Feng Ruicheng, Cao Hui*, Li Haiyan, Rui Zhiyuan and Yan Changfeng

Effects of Vacancy Concentration and Temperature on Mechanical Properties of Single-Crystal γ-TiAl Based on Molecular Dynamics Simulation

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Abstract: Molecular dynamics simulation is used to analyze tensile strength and elastic modulus under different temperatures and vacancy concentrations. The effects of temperature and vacancy concentration on the mechanical properties of γ-TiAl alloy are investigated. The results show that the ultimate stress, ultimate strain and elastic modulus decrease nonlinearly with increasing temperature and vacancy concentration. As the temperature increases, the plastic of material is reinforced. The influence of temperature on strength and elastic modulus is larger than that of vacancy concentration. The evolution process of vacancy could be observed clearly. Furthermore, vacancies with different concentrations develop into voids first as a function of external forces or other factors, micro cracks evolve from those voids, those micro cracks then converge to a macro crack, and fracture will finally occur. The vacancy evolution process cannot be observed clearly owing to the thermal motion of atoms at high temperature. In addition, potential energy is affected by both temperature and vacancy concentration.

Keywords: γ-TiAl alloy, molecular dynamics, vacancy, temperature, mechanical properties

Introduction

Because of its low density, high conductivity, high specific strength and stiffness, and good flame-retardant and oxidation-resistant capability, γ-TiAl alloys has become a new type of high-temperature structure material with huge development potential and application prospects at high temperatures [1–8]. It has been widely used in the aerospace and automotive industries. The studies of its mechanical properties are widely conducted by researchers. For high-temperature structure materials, the elastic modulus and plastic of γ-TiAl alloy are important mechanical properties [9]. In terms of experiments, the mechanical properties of γ-TiAl alloy with different elements and different processing technologies have been studied more than γ-TiAl alloy with defects [10–13]. In practice, γ-TiAl alloy contains various defects, such as vacancies and cracks, and research on the effect of these defects on the mechanical properties will help us better understand γ-TiAl alloy and make it more useful. The research on γ-TiAl alloy under the condition of experiments is restricted, because it is difficult to design experiments at the nanoscale; therefore, atomic-scale methods such as molecular dynamics simulation are widely used to research the mechanical properties of γ-TiAl alloy. The relationship between atomic-scale defects and mechanical properties is increasingly elaborated [14]. The mechanical properties of single-crystal bulk Mg2Si were investigated by Yu [15], and the results show that the ultimate stress decreases nonlinearly with increasing vacancy concentrations. Once the defects are present, there is a substantial decrease in the ultimate stress, which decreases in higher concentrations. The mechanical properties of CoSb3 that contain vacancy defects were investigated by Yang [16], who found that the ultimate stress and elastic modulus decrease with increasing temperature and vacancy concentration.

From the above research, it can be found that increasing attention is paid to the influence of temperature and vacancy concentration on the mechanical properties, but research on the mechanical properties of γ-TiAl alloy with defects is less common. γ-TiAl alloy is a material that has development potential and application prospects at high temperature; therefore, it is necessary to study the influence of temperature on its mechanical properties. It is noted that there is still no common view

***Corresponding author: Cao Hui,** Mechanical and Electronical Engineering College, Lanzhou University of Technology, Lanzhou 730050, China; Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, Lanzhou, China, E-mail: 1042126484@qq.com
Feng Ruicheng, Li Haiyan, Rui Zhiyuan, Yan Changfeng, Mechanical and Electronical Engineering College, Lanzhou University of Technology, Lanzhou 730050, China; Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, Lanzhou, China

of the exact limit of the vacancy fraction in the literature [16]. Therefore, in our simulation, according to the vacancy concentration and temperature in [15–19], that in our simulation, three vacancy concentration of 0.09 %, 0.12 % and 0.16 % which are generated from vacancy atoms coordinate in normal distribution, as well as five temperatures of 300 K, 800 K, 1,000 K, 1,100 K and 1,200 K are selected to study the mechanical properties of γ-TiAl alloy by molecular dynamics simulation.

Computational model and method

The embedded atom method (EAM) is used in the simulation, and the specific parameters of its expression are fitted by using data from reliable experiments and calculations of the primary principle method. It is verified that this potential can describe related lattice deformation in γ-TiAl alloy [20, 21]. The lattice constants are $a_0 = b_0 = 4.0010$ Å and $c0 = 4.1810$ Å, which are consistent with the experimental values $a_0 = b_0 = 4.0050$ Å and $c0 = 4.0707$ Å; therefore, the chosen EAM potential is reasonable [22]. a_0, b_0 and c_0 are unequal, which also shows that the γ-TiAl alloy structure is different from an ordinary face-centered cubic (FCC) structure. γ-TiAl alloy has face-centered tetragonal (FCT) structure with an $L1_0$ structure [23], as shown in Figure 1. The x, y, and z coordinate axes correspond to the crystallographic orientations [100], [010], and [001], respectively.

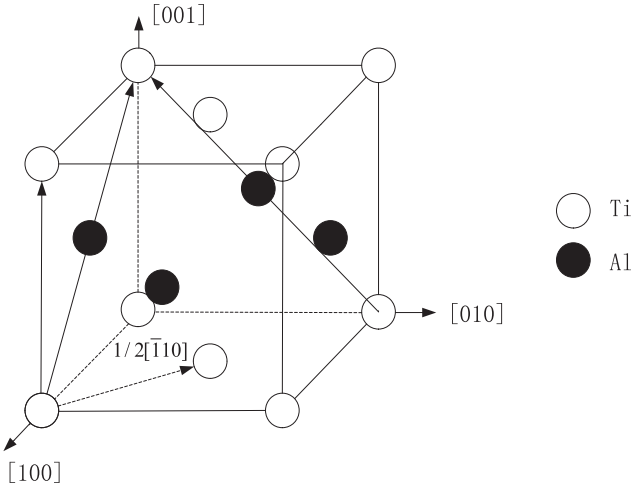

Figure 1: $L1_0$ structure of γ-TiAl.

Atom models of γ-TiAl alloy at three vacancy concentrations are shown in Figure 2. The size of model is $80a_0 \times 2b_0 \times 40c_0$. The model has 26,082 atoms. The LAMMPS software program is used for molecular dynamics

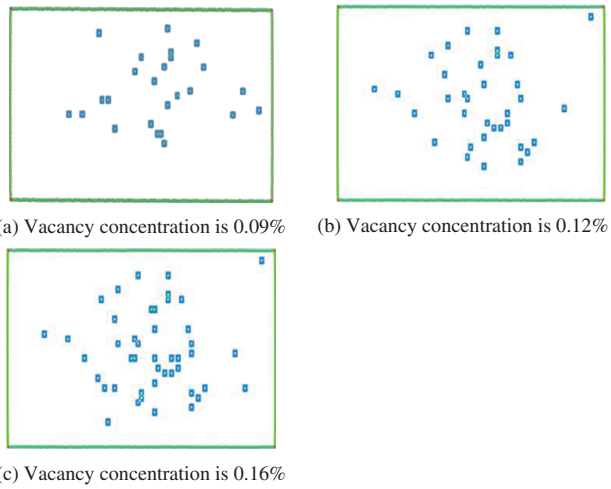

Figure 2: Atom model of γ-TiAl alloy at three vacancy concentrations.

simulation, and the center symmetry parameter of the OVITO software program is used to highlight defective atoms, and view the evolution of the defects during the shape change and fracture process. Center symmetry parameter is chosen to show the vacancy defects and boundary in Figure 2(a), (b) and (c). The atomic coordinates of the precast vacancy in normal distribution are mentioned above. Normal distribution is applied to study the error due to accidental factors; the impact of these causal factors is small, and they are independent of one another. Small and independent causal factors, such as vacancy caused by the random variables, obey the normal distribution. Thus, the atomic coordinate vacancy obeys the normal distribution method to precast different concentrations vacancies. The distribution of the normal distribution density is [24]:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma_x} \exp\left[-\frac{(x-\mu_x)^2}{2\sigma_x^2}\right] \quad -\infty < x < +\infty \tag{1}$$

where μ_x represents the mean value of the normal distribution, and σ_x represents the standard deviation. The vacancy coordinates x, y, and z obey the normal distributions of $\mu = 40$, $\sigma = 100$; $\mu = 0$, $\sigma = 2$; and $\mu = 20$, $\sigma = 100$, respectively. 25, 35 and 45 points are chosen randomly on three normal distribution curves, and then the atoms of these locations are deleted. Three different vacancy concentrations of 0.09 %, 0.12 % and 0.16 % are precast, and these points are generated by normal distribution. The vacancy positions are randomly generated to test the impact on the result of the simulation. The "velocity loading" is used; that is, one end is fixed, and the other end is loaded. Because the system is not balanced before loading, the model under isothermal–isobaric ensemble (NPT) first relaxes for 100 ps

to balance. The relaxation process in three directions is set to the periodic boundary condition. Loading is begun after relaxation. The loading process is under the canonical ensemble (NVT), using the Nose-Hoover method to control the temperature. The time step is 1 fs, and the strain rate is 1×10^{8}/s. The × and z directions are set to the free boundary conditions in the process of loading. The y direction is still the periodic boundary condition, to obtain a realistic simulation sample and reduce the residual stress in the specimen. The velocity Verlet algorithm is used to calculate the atomic trajectory.

Results and discussion

Atomic trajectory at 300 K

To observe the vacancy evolution process conveniently, one atomic layer is cut out to analyze the evolution of the vacancy. The center symmetry parameter is used in Figure 3(a) to (f) to display the vacancies and defects such as dislocations. Stress nephograms are showed in Figure 3(g) and (h) to observe the change in the stress.

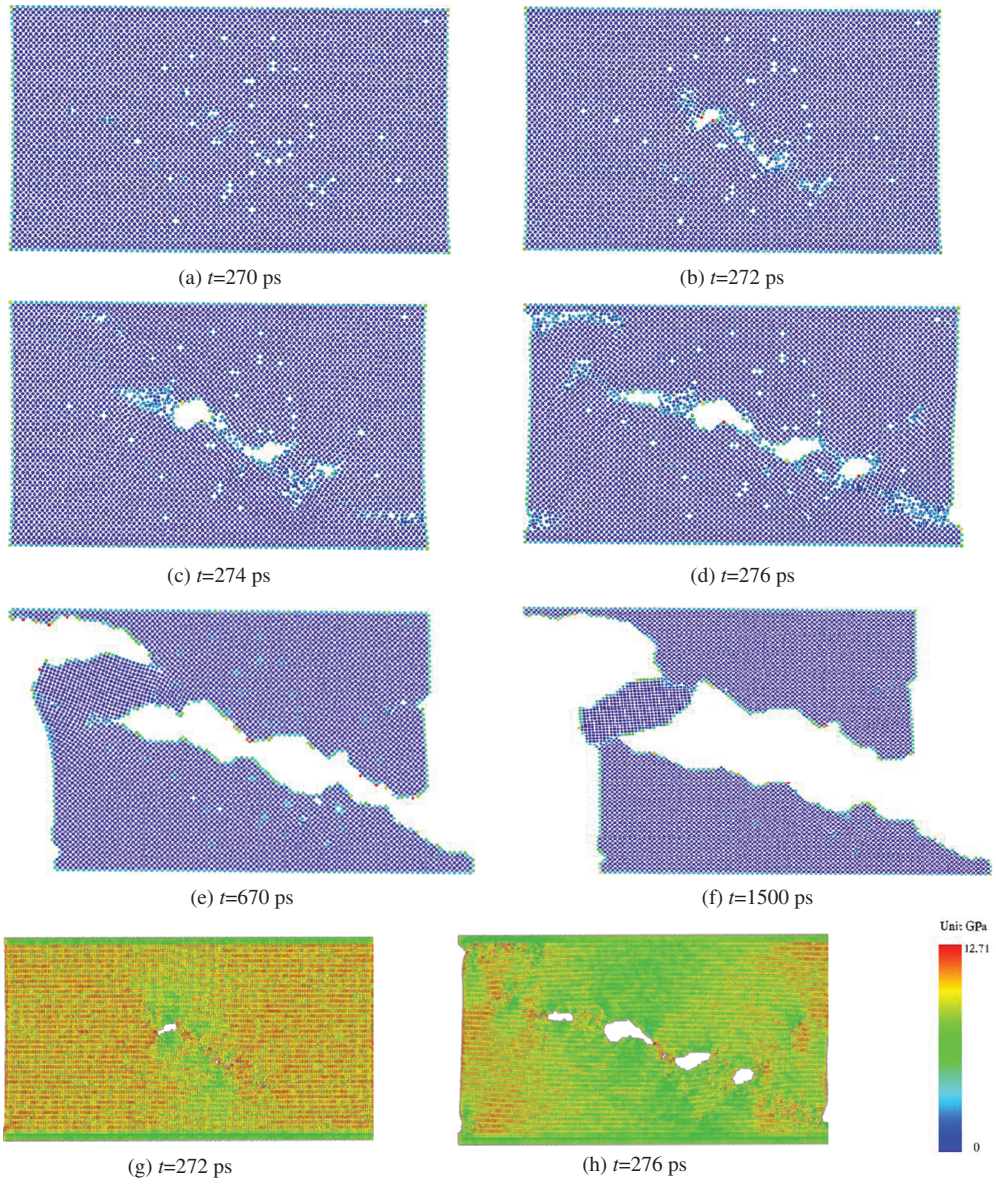

Figure 3: Atomic trajectory at different times at 300 K.
Note: Dark blue represents perfect atom while light blue are defect atoms from Figure 3 (a) to (f), the color scale employed corresponds to stress is increasing from blue, the weakest, to red, the strongest.

Under a vacancy concentration of 0.16 % and temperature of 300 K, atomic trajectories at different times are shown in Figure 3. With applied loading, atoms surrounding the vacancy exhibit a disordered phenomenon, which leads to lattice distortion and stress concentration. Plastic deformation of γ-TiAl alloy occurs in the place of stress concentration. Owing to the plastic deformation of material caused by stress concentration, the local stress exceeds the bond forces among the atoms in the alloy. The atomic bonds would then be broken to form voids under the external force stress concentration around the void, causing atomic bond ruptures that form micro-cracks. Because the different locations of the vacancies form multiple voids, these voids gradually form multiple micro-cracks that propagate randomly. With the interaction among micro-cracks, they eventually converge to form one crack. The crack tip blunting then leads to crack propagation suppression. In the evolution process of vacancies, this will produce constant dislocation emission. The dislocation emission and accumulation lead to fluctuating stress–strain curves, yet dislocation emission and accumulation causes stress redistribution. The temperature is higher, and the thermal motion of atoms is more intense, but the evolution process of vacancies is not obvious. Thus, in this paper, the vacancy evolution process at room temperature is chosen to observe the evolution process from vacancies to cracks. The effect of temperature on the material mechanical properties is observed at only four other temperatures.

Stress–strain curves under different temperatures and vacancy concentration conditions

Comparing the stress–strain relation for each vacancy concentration at five temperatures, stress–strain curves for three vacancy concentrations of 0.09 %, 0.12 % and 0.16 % are shown in Figure 4(a), (b) and (c)

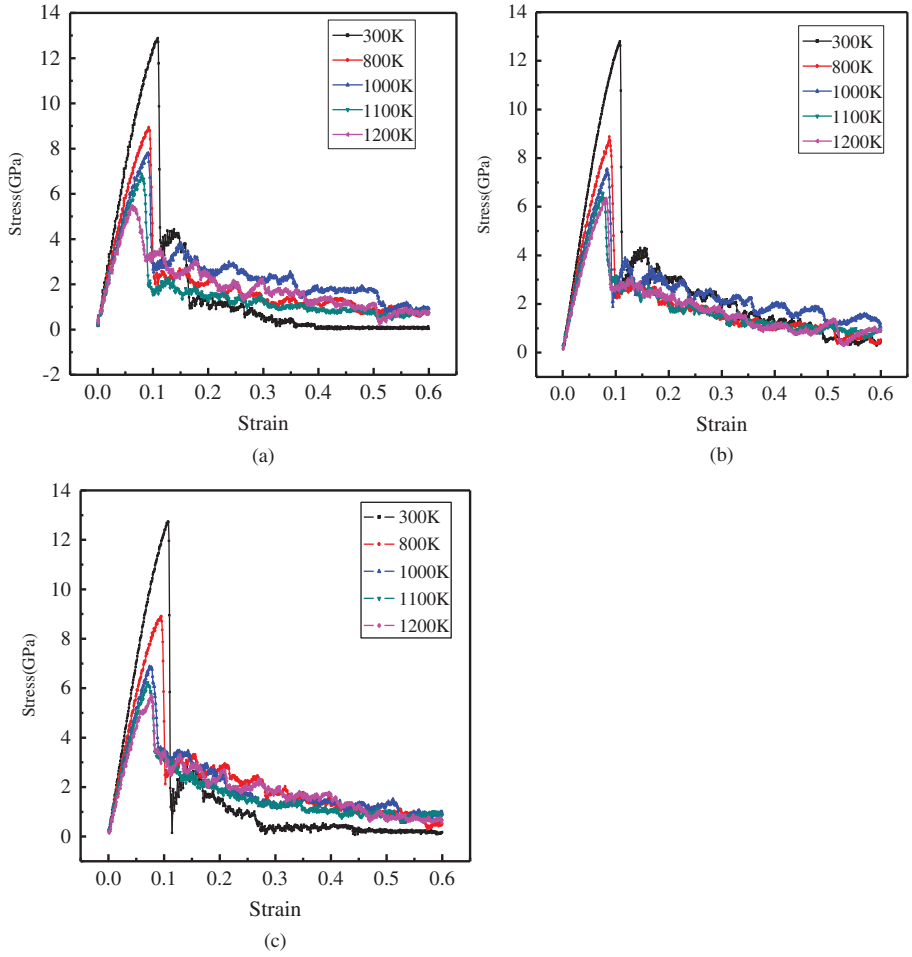

Figure 4: Stress–strain curves at different temperatures and vacancy concentrations.

respectively. It is shown that the vacancy concentration has no effect on the basic shape of the stress–strain relation, and all of them have three stages: the elastic deformation stage, the plastic deformation stage and the stress drop to zero stage. The temperature has a slight effect on elastic deformation stage. As the temperatures increase, the thermal motion of atoms becomes very intense, and atomic movement out of the original balanced position cause plastic deformation to more likely occur. It can be seen from the stress–strain curve that the yield phenomenon does not appear at 300 K; that is, γ-TiAl alloy shows brittleness at room temperature. It can be seen that the higher the temperature, the more obvious the yield phenomenon. With increasing temperature, γ-TiAl alloy obviously becomes plastic. The stress increases linearly with increasing strain at the elastic deformation stage. When the strain reaches the critical value, stress increases nonlinearly. When stress reaches its maximum namely, the ultimate stress value the material enters the stage of plastic deformation. At this point, the stress is greater than the binding force among atoms; therefore, the atom bonds rupture, leading to material fracture.

The work of vacancy was focused on formation and migration [25–27], and vacancy evolution to crack in TiAl had been done a little in experiment, however, the MD results did not compare with it. In view of other metals, our results would be verified. For example, in the experiments, nanocrystalline Ni specimens containing different numbers of vacancies were produced by electrode position and annealing, it is found that the yield stress and fracture stress for the specimen containing more vacancies were lower than those for the one containing fewer vacancies [28], which have the same results obtained by us.

The ultimate stresses at different temperatures and vacancy concentrations are shown in Figure 5. It can be seen from the curves that with increasing temperature and vacancy concentration, the ultimate stress value declines nonlinearly. It can be seen from Xu's [25] investigation that point defects have significant effects on mechanical properties of materials such as strength and ductility. When the vacancy concentration is 0.09 %, temperature changes from 300 K to 1,200 K, the ultimate stresses are 12.84 GPa, 8.90 GPa, 7.54 GPa, 6.60 GPa and 6.36 GPa; thus, the ultimate stress decreases by 50 %. When the vacancy concentration is 0.12 %, the ultimate stresses are 12.89 GPa, 8.93 GPa, 7.80 GPa, 6.89 GPa and 6.33 GPa, a reduction of 51 %. When the vacancy concentration is 0.16 %, the ultimate

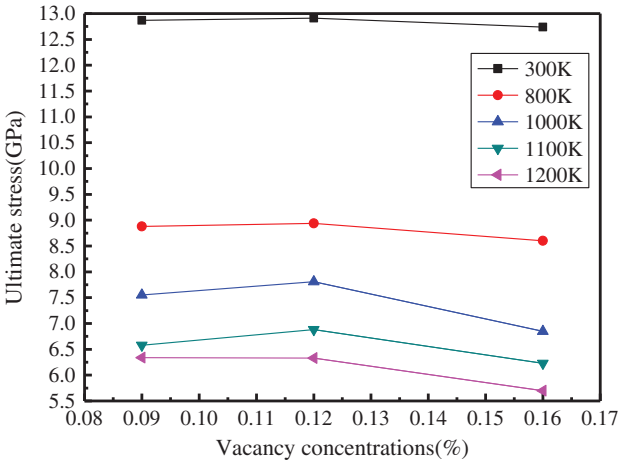

Figure 5: Ultimate stress curves at different temperatures and vacancy concentrations.

stresses are 12.71 GPa, 8.62 GPa, 6.83 GPa, 6.25 GPa and 5.70 GPa, a reduction of 55 %. At 300 K, with vacancy concentrations ranging from 0.09 % to 0.16 %, the ultimate stress decreases by 1 %; at 800 K, the ultimate stress decreases by 3 %; at 1,000 K, the ultimate stress decreases by 9 %; at 1,100 K ultimate stress decreases by 6 %; and at 1,200 K, the ultimate stress decreases by 10 %. When the vacancy concentration is different, there is different strength as mentioned in [25]. The temperature has a great influence on the strength of the material: the higher the temperature, the lower the strength of the material. Because of the increase in temperature, the material thermal motion becomes severe, the distance between internal atoms increases, mutual attraction is reduced, and plastic deformation is more likely to occur. In addition, the vacancy concentration also has an effect on the material strength. The vacancy concentration increases from 0.09 % to 0.16 %, and the strength of the materials decreases. The vacancy concentration has a less significant effect than the temperature on the ultimate stress.

Ultimate strain curves at different temperatures and vacancy concentrations are shown in Figure 6. It can be seen from the curves that with increasing temperature and vacancy concentration, the ultimate strain value declines nonlinearly, which have the same results investigated by Yu [15] and Yang [16]. The trend is similar to the change in the ultimate stress value. When the vacancy concentration is 0.09 %, from 300 K to 1,200 K, the ultimate strains are 10.9 %, 9.2 %, 8.7 %, 7.6 % and 7.2 %, reduction of 33 %. When the vacancy concentration is 0.12 %, the

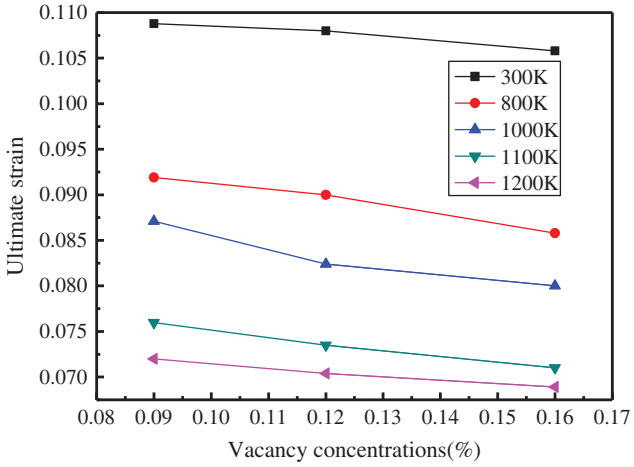

Figure 6: Ultimate strain curves at different temperatures and vacancy concentrations.

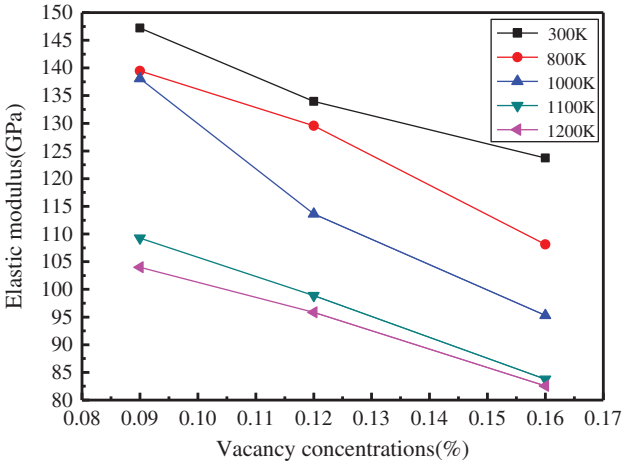

Figure 7: Elastic modulus curves at different temperatures and vacancy concentrations.

ultimate strains are 10.8 %, 9.0 %, 8.3 %, 7.4 % and 7.1 %, reduction of 35 %. When the vacancy concentration is 0.16 %, the ultimate strains are 10.6 %, 8.6 %, 8.0 %, 7.1 % and 6.9 %, reduction of 35 %. At 300 K, with vacancy concentrations ranging from 0.09 % to 0.16 %, the ultimate strain decreases by 3 %; at 800 K, the ultimate strain decreases by 7 %; at 1,000 K, the ultimate strain decreases by 9 %; at 1,100 K, the ultimate strain decreases by 8 %; and at 1,200 K, the ultimate strain decreases by 7 %. The reduced attraction causes the plastic deformation to be more likely to occur. In addition, the vacancy concentration also has an effect on the material strength: with increasing vacancy concentration, the strength of materials decreases. It can be seen that the vacancy concentration has a less significant effect than the temperature on the ultimate strain.

The elastic modulus at different temperatures and vacancy concentrations is shown in Figure 7. It can be seen from the curves that with increasing temperature and vacancy concentration, the elastic modulus value declines nonlinearly which is consistent with Yang's [16] and Chang's [18] investigation. When the vacancy concentration is 0.09 %, from 300 K to 1,200 K, the elastic moduli are 147.3 Gpa, 139.7 Gpa, 138.0 Gpa, 109.3 GPa and 103.9 GPa, a reduction of 29 %. When the vacancy concentration is 0.12 %, the elastic moduli are 134.0 Gpa, 129.4 Gpa, 113.7 Gpa, 98.8 GPa and 95.6 GPa, a reduction of 28 %. When the vacancy concentration is 0.16 %, the elastic moduli are 123.5 Gpa, 108.4 Gpa, 95.4 Gpa, 83.9 GPa and 82.6 GPa, a reduction of 33 %. At 300 K, with vacancy concentrations ranging from 0.09 % to 0.16 %, the elastic modulus decreases by 16 %; at 800 K, the elastic modulus decreases by 23 %; at 1,000 K, the elastic modulus decreases by 31 %; at 1,100 K, the elastic modulus decreases by 23 %; and at 1,200 K, the elastic modulus decreases by 21 %. It can be seen that the vacancy concentration has a less significant effect than the temperature on the elastic modulus.

With vacancy concentrations of 0.09 %, 0.12 % and 0.16 %, the changes in potential energy curves with time at five temperatures are shown in Figure 8. It can be observed from Figure 8 that the influence of temperature on the potential energy is very large. When the temperatures rise, the potential energy increases, the greater the potential energy, the more unstable the system and the more likely the occurrence of plastic deformation. The vacancy concentrations has no effect on the shape of the potential energy curve, but it will affect the time at which the potential energy reaches the peak time: the greater the vacancy concentration, the lower the maximum potential energy. Investigating the effect of vacancy concentration on potential energy at 300 K, the specimen with higher vacancy concentrations store higher potential energy before the fracture, and the energy is released in the process of fracture. As the essential of materials is different, the opposite conclusion with Dewapriya's [17] was got. However, temperature is higher than 300 K, the specimen with higher vacancy concentrations store lower potential energy before the fracture.

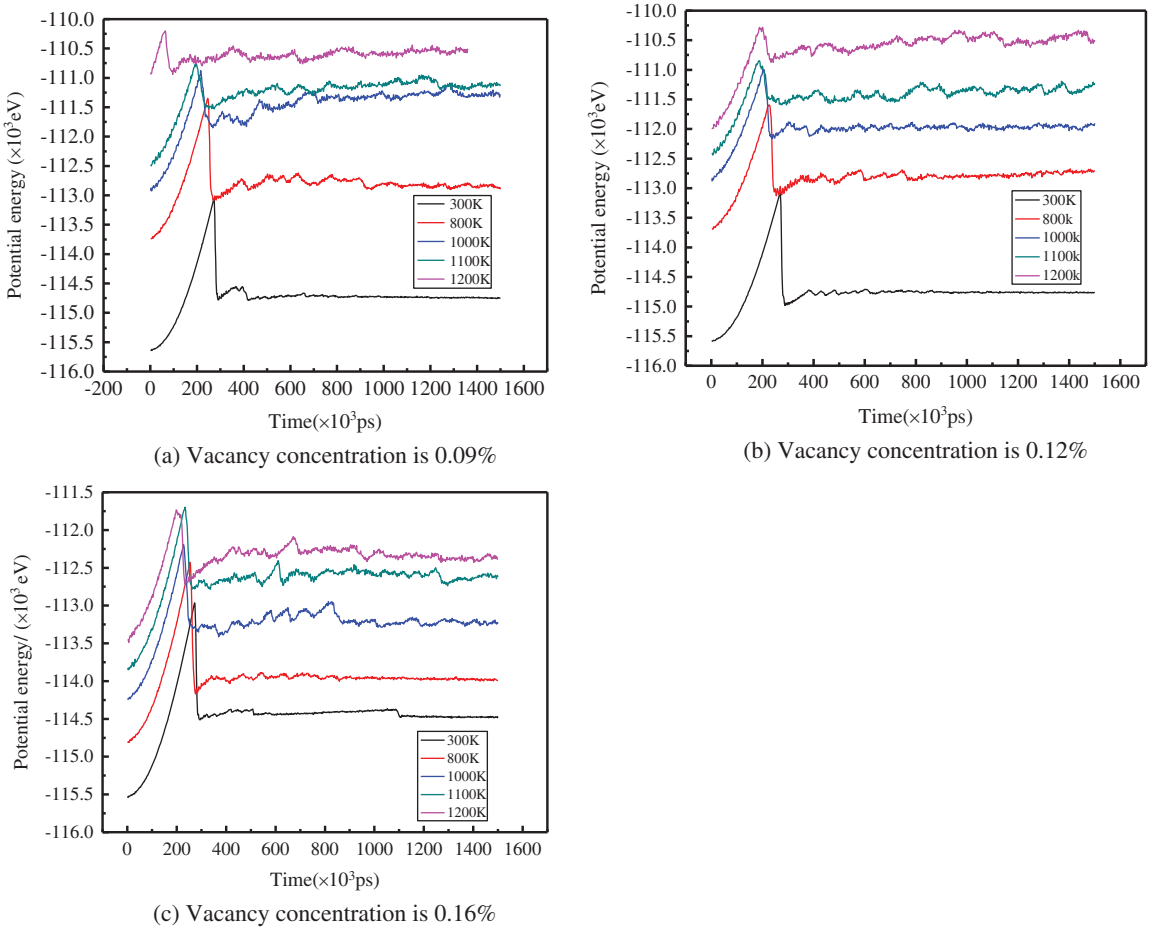

Figure 8: Potential energy curves at different temperatures and vacancy concentrations.

Conclusion

In this paper, the ultimate stress, ultimate strain and elastic modulus of single crystal γ-TiAl alloy is analyzed based on the molecular dynamics method under different temperatures and vacancy concentrations, and the effects of temperature and vacancy concentration on the mechanical properties of the material are determined. The results show the following:

(1) As the vacancy concentration increases, tensile strength decreases, and the ultimate stress and strain decline nonlinearly. Owing to the small number of vacancies, the elastic modulus of the material varies slightly, but the downward trends of the three quantities are not obvious.

(2) As the temperatures increases, the ultimate stress and strain decline nonlinearly, and the elastic modulus of the material decreases obviously. The downward trends of the five curves are more obvious.

(3) During the stretching process, vacancies with different concentrations develop into voids first as a function of external forces or other factors. The voids evolve into micro-cracks, and then micro-cracks converge into a macro-crack, ultimately resulting in fracture. In addition, there are dislocation emissions in the process of the vacancy evolution, and the nucleation and emission of the dislocation will affect the stress value. In the whole process, the stress is always concentrated on the vacancy, the dislocation accumulation and the crack tip. Stress is redistributed as the time step increases. When the temperature is high, the thermal motion of atoms is obvious, and the vacancy evolution process is not observed clearly.

(4) The vacancy concentration has no effect on the shape of the potential energy curve but will affect the time in which the potential energy reaches the peak time: the greater the vacancy concentration, the lower the maximum potential energy.

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References

[1] Z.Y. Rui, G.T. Zhang, R.C. Feng, et al., J. Funct. Mater., 46 (2015) 1103–1105.
[2] H. Clemens and S. Mayer, Adv. Eng. Mater., 15 (2013) 191–215.
[3] H. Clemens and W. Smarsly, Adv. Mater. Res., 27 (2011) 551–556.
[4] R. Cao, J.H. Chen, H. Zhu, et al., J. Mater. Sci. Eng., 5 (2004) 013.
[5] Y.W. Kim and S.L. Kim, Intermetallics, 53 (2014) 92–101.
[6] Y.Y. Chen, S.Z. Zhang, F.T. Kong, et al., Chinese J. Rare Met., 36 (2012) 154–160.
[7] R.C. Feng, Z.Y. Rui, Y.R. Zuo, et al., Strength mater+, 4 (2014) 417–421.
[8] R.C. Feng, Z.Y. Rui, G.T. Zhang, et al., Strength mater+, 46 (2014) 183–189.
[9] J.L. Su and X.F. Lian, Chinese J. Nonferrous Met., 25 (2015) 338–343.
[10] Z.C. Liu and J.P. Lin, Trans. Mater. Heat Treat., 22 (2001) 7–13.
[11] S.J. Li, Y.L. Wang, J.P. Lin, et al., Rare Metal. Mat. Eng., 3 (2004) 144–148.
[12] D.R. Li, S.Y. Xu, Y.X. Cai, et al., Rare Metal. Mat. Eng., 2 (2013) 277–279.
[13] X. Lu, X.B. He, S.Q. Li, et al., J. Univ. Sci. Technol. B, 30 (2008) 254–257.
[14] A. Ito and S. Okamoto, J. Commun. Comput., 10 (2013) 9–18.
[15] R. Yu, S. Yang, G. Chen, et al., J. Electron. Mater., 43 (2014) 1668–1673.
[16] X.Q. Yang, P.C. Zhai, L.S. Liu, et al., Phys. B, 407 (2012) 2234–2238.
[17] M.A.N. Dewapriya and R.K.N.D. Rajapakse, J. Appl. Mech., 81 (2014) 081010.
[18] W.J. Chang, Microelectron. Eng., 65 (2003) 239–246.
[19] Y.J. Liang, Q. Han and S. Huan, J. Therm. Stresses, 38 (2015) 926–933.
[20] B.W. Zhang, W.Y. Hu and X.L. Shu, Theory of Embedded Atom Method and Its Application to Materials Science, Hunan University Press, Changsha (2003).
[21] R.R. Zope and Y. Mishin, Phys. Rev. B, 68 (2003) 024102.
[22] F.L. Tang, H.M. Cai, H.W. Bao, et al., Comput. Mater. Sci., 84 (2014) 232–237.
[23] S.R. Chubb, D.A. Papaconstantopoulos and B.M. Klein, Phys. Rev. B, 38 (1988) 12120.
[24] C. Wang, Mechanical Reliability Engineering, Metallurgical Industry Press, Beijing (1992).
[25] D.S. Xu, H. Wang, R. Yang, et al.,International Conference on the Fundamentals of Plastic Deformation Materials Science and Engineering, 13–17, 2008, Materials Science and Engineering, Hong Kong (2009).
[26] H. Wang, R.C. Reed, J.C. Gebelin, et al., Calphad, 39 (2012) 21–26.
[27] Z.X. Li, B.Y. Wang, D.N. Wang, et al., Intermetallics, 18 (2010) 2259–2261.
[28] M. Yuasa, H. Matsumoto, M. Hakamada, et al., Mater. trans., 49 (2008) 2315–2321.