scanning speed increases from 0.6 to 0.8 Å/ps, the number of dislocations significantly escalates, which is due to the simultaneous increase in the cooling rate, resulting in more final forming dislocations. Conversely, when the scanning speed decreases from 0.6 to 0.2 Å/ps, the number of dislocations increases again. This is because the decrease in the scanning speed promotes an increase in the laser energy

density, leading to stress mismatch in the molten pool. The coupling relationship between the temperature and stress fields during the laser powder bed fusion process further causes uneven distribution in the temperature field. Under the combined effect of these dual fields, dislocation defects in the melting pool are further extended and expanded, resulting in an increase in the number of final forming dislocation defects. This interpretation corresponds with that of Wang et al.'s experiment on effects of LPBF process parameters on molten pool defects [51].

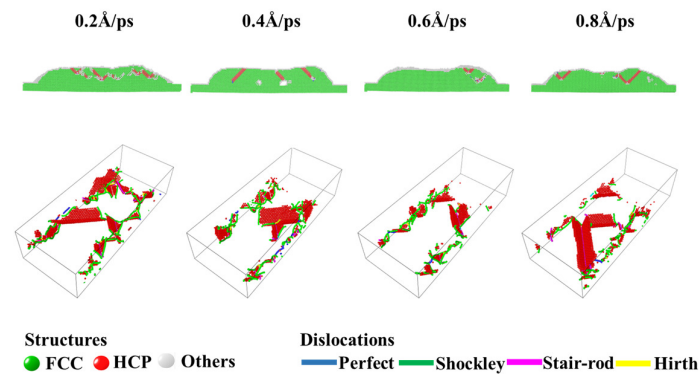


Figure 10. Defect analysis at the end of the LPBF process under different scanning speeds with the laser power of 600 eV/ps.

4. Conclusions

In this study, based on the molecular dynamics numerical simulation method, the microevolution process of γ -TiAl alloy formation through the laser powder bed fusion process was clarified. Also, the impact of different process parameters on the defect formation in the laser forming of γ -TiAl alloy was investigated, which also provides a theoretical reference for the optimization of laser powder bed-fused components in the aerospace and other fields, such as aero-engine turbine blades. The results are as follows:

- (1) As the laser scanning speed decreases, the exposure time significantly increases, further promoting the displacement and diffusion processes of powder particles, which are conducive to improving the final forming quality;
- (2) The melting and crystallization process of γ -TiAl alloy in the LPBF process does not alter the original crystal structure. However, the atomic order of the atoms after powder bed forming is slightly reduced by 19% due to the thermal-stress coupling introduced by the laser heating process;
- (3) When the laser power increases from 200 to 400 eV/ps, the stable value of atomic displacement rises from 6.66 to 320.87, while it rises from 300.54 to 550.14 when the scanning speed is attenuated from 0.8 to 0.4 Å/ps, which indicates that, compared with the scanning speed, the atomic mean-square displacements are relatively more sensitive to the fluctuation of laser power;
- (4) The increase in the laser power or scanning speed exacerbates the high heating and cooling rate brought about by the rapid heating and cooling characteristics of laser processing, which hinders the displacement and diffusion of particles, causing stress concentration and ultimately inducing the initiation and extension of defects.

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Abbreviations

HCP	Hexagonal Close-Packed
LPBF	Laser Powder Bed Fusion
EAM	Embedded Atom Method
MSD	Mean Squared Displacement
FCC	Faced-Centered Cubic
RDF	Radial Distribution Function
FCT	Face-Centered Tetragonal

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