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ARTICLE

Effects of Al Content on the Mechanical Properties of Single Crystal TiAl Alloy

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Abstract: The effects of Al content on the mechanical properties and the crack propagation mechanism of single crystal TiAl was discussed using molecular dynamics simulation. The stress-strain curves and evolution process of the defects were obtained under different Al contents. The results show that the Al content would affect the elastic modulus and the strength of the TiAl alloy. Defects such as stacking faults, dislocations and vacancies and their migrations result in better plasticity of TiAl when the Al content is below 45 at%. However, the specimen exhibits obvious brittleness with the Al content greater than 45 at%. Furthermore, the plasticity deformation dominates the main mode under the low Al content, while the crack fracture presents brittleness when the Al content is high. Therefore, Al contents would affect the mechanical proprieties of TiAl alloy, i.e. the plasticity of TiAl would increase with the decreasing Al content. In addition, the mechanism of crack propagation would vary with the change of Al content.

Key words: TiAl specimen; Al content; molecular dynamics; plasticity; crack propagation

TiAl alloy has many outstanding properties including low density, high stiffness, good flame retardant ability, excellent resistance to sea water corrosion and stress corrosion resistance, low linear expansion coefficient and high thermal conductivity, high strength and oxidation resistance at 600~750 °C, remarkable high temperature creep resistance and machinability[1-4]. Therefore, it is regarded as a new type of high temperature structural materials with huge developing potential and competitiveness, which was used in the engine with high-pressure compressor blades, high-pressure turbine blades, low pressure turbines, excessive catheter beam, exhaust valve, nozzle, etc[5]. However, several reviews described the development of TiAl alloy restricted by its shortcomings, such as brittleness at room temperature, poor fracture toughness, the oxidation resistance above 800 °C and processing performance[6,7].

The mechanical properties of TiAl alloy are closely related to the atomic configuration which depends on its composition strongly[8,9]. In order to prepare more useful TiAl alloy, the effects of Al content on the mechanical properties of the TiAl specimen should be studied. Much work so far has focused on the relationships between microstructure and mechanical properties. For some industrial applications, Al was commonly added to Ti as α stable phase to improve both the mechanical properties and thermal resistance of the alloy[10], and it would affect the configuration of TiAl alloy. Moreover, the microstructure would change with different Al contents, and the phase transformation would appear[11-13]. Besides, the Al content would affect hardness values[11]. The tensile deformation behaviors of TiAl alloy of different composition were investigated at room temperature. It is found that the average thickness of TiAl(γ) lamellae as well as the average spacing of Ti_3Al(α_2) lamellae decreases with the decreasing Al content[14]. During the process of cyclic loading for Ti-5at%Al, it is found that the crystals orientation and twinning are the major plastic deformation mechanism in the single crystals[15,16].

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These studies mentioned above mainly focused on the process of various phase transformation under different Al contents, while surprisingly little attention has been devoted to the effects of Al content on crack propagation. In terms of experiments, the effects of Al content on lamellar structure in macro scale were studied. But the essence of the deformation behavior of TiAl alloy affected by Al content in atomic scale was not explained. Molecular dynamics simulation provided us with a simple and economical method[17]. It can be used to simulate the process which is hard to achieve in experiment. Therefore, molecular dynamics simulation has been widely used by researchers. For Ti-5at%Al and Ti-10at%Al alloy, the phase transformation in the $\beta \rightarrow \alpha$ area was studied[18]. In the tensile process of Ti-5at%Al and Ti-10at%Al alloy, it is found that the ductility would decrease with the increasing Al content, which results in the earlier necking and cracking[19].

At present, the effects of Al content on the mechanical properties of TiAl alloy have been researched incompletely. In addition, there are various defects in materials both in production process and practical application. The crack, in particular, is one of the most important defects, whose propagation mechanism is greatly influenced by Al content in TiAl alloy. However, there are relatively few studies devoted to the mechanism of crack propagation. It is the purpose of the present paper to provide the relationship between mechanical properties and atomic configuration and to make up the research gap of TiAl specimen from the atomic scale. The primary focus of this paper is on the effects of Al content on the mechanical properties and the crack propagation of single crystal TiAl specimen by molecular dynamics simulation.

1 Simulation Model Construction

Ti and Al atoms were arranged alternately along [001] orientation in the TiAl specimen. TiAl specimens with different Al contents were obtained by substituting Al atoms for Ti atoms randomly using the same method in Ref. [18]. In the present paper, the Al content is 42 at%, 45 at%, 48 at%, 50 at% and 60 at%. The embedded atom method (EAM) was used to describe the atomic interaction which was developed by Zope et al[20]. The potential fitted to both experimental and first-principles data of various crystal properties and structures in Ti-Al system could give a good description of basic properties such as point defects, planar fault energies and elastic constants[21]. It is widely used to describe interatomic force of TiAl[21-23]. This suggests that the selection of potential function is appropriate. As shown in Fig.1, there is a pre-existing center crack by canceling the atomic interaction of the length $10a_0$ in the model. In this simulation, the free surface of crack is (010), and the propagation direction is <100>. The size of the model is $150a_0 \times 50b_0 \times 12c_0$ (a_0, b_0 and c_0 are the lattice constants, which is 0.4001, 0.4001 and 0.4181 nm, respectively), and the model contains 368 424 atoms. *X*, *Y* and *Z* axis represent [100], [010] and [001] orientation, respectively.

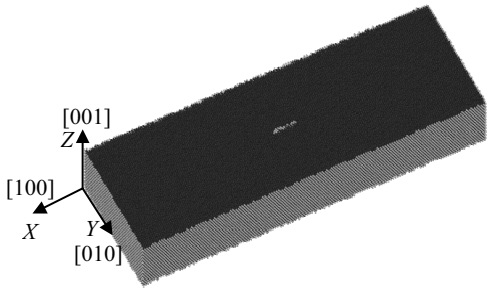

Fig.1 Atomic model of TiAl specimen

The *X*, *Y* directions were set to free boundary conditions, while the *Z* direction was set to periodic boundary condition. The models were performed under the NPT ensemble for a period of time to reach equilibrium state after the atomic models of TiAl alloy were established. And the tensile loading was carried out by imposing velocity to atoms in the fixed layers at the upper of models along the *Y* direction, while the fixed layers at the lower of models were velocity free under the NVT ensemble. Moreover, the simulation was performed with the temperature of 300 K and the strain rate of 4×10^8 s^{-1}. The LAMMPS was used for molecular dynamics simulation, and the center symmetry parameters (CSP) of the visualization software OVITO were chosen to measure the disorder phenomenon of local lattice and the location of the atom. Using this method, the defects and their evolution during the process of deformation and fracture can be highlighted and distinguished easily. The *P* values of centrosymmetry parameter reflect the kinds of defects. Eq. (1) was employed to calculate CSP value of each atom[24]:

$$P = \sum_{i=1}^{6} \left| \vec{R}_i + \vec{R}_{i+6} \right|^2 \quad (1)$$

where, $\vec{R}_i$ and $\vec{R}_{i+6}$ are the vectors from the central atom to a particular pair of the nearest neighbors.

2 Results and Discussion

2.1 Process of crack propagation with different Al contents

Under the Al content of 42 at%, the stress-strain curve is shown in Fig.2. The stresses, under different Al contents, used to depict the relationship of stress-strain were all calculated using the Virial theorem, which was commonly used in molecular dynamics simulations[25-27]. Fig.2a, 2b, 2c and 2d are the atomic trajectories corresponding to the point A, B, C and D, respectively in stress-strain curve. It can be seen that the stress always concentrates on the tip of crack and redistributes with the crack propagation. At the point A, the value of stress reaches its maximum named the yield stress. Combined with the atomic trajectory, it is shown that partial dislocations nucleate due to the stress concentrations on two crack tips. This indicates that plastic deformation begins and crack propagates along <100> direction. At this time, the

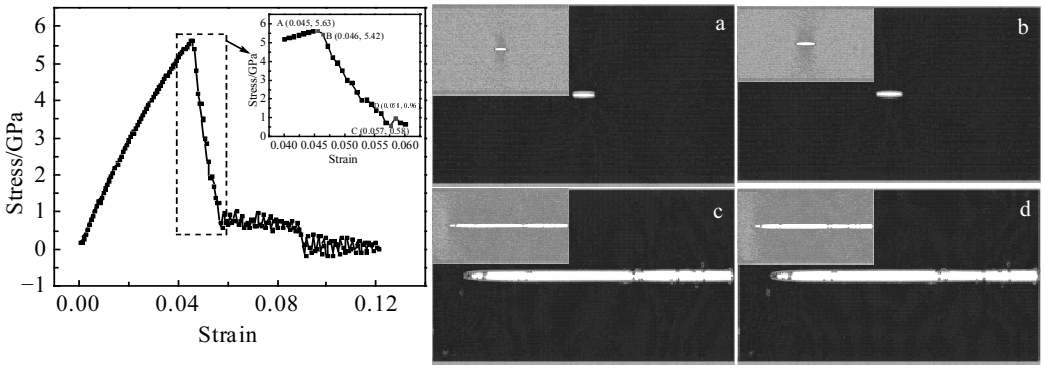

Fig.2 Stress-strain curves of TiAl specimen with Al content of 42 at% (atomic color from green to red represent stress value increasing): Fig.2a~2d corresponding to point A~D of the inset of stress-strain curve

stacking fault of the partial dislocation acting as the boundary is nearly simultaneous nucleation on different {111} plane. Due to this, the stress rapidly decreases. After the stress reaches to the yield stress, it can be seen from the atomic trajectory that in the point B, crack widens gradually and propagates along [100] orientation. In general, the propagation of crack would carry partial stress. As a result, the stress would decrease at point B. After that, dislocations are still nucleation and emission. Dislocation nucleation causes stress to increase and dislocation emission carries partial stress, leading to the stress decreasing until point C. Combined with the atomic trajectory, we can see that the direction of crack propagation changes from [100] orientation to [$\bar{1}$00] orientation after the specimen fracture. The material fractures in one direction should be the reason for stress decreasing to the minimum value. The stress increase, as shown in the point D, should be attributed to the change of crack propagation direction. The emission of dislocation releases the stress concentration on crack tip, which leads to the crack propagation. During the tensile process, the mechanism of crack propagation is mother-child. Owing to stress concentration, a void appears in front of crack tip and gradually grows to micro crack, finally combines with the main crack and propagates with dislocations emission.

Under the Al content of 48 at%, the stress-strain curve is shown in Fig.3. Fig.3a, 3b, 3c and 3d are the atomic trajectories corresponding to the point A, B, C and D, respectively which are in stress-strain curve. The stress value decreases to the minimum immediately after it reaches to the maximum and finally fluctuates near zero, which indicates a brittle fracture of material. In contrast to the investigation of Mine[28], crack deflection appears during the crack propagation, while does not occur in our simulation. The discrepancy is that the samples in experiment and simulation are different; lamellar spacing and microelement would affect crack propagation behavior. It can be clearly seen that the stress-strain curve is different for these two samples. Firstly, the slope of stress-strain curve in Fig.3 is larger than that in Fig.2, which shows that when the Al content is 42 at%, it is easier to deform compared with the Al content of 48 at%. Secondly, the slope of stress drop is slower in Fig.2 than that in Fig.3 because the plasticity deformation occurs, and the ductility of TiAl alloy increases. Lastly, the stress drops to 0 rapidly in Fig.3, while fluctuation appears in Fig.2. The reason is that there are dislocations glide, pile-up, reaction with each

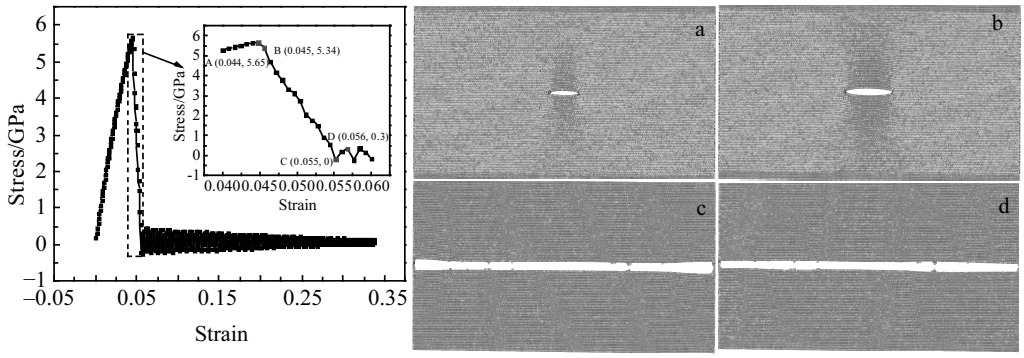

Fig.3 Stress-strain curves of TiAl specimen with Al content of 48 at% (atomic color from green to red represent stress value increasing): Fig.3a~3d corresponding to point A~D of the inset of stress-strain curve

other, vacancies and stacking faults generation and reaction with dislocation, and all of these would change the stress.

There is a plastic deformation accompanied with partial dislocations nucleation from crack tip when the Al content is 42 at% and 45 at%. When the Al content is 48 at%, 50 at% and 60 at%, plastic deformation does not appear. The crack displays the brittle deformation and fracture. There are no defects such as vacancies, dislocations and stacking faults in the process of crack propagation. As the stacking fault energy of Al is high, stacking fault is harder to appear when the Al content is higher, while it appears at the Al content of 42 at% and 45 at%, leading to the better plasticity of TiAl specimen than that of 48 at%, 50 at% and 60 at%. From the research of Tetsui[29,30], we know that there was a good process ability and creep resistance when the Al content was 42 at%. This can be attributed to the formation and reaction of defects. Due to defects free, the repulsive force which is hindering the crack propagation is small. So, the crack propagation under the Al content of 48 at%, 50 at% and 60 at% is faster than that of 42 at% and 45 at%. As a result, the good plasticity give rise to that the crack is hard to propagate at low content of Al, that is why when Al content is lower, the crack propagation is slower.

On the one hand, various defects under different Al contents affect the plasticity of TiAl specimen and the mechanism of crack propagation. On the other hand, the atomic bond and binding force of Al/Ti, Ti/Ti and Al/Al are different with Al contents. It is generally accepted that there is a strong binding force between Ti and Al because of polarization effect, leading to the anisotropic of Peierls stress. From the results, we can find that the Al content and atomic bond of Al/Al is increased, while those of Ti/Ti and Al/Ti are decreased. As a consequence, partial dislocation is hard to activate due to large Peierls stress. Besides, the binding force between Al/Al is smaller than that of Al/Ti. Therefore, the atomic bond of Al/Al is easier to fracture. This can explain the brittle fracture of TiAl specimen with high Al content. In addition, atomic bond fractures lead to crack propagation. Fig.4 illuminates the atomic bond around crack tip at the Al content of 42 at% and 48 at% at 112 ps. Atoms was deleted to observe atomic bond clearly.

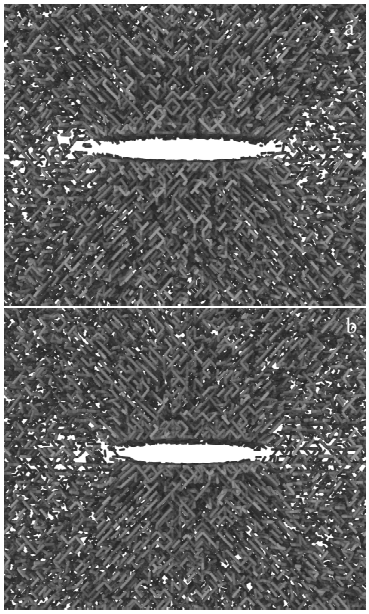

Fig.4 Atomic bond of crack tip of TiAl specimen with different Al contents: (a) 42 at% and (b) 48 at% (red represents Ti atomic bond, and blue represents Al atomic bond)

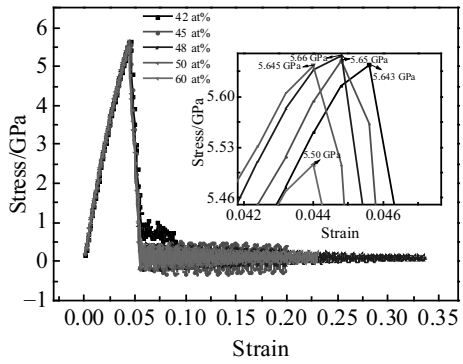

Fig.5 Stress-strain curves of TiAl specimen with different Al contents

2.2 Stress-strain curves

To achieve a better understanding of the mechanical properties of TiAl alloy with different Al contents, the stress-strain curves with different Al contents are shown in Fig.5. In the process of tension, the stress rises rapidly in elastic deformation stage. It is shown that the slope of each curve is slightly different which indicates that Al content would affect the elastic modulus of the TiAl specimens. When the Al content is 60 at%, the slope of stress-strain curves is the smallest. Except for this Al content, the slopes of other stress-strain curves decline significantly with the decreasing Al content which manifests an easier deformation. When the Al content is 42 at% and 45 at%, the behavior of dislocation affects the slope of stress-strain curves. It can be obtained from the partial enlargement of stress-strain curves that yield stress changes irregularly. This result is different from the experiment result which indicates that peak stress increases as Al content decreases[31]. It is reasonable to infer that the condition of experiment and simulation and the selection of Al content play very important roles in the discrepancy of experiment and simulation results. When the Al content is 45 at% and 48 at%, the yield strength is 5.65 and 5.66 GPa, respectively. When the Al content is 42 at% and 50 at%, the yield strength would be nearly the same level and slightly less than that under the Al content of 45 at%. When the Al content is 60 at%, it has the minimum yield stress and the worst strength. These values are larger than those of experiments[32,33], which can be attributed to the high strain rate in

molecular dynamics simulation and alloying elements of the samples in experiment. Furthermore, in experiment study[14], when Al content ranges from 46 at% to 49.3 at%, the yield stress increases with the decreasing Al content. In our simulation, when Al content is 48 at% and 50 at%, yield stress shows the same relation compared with experiment results. From the yield strength under different Al contents, we know that the variation of Al content has a little influence on the yield strength of TiAl alloys. The results are in good agreement with the experiment results[34]. The stress is released through the generation and reaction of vacancies, dislocations and stacking faults. In order to improve the plasticity of TiAl specimen at room temperature, it is necessary to reduce the Al content appropriately to overcome the low plasticity at room temperature.

2.3 Defects evolution behavior

Dislocation is one of the main factors that affect deformation behavior and mechanical properties of materials. In order to deeply investigate the crack propagation mechanism, the dislocation behavior was studied. The type, amount and emission time of the dislocation have an effect on both the speed and mechanism of crack propagation. Atomic trajectory is given to study the dislocations behavior in TiAl specimen with different Al contents. The process of defects evolution at the Al content of 42 at% is revealed in Fig.6. Centrosymmetry parameter is used to delete perfect crystal structure, and then defect atom is exhibited.

The process of dislocation evolution, in left crack tip, is shown from Fig.6a to 6f. Firstly, the lattice distorts and partial dislocations nucleate because the stress concentrates on crack tips. It can be seen from Fig.6a that dislocation nucleates at the left crack tip at t=130 ps. At the same time, dislocation would nucleate at the right crack tip. With the further increase of the applied strain, $1/6[12\bar{1}]$ Shockley partial dislocations would occur in front of the left crack tip. Because of the lattice resistance, dislocations glide along the lattice close to surface. This would destroy the normal stacking sequence of local atoms, leading to the generation of extrinsic stacking fault (ESF). Stacking fault glides along {111} plane. The activate slip system has a relationship with critical resolved shear stress. The width of stacking fault gradually increases, accompanied by the dislocation gliding in {111} plane. It would decrease owing to the planar faults propagation. Every two faults encounter here and partial dislocations reaction generates a stair-rod dislocation, illustrated in Fig.6k, which was analyzed by common neighbor analysis (CNA). Fig.6l is the same deformation process as Fig.6k, which is seen in a different direction. Besides, dislocation line can be seen in Fig.6l. The generation of stair-rod dislocation is as follows:

$$\frac{1}{6}\left[\bar{1}21\right]+\frac{1}{6}\left[1\bar{1}2\right]=\frac{1}{6}\left[01\bar{1}\right] \quad (2)$$

Another interesting finding is that the different kinds of partial dislocations on different slip plane cause the different types of stair-rod dislocation. The stair-rod dislocation connects the two stacking faults from the two remaining partials and forms a triangular structure, such as Lomer-Cottrell lock. For the stability of stair-rod dislocation and Lomer-Cottrell lock, it often hinders other dislocations movement, illustrating that the interaction of dislocations can improve the plasticity. Under the greater strain, the stair-rod dislocation and Lomer-Cottrell lock would be overcome. Stacking fault and partial dislocation continue to glide along slip plane, and finally accumulate at boundary leading to the stress concentration. As dislocation and stacking fault appear at crack tip, it would cause the crack tip blunting and bring on crack hard to propagate. With the further increasing of the applied strain, dislocations move along the slip system continuously and pile-up in the boundary as shown in Fig.6e and Fig.6f. As the location of dislocation nucleation has a relationship with the point of stress concentration, and the glide direction is influenced by the different Schmid factors of the active slip direction, the location and glide direction of dislocation is different at two crack tips. Furthermore, the amount and types of dislocations is also increased, because a perfect dislocation would break into partial dislocation and stacking fault in the process of dislocation movement.

The process of single vacancy evolution is shown from Fig.6i to 6j. Divacancy and vacancy cluster can be seen in Fig.6f and Fig.6k, respectively. Point defects have significant effects on mechanical properties of materials such as strength, ductility, fatigue and creep, owing to their interactions with dislocations and other defects during deformation[35]. It is commonly known that the vacancy is a kind of point defects. The coordination number of perfect lattice is 12, and there are 12 atoms around a single vacancy. Vacancies are generated by the reaction and movement of dislocations. Its generation and movement would offer a repulsive force, causing crack to propagate slowly, and thus improve the fracture toughness of specimen. The simulation can reflect the progress of generations and variations of various defects roughly. But there are artificial results with the restriction of the simulation size. The effects of fixed boundary condition on dislocation emission was investigated by Sun[36], and the results indicated that the emission of dislocation from crack tip was not affected by the fixed boundary condition. Therefore, the effects of boundary condition would be ignored in our simulations.

The mechanism of crack propagation mentioned above was studied from atomic scale. A large number of experiment investigations revealed that the mechanical properties of TiAl are greatly influenced by Al content[37-39]. There is a difference between the experimental observation and molecular dynamics simulation results, which can attribute to the loading rate, boundary condition and potential function and so on.

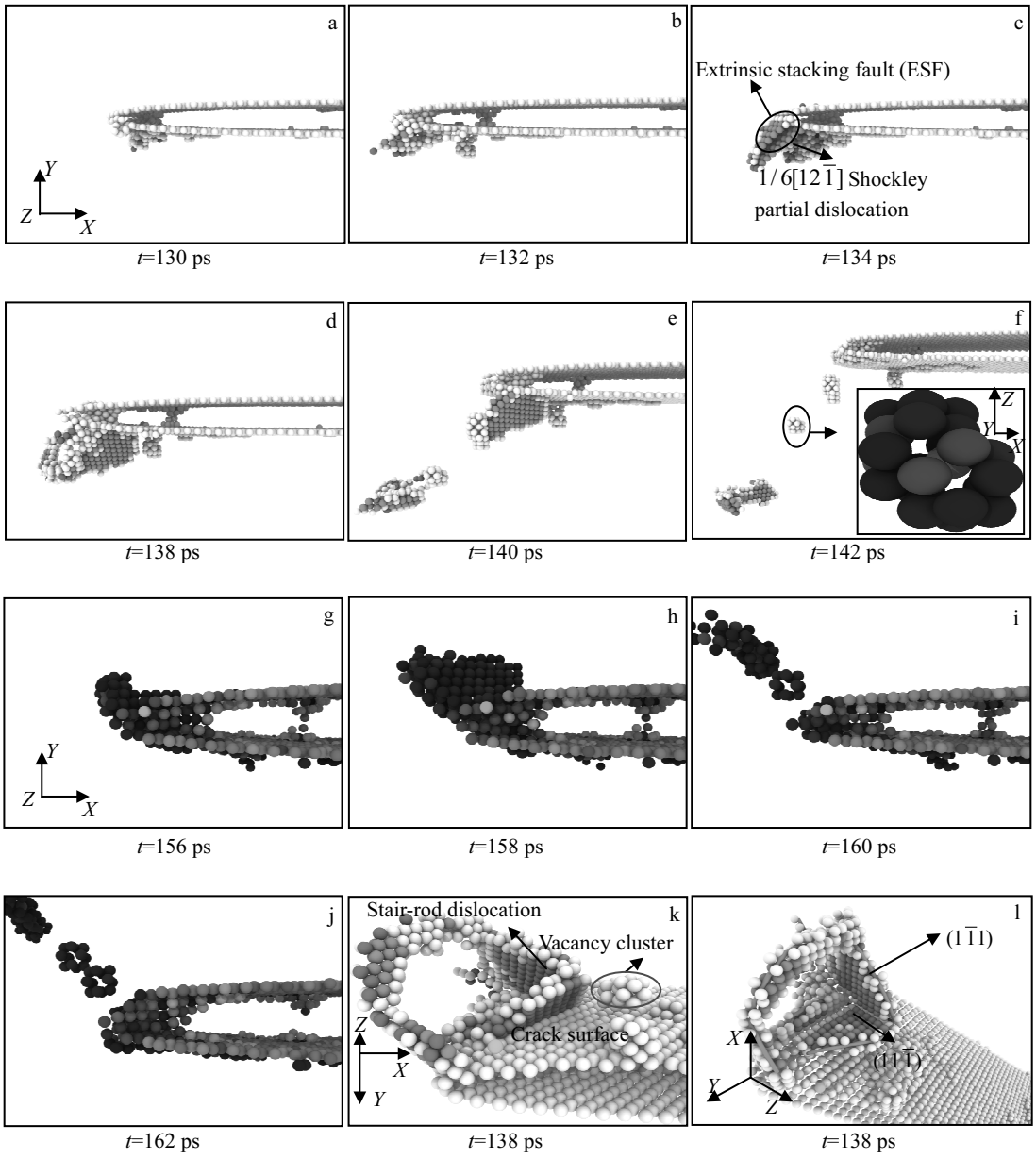

Fig.6 Defect evolution at crack tips with Al content of 42 at%

The simulation results that mentioned above can also be used to guide experiment, providing an effective method to design and produce TiAl specimen in practice.

3 Conclusions

1) The plasticity of the specimens increases with the decreasing Al content. It is dislocation emission, pile-up, interaction with each other, vacancies and stacking faults result from dislocations reaction and glide, dislocation locks that improve plasticity. Thus, lower Al content would improve the plasticity of TiAl specimen. In addition, Al content would affect the elastic modulus and the yield strength of the specimens.

2) As Al contents are different, the crack propagation mechanism is different. In detail, when Al content is lower, the crack propagates in the form of plastic deformation; when Al content is higher, the crack is brittle fracture.

3) During the process of crack propagation, stress always concentrates on crack tips. Defects result in the stress released and redistributed. Furthermore, the type and amount have an effect on the mechanism and speed of crack propagation.

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Al 含量对单晶 TiAl 合金力学性能的影响

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摘　要：通过改变 TiAl 中 Al 的含量，用分子动力学方法研究了 Al 含量对含有裂纹的单晶 TiAl 试件性能及裂纹扩展的影响，分析了不同 Al 含量下的应力-应变曲线，缺陷的演化过程。模拟结果表明：Al 含量不同，材料的弹性模量和强度也不同。Al 含量低于 45 at%时，由于层错和位错的产生以及位错反应和运动产生的空位和空位的迁移提高了试件的塑性使得试件表现出良好的塑性，而大于该含量时，试件呈明显的脆性；Al 含量较低时，裂纹以塑性变形的方式扩展，Al 含量较高时，裂纹以脆性方式断裂。即 Al 含量会影响材料的性能；随着 Al 含量降低，试件的塑性增强，此外，Al 含量对裂纹的扩展机制也有很大影响。

关键词：TiAl 试件；Al 含量；分子动力学；塑性；裂纹扩展

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