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ARTICLE

Effect of Cutting Depth on Mechanical Properties of Single Crystal γ-TiAl Alloy

Li Haiyan[1,2], Qiao Haiyang[1], Feng Ruicheng[1,2], Wang Qi[1], Wang Maomao[1], Li Jian-hua[1,2]

[1] Lanzhou University of Technology, Lanzhou 730050, China; [2] State Key Laboratory of Advanced Processing and Recycling of Nonferrous Metals, Lanzhou 730050, China

Abstract: The nano-cutting and tensile model of monocrystalline γ-TiAl alloy was established by large scale molecular dynamics simulations method. The effect of different cutting depths on tensile process of workpiece was analyzed. For one thing, the relationship between lattice transformation and micro-defect evolution was studied. For another, the influences of cutting depths on stress-strain curve, the nucleation of dislocation and position of fracture surface were discussed. The results show that the amount of lattice transition rises with the increases of cutting depth and it is consistent with micro-defect evolution during nano-cutting. Within a certain range of cutting depth, the yield stress and elastic modulus of workpiece are improved correspondingly. In addition, cutting depths have great influence on the position of dislocation nucleation and fracture surface of workpiece during tensile process. The dislocation of machined workpiece is nucleated at subsurface, while dislocation of unmachined workpiece is nucleated at edge of workpiece. The port position of workpiece is closer to drawing end with the increase of cutting depth.

Key words: nano-cutting; tensile; molecular dynamics simulations; lattice transformation; dislocation

With the rapid development of science and technology, ultraprecision machining and nano-scale processing occupy a dominant position in a wide range of fields, such as aerospace, defense, military, medicine, biology and optics[1]. In recent years, machining accuracy determines the service life of mechanical components, and also affects the working life of mechanical systems. During micro-nano scale processing, different dislocations, lattice deformation and microstructure evolution are introduced, which affects mechanical properties of workpiece. Therefore, it is necessary to carry out research on mechanical properties of workpiece with different depths of cutting.

At present, there are a lot of work to study mechanism of nano-cutting, chip morphology, dislocation evolution, temperature, residual stress distribution and mechanical properties of material, etc. In the first place, scholars have done a lot of work on the research of nano-cutting. For example: Wang et al[2] studied residual stress in the process of machining by means of simulation. It was found that tensile residual stress decreases and compressive residual stress rises underneath surface with increases of cutting depth. Chavoshi et al[3] analyzed chip related phenomena in nanometric cutting of single crystal silicon at elevated temperatures. The results showed that smaller released thermal energy and larger value of chip ratio as well as shear plane angle were obtained when cutting was performed at higher temperatures. Li et al[4] discussed plastic deformation mechanism of nanocrystalline copper for different processing conditions. It turned out that plastic deformation of single crystal copper is mainly dependent on interaction between dislocations, while plastic deformation of polycrystalline copper is mainly determined by interaction between dislocation and grain boundary. Liu et al[5] explained evolution of stacking fault tetrahedron (SFT) of single crystal copper processing. It was found that SFT is

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Corresponding author: Qiao Haiyang, Master, Lanzhou University of Technology, Lanzhou 730050, P. R. China, Tel: 0086-931-7823072, E-mail: 244294726@qq.com

nucleated at intersection of differently oriented stacking fault planes, and SFT evolved from preform with incomplete surfaces to a solid defect. Lai et al[6] researched on partially overlapped nano-cutting of monocrystalline germanium. The atomic sights on the subsurface deformation showed that the thickness of deformation layer after multiple machining is much less than that after single cutting with the same nominal depth of cutting. Zhu et al[7] studied nanometer cutting of single crystal Nickel. The results revealed that generation of complex stacking fault is the main reason for fluctuation of cutting force, and the structure of complex stacking fault leads to work hardening of material.

In the second place, mechanical properties of material were studied. Naiyer et al[8] analyzed effect of nitrogen content on crack growth behavior in Fe-N alloy at high temperature. It turned out that at higher temperatures of 900 and 1100 K, more slip systems are activated, which result in the crack tip becoming obtuse ahead of time and being accompanied by cavity nucleation and growth. Song et al[9] studied effect of hydrogen atoms on crack propagation behavior of α-Fe. The results showed that a model has good ductility when local hydrogen concentration is high in the front region of crack tip. The peak stress of α-Fe decreases with increase of hydrogen concentration. Feng et al[10] discussed effects of vacancy concentration and temperature on mechanical properties of γ-TiAl. The results revealed that the ultimate stress, ultimate strain and elastic modulus decrease linearly with increase of temperature and vacancy concentration. Wang et al[11] explained orientation effects on tensile properties of single crystal nickel with nanovoid. It was found that void volume fraction has a significant effect on Young's modulus, initial yield stress and initial yield strain.

Based on the above research, it can be found that a large number of scholars have focused on nano-cutting or effects of defect on tensile properties. There are few researches on combination of nanometric cutting and tension. In addition, the research on tensile properties of defects is mainly prefabricated by man. There are many artificial subjective factors, such as cracks, vacancies, twins, and dislocations. In practice, some dislocations and stacking faults were produced in product after processing, which have a great impact on performance of workpiece. It is determined by non-human factors. At present, only Chen[12] research group of Harbin Institute of Technology analyzed the influence of machining introduced sub-surface defects upon mechanical properties of single crystal copper. However, the study about γ-TiAl alloy has not been found. In this paper, γ-TiAl alloy was used as the research object. Because of its low density and remarkable high temperature performance, it has a good application prospect in aerospace, automobile and other fields[13].

In this work, a series of simulations on nano-cutting and stretching process of single crystal γ-TiAl were implemented by molecular dynamics (MD) method. Firstly, evolution of lattice transition and dislocation were investigated during nano-cutting. Secondly, influence of cutting depth on stress-strain curve was discussed. Lastly, effects of different depths of cutting on position of dislocation nucleation and port of workpiece were studied during stretching.

1 Simulation Model and Computation

1.1 MD simulation model

γ-TiAl alloy has face-centered tetragonal (fct) with the L_{10} structure[14], as shown in Fig.1. The x, y and z coordinate axes correspond to the crystallographic orientations [100], [010] and [001], respectively. The lattice constants are a_0=b_0= 0.4001 nm and c_0= 0.4181 nm, which are consistent with the experimental values a_0=b_0=0.4005 nm and c_0=0.40707 nm[15].

MD simulation was performed in large-scale atomic/ molecular massively parallel simulator (LAMMPS)[16], and the nano-cutting model shown in Fig.2 consists of single-crystal γ-TiAl and a diamond tool. The size of the model is 18 nm×11 nm×10 nm along the [101], $[0\bar{1}0]$ and $[10\bar{1}]$, respectively. The model of single-crystal γ-TiAl contains 124 188 atoms, and diamond tool has about 7793 atoms. The periodic boundary conditions are only applied in direction x in order to eliminate the boundary effect. There are three kinds of atoms in the workpiece: boundary atoms, thermostat atoms and Newtonian atoms. Here the bottom and right boundary atoms are fixed in space to support the whole system. Initial temperature of workpiece is chosen as 293 K. The heat dissipation is achieved by keeping thermostat atoms at constant temperature of 293 K using velocity rescaling method during MD simulation process. Newton atoms are main atoms used to investigate various aspects pertaining to cutting process, and the motion of Newton atoms obeys Newton's second law.

Fig.3 shows the process of tension test. To start with, the specimen is scratched by tool at a certain velocity and cutting depth. Secondly, cutting is completed to make a tool withdraws, and after a period of relaxation, the workpiece is stabilized and then stretched. During stretching process, the atoms of thermostat layer and boundary layer are removed, and then the temperature of system is controlled to be 293 K with Nose-Hoover. The thickness of right end is fixed at 2 nm,

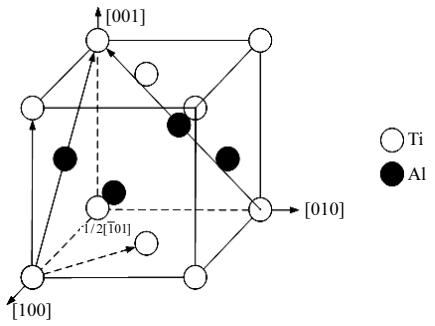

Fig.1 L_{10} structure of γ-TiAl

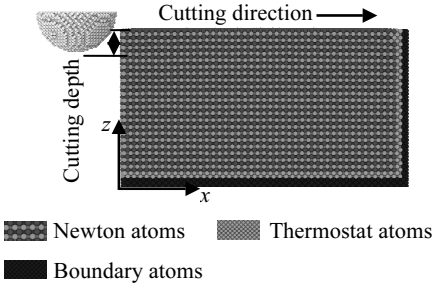

Fig.2 MD simulation model of nano-cutting process (green and red represents Ti, Al, respectively)

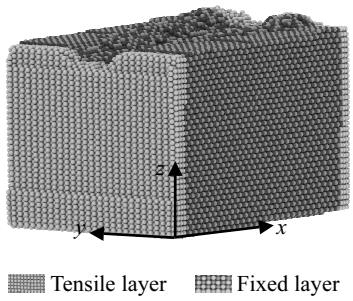

Fig.3 MD simulation model of stretched process

and left end is uniaxial stretched at a speed of 50 m/s using the fix move command.

1.2 Interatomic potential

In MD simulation, the appropriate empirical potential function is usually chosen to depict interaction between atoms. Cao et al[17] studied the nano twin deformation mechanism of γ-TiAl by embedded atom method (EAM). The EAM method has been successful in accurately describing properties of a metallic system[18-20], which is expressed as a multi-body potential energy function in the following form:

$$E = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{ij(i\neq j)} \phi_{ij}(r_{ij}) \quad (1)$$

$$\rho_i = \sum_{j(j\neq i)} f_j(r_{ij}) \quad (2)$$

where, F_i is the embedding energy of atom i whose electron density is ρ_i, ϕ_{ij} is the relative potential energy of atom i and atom j, r_{ij} is the distance between atom i and atom j, $F_i\rho_i$ is the sum of electron cloud density produced by all other atoms' extranuclear electron to atom i, $f_j(r_{ij})$ is the electron density produced by atom j.

The interaction between Al-C and Ti-C is described by Morse potential, and the expression is given by

$$V(r_{ij}) = D_e[e^{2\alpha(r_e - r_{ij})} - 2e^{\alpha(r_e - r_{ij})}] \quad (3)$$

where, D_e represents the cohesive energy between atoms i and j, α is the elastic modulus of material, r_{ij} is the instantaneous distance between atoms i and j, and r_e is the equilibrium distance between atoms i and j. The parameter of Morse potential can be adopted from Zhu et al[21] as $D_{Ti\text{-}C}$=0.982 eV, $\alpha_{Ti\text{-}C}$=22.83 nm^{-1}, $r_{Ti\text{-}C}$=0.1892 nm, $D_{Al\text{-}C}$=0.28 eV, $\alpha_{Al\text{-}C}$=27.8 nm^{-1}, $r_{Al\text{-}C}$=0.22 nm. Since stiffness of diamond is much higher than that of γ-TiAl alloy, thereby, the tool is a rigid body during MD simulation. Table 1 shows the MD simulation parameters.

The selection of cutting speed is based on following references and combined with characteristics of γ-TiAl alloy. Su et al[22] simulated the influence of cutting speed on copper nano-cutting by molecular dynamics, and cutting speed was selected as 10~2000 m/s. The results show that dislocation can be produced at appropriate cutting speed (100~400 m/s), which accords with real physical situation, but only disordered atoms at higher cutting speed. Gong et al[18] have studied molecular dynamics simulation of nano-machining of single crystal nickel, and cutting speed is selected as 100~1200 m/s. Therefore, when actual plastic deformation mechanism is fully reflected, the cutting speed of 400 m/s can not only shorten simulation time but also improve computational efficiency.

This paper uses common neighbor analysis (CNA)[23] technology to identify transformation of lattice structure during nano-cutting and stretching, such as in the workpiece material fcc (face-centered cubic) could be converted to bcc (body-centered cubic) or hcp (hexagonal close-packed). Moreover, the dislocation extraction analysis (DXA) was performed to dislocation evolution in the workpiece.

2 Results and Discussion

2.1 Defects in the nano-cutting process

In order to conveniently compare the influence of cutting and non-cutting on crystal structure of workpiece during stretching process, the quantity of crystal transformation of workpiece was studied in the cutting process.

Due to a small depth of cutting, the number of crystal structures of bcc and ico is small. Therefore, only hcp is chosen as the research object of crystal structure for facilitating analysis. The number of hcp varies with different cutting depths during nano-cutting, which is illustrated in Fig.4. In the first place, three curves show a peak distribution, which increases first and then decreases with increase of cutting distance. The

Table 1 MD simulation parameters

Machining parameters	Value
Potential function	EAM, Morse
Workpiece	Single crystal γ-TiAl
Workpiece size/mm	18×11×10
Tool	Diamond
Tool edge radius, R/nm	1.5
Lattice structure	$L1_0$
Cutting speed/m·s^{-1}	400
Cutting depth/nm	0.5, 1, 1.5
Cutting direction	$<110>[\bar{1}01]$
Time step/fs	1

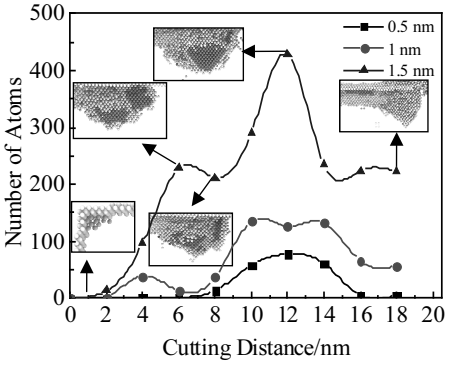

Fig.4 Lattice transformation at different cutting depths

highest peak of three curves corresponds to 12 nm. It is because cutting force, temperature, and energy increase as cutting distance increases, which provide good condition for crystal structure transformation. The nano-scale cutting process can be divided into three stages, namely, initial stage, middle stage and later stage. However, the maximum number of crystal structure appears in the middle stage, that is, more defects. In the second place, the number of crystal structure transitions increases with the increase of cutting depth. In particular, the number of crystal structures at a cutting depth of 1 nm is slightly higher than that of 0.5 nm, but the number of crystal structures at a cutting depth of 1.5 nm is much higher than that of 1 nm.

The different cutting depths have a greater impact on number of crystal structure transitions. The crystal structure transition time is faster with increase of cutting depth. The lattice transition starts at 8, 3 and 2 nm when the cutting depth is 0.5, 1 and 1.5 nm, respectively. The fluctuation of three curves is caused by evolution of a stack fault. The concrete explanation is that, taking the cutting depth of 1.5 nm as an example, the number of lattice transitions conforms to microstructure evolution during nano-cutting process. The five local graphs in Fig.4 are microstructure evolution of subsurface defect with different cutting distances, where red and white are hcp and other atom (boundary atom and defective fcc), respectively. The hcp atoms are not generated, but a small amount of defective fcc (Dfcc) atoms are produced in front of tool, which is a disordered state when cutting to 1 nm. As cutting distance reaches 6 nm, a stacking fault is formed in workpiece. A certain number of stacking faults can lead to work hardening of workpiece, which improves strength and hardness of workpiece. Due to the extrusion of tool, hcp is transformed into other atom, so other atom increases and hcp atom decreases slightly when cutting to 8 nm. The number of hcp atoms are maximum account for large cutting force, cutting temperature and lattice reconfiguration when cutting to 12 nm. At the end of cutting, the hcp atoms eventually transform into other atoms, except for both sides of the cutting groove, which are removed in the form of chips.

The formation of dislocation reflects plastic deformation of workpiece in nanometric cutting process, so length of dislocation line at each stage was studied. The length of dislocation line was quantitatively intercepted by ovito visual analysis software. Fig.5 shows the effect of different cutting depths on length of dislocation line. It can be seen that the length of dislocation line gradually increases with the increase of cutting depth. The length of dislocation line at cutting depth of 1.5 nm is much longer than that of 1 nm. It indicates that the greater the cutting depth, the greater the plastic deformation of the workpiece.

In addition, the more likely plastic deformation occurs with greater cutting depth, which accords with initial cutting stage of Fig.4. As shown in Fig.5, the curve at cutting depth of 1 nm is most unstable. The following are specific explanations. It can be clearly seen from partial view of Fig.5 that the length and number of dislocation lines are dynamic with cutting distance. The types of dislocations are illustrated in Table 2. The Shockley partial dislocation is formed first when cutting distance exceeds 2 nm, and then slips to upper left under the push of a tool. It disappears into the chip when cutting distance is 6 nm. The type and length of dislocation increase as the cutting progresses. In particular, the length of Shockley's partial dislocation is longest and easiest to be formed. It is because Shockley dislocation is formed on the (111) plane, which is a compact plane, and requires relatively small shear-slip stress. The length of dislocation reaches their peak when cutting distance is 10 and 11 nm, corresponding to

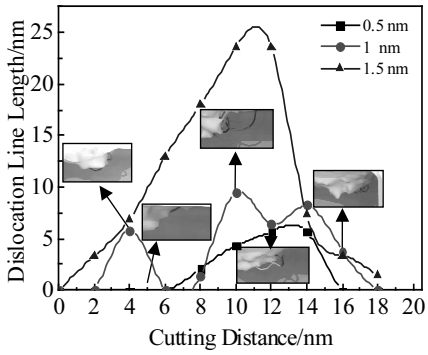

Fig.5 Length of dislocation line at different cutting depths

Table 2 Dislocation type

Color	Dislocation type
	Other
	1/2<110>(Perfect)
	1/6<112>(Shockley)
	1/6<110>(Stair-rod)
	1/3<001>(Hirth)
	1/3<111>(Frank)

the cutting depth of 1 and 1.5 nm, respectively. Subsequently, the dislocations react with each other, which results in a slight decrease of dislocation line when cutting distance is 12 nm. The reaction formula is as follows:

$$\frac{1}{6}[\bar{1}\,\bar{1}\,2]+\frac{1}{6}[\bar{1}\,1\bar{2}]\rightarrow\frac{1}{3}[\bar{1}00] \quad (4)$$

That is, two Shockley partial dislocations react to generate a Hirth dislocation. So the length of dislocation line get smaller, leaving only a small amount of Shockley dislocation when cutting distance is to the end. It is because boundary is set to a rigid body, and dislocation cannot continue to slide and expand in a rigid body, which is removed by chip. Finally, the highest peak of dislocation line is basically in middle of the cutting, which is consistent with Fig.4. It is fully illustrated that defect is most obvious at the middle of cutting.

2.2 Effect of cutting depth on yield stress and elastic modulus of materials

A stress-strain curve well reflects mechanical properties of workpiece, so influence of different cutting depths on mechanical properties of workpiece was studied. The effect of different cutting depths on stress-strain curve is illustrated in Fig.6, where, black, red, blue and green represent cutting depth of 0.5, 1, 1.5 and 0 nm, respectively. It can be seen elastic stage of four curves is basically the same; however, plastic stage is quite different. The modulus of elasticity at different cutting depths can be calculated by Fig.6. The modulus of elasticity at cutting depths of 0.5, 1, 1.5 and 0 nm are 235, 228, 213 and 175 GPa, respectively. The experimental values of modulus of elasticity for γ-TiAl alloy is 160~176 GPa[24]. It is due to difference of macro and nano scales and deviation of simulation and experimental values, but they still have good consistency. The elastic modulus of machined workpiece is higher than that of non-machined workpiece, because defects are generated inside workpiece subjected to cutting which improves bonding strength of TiAl. In addition, it can be seen from Fig.6 that strain rates of TiAl ranging from 0.01 to 0.04 and Ref. [24] are in good agreement. Next, the maximum stress value is 1.03, 1.26, 1.12 and 1.02 GPa when cutting depth is 0, 0.5, 1 and 1.5 nm, respectively. It can be seen clearly that stress of workpiece will increase at a certain cutting depth, which is attributed to effect of microstructure and dislocation density on a work hardening in cutting process. Last but not the least, fracture becomes easier with increasing cutting depth, from the point of view of workpiece fracture. The curve fluctuation of plastic phase results from evolution of microstructure and dislocation during the stretching process.

2.3 Effect of cutting depth on number of lattice transition, dislocation evolution and fracture in tensile process

For the sake of study law of lattice transition before and after nanometer cutting, a quantity of hcp lattice transition was analyzed quantitatively in tensile stage. The number of lattice transition varies with time step during stretching which is depicted in Fig.7. As can be seen four curves are similar at initial tensile stage. To put it another way, the number of lattice transition increases rapidly. Nevertheless, difference is obvious in plastic stage. Especially, the number of lattices transition at cutting depth of 1.5 nm is 254 instead of 0 at the beginning of drawing, which conform to last local graph in Fig.4. From the overall view of Fig.7, the maximum value of lattice transition decreases gradually from cutting depth of 0.5, 0, 1 to 1.5 nm in early stage of stretching. The number of lattice transition increases firstly, then decreases and finally reaches the stable state when cutting depth is 0.5 and 1.5 nm. It is the cause that stress and temperature contribute to lattice transition. However, number of hcp atoms decreases originating from reconstruction of crystal when stress exceeds a certain range. Finally, the number of lattice transition is stable because workpiece has broken. The crystal structure rule is opposite to that in Fig.4 when the cutting depth is 0.5 and 1.5 nm. It indicates that nano-cutting has a greater influence on number of crystal lattices transition in tensile stage. This is because removal rate of material is large at cutting depth of 1.5 nm, resulting in large plastic deformation. The number of lattice transition is always higher when cutting depth is 0 and 1 nm, which is the result that more slip systems are activated and lead to more stacking fault in tensile stage.

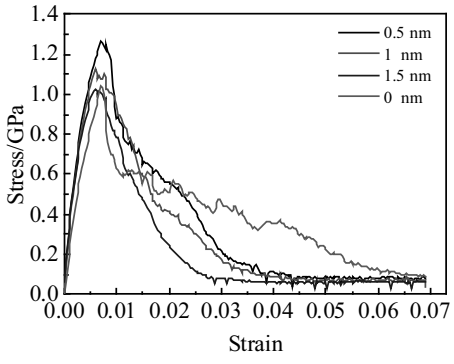

Fig.6 Stress-strain curves at different cutting depths

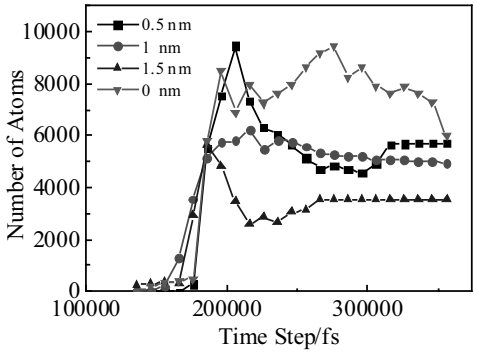

Fig.7 Changes curves of the number of lattice transitions with time step at different cutting depths

The fluctuation of curve in graph is caused by a stacking fault evolution in workpiece.

In this paper, the dislocation line is extracted by DXA method and position of dislocation nucleation is described during drawing. The effect of different cutting depths on dislocation nucleation is illustrated in Fig.8. Fig.8a~8c and 8d~8f represent cutting depth is 0.5 and 0 nm, respectively. The types of dislocation in Fig.8 are shown in Table 2. It can be seen clearly that nucleation position of dislocation is very different. The dislocation nucleation of machined workpiece is easier on subsurface, because the stress of machined subsurface is high and multiple dislocation slip systems have been activated, then expands from subsurface of workpiece to inside, as depicted in Fig.8a and 8b. However, the stress at boundary of unmachined workpiece is more intensive, so dislocation extends from boundary to inside of workpiece, as shown in Fig.8d and 8e. As drawing continues, workpiece has a large plastic deformation, so that workpiece is quickly filled with dislocation, as illustrated in Fig.8c and 8f. From overall view of Fig.8, there are more Shockley dislocation nucleation in initial stretching. The Perfect, Other, Stair-rod and Hirth dislocations are gradually nucleated and expanded with stretching. This is because Perfect, Stair-rod and Hirth dislocations must be formed through a synthetic reaction between dislocations.

It is found that cutting depth has a great influence on a fracture surface during tensile process. Therefore, the fracture of workpiece needs to be further studied. Fig.9 shows the effect of cutting depths on fracture location of workpiece, where green and red represent perfect fcc and stacking fault, respectively. Besides, Fig.9a, 9b, 9c and 9d represent cutting depth of 1.5, 1, 0.5 and 0 nm, respectively. From overall view of Fig.9, four tensile models have undergone large plastic deformation and some small holes are produced, as shown in Fig.9c and 9d. However, the fracture surface of workpiece becomes flatter with increase of cutting depth. It is due to the high surface stress of workpiece and high removal rate of chips, which causes rapid fracture of workpiece. Last but not the least, it is found that fracture location of workpiece has certain regularity with increase of cutting depth. In other words, the

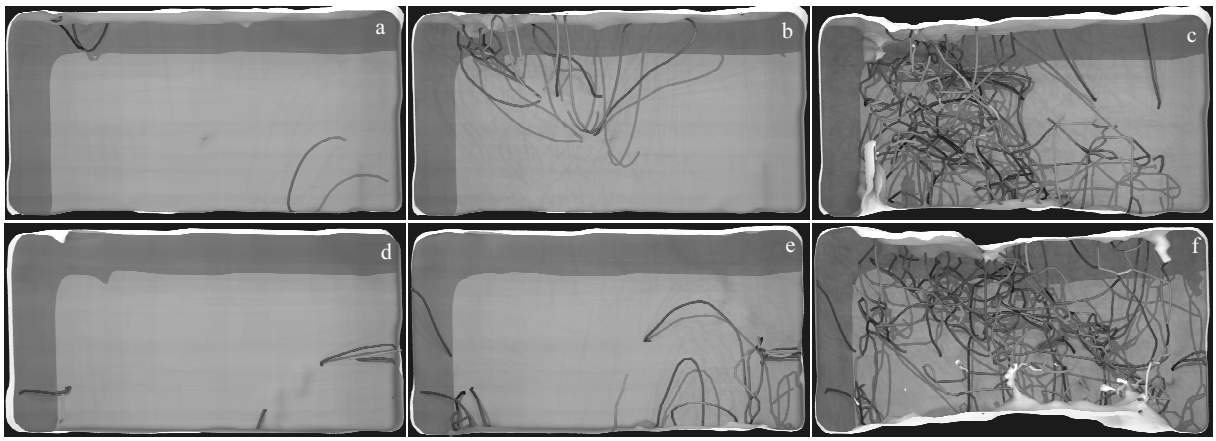

Fig.8 Effect of cutting depth on dislocation nucleation during stretching: (a~c) 0.5 nm and (d~f) 0 nm

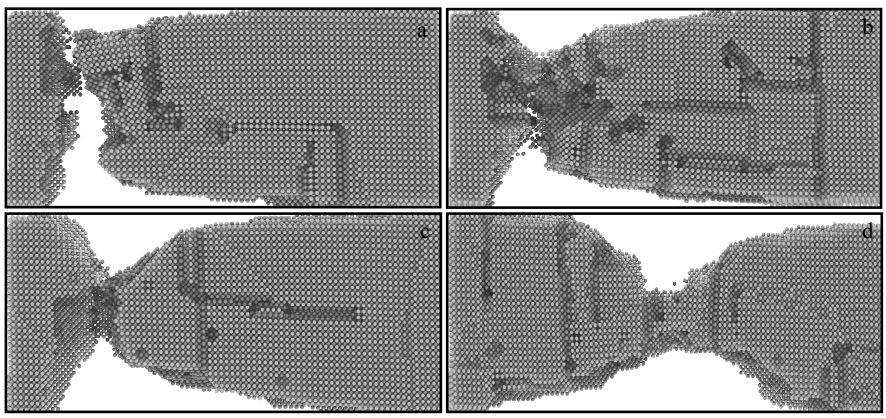

Fig.9 Effect of different cutting depths on workpiece fracture: (a) 1.5 nm, (b) 1 nm, (c) 0.5 nm, and (d) 0 nm

fracture position is closer to tensile end with increase of cutting depth. This is owing to that the stress on surface of workpiece becomes more intensive with increase of cutting depth. Furthermore, the stress at tensile end of workpiece is inherently concentrated, so it is affected by these two factors.

3 Conclusions

1) In cutting process, the number of lattice transition and length of dislocation line increase with increase of cutting depth. Moreover, synthetic reaction between dislocations results in fewer dislocation lines. During the tensile process, the number of lattice transition decreases with increase of cutting depth, in which the law of inverse ratio is formed before and after cutting.

2) The yield stress and elastic modulus of workpiece increase in a certain range of cutting depth, which makes workpiece have well mechanical properties.

3) The dislocation of machined workpiece is nucleated at subsurface of workpiece. However, the dislocation of unprocessed workpiece is nucleated at edge of workpiece. Besides, the fracture of workpiece is closer to tensile end and workpiece breaks down quickly as cutting depth increases.

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切削深度对单晶 γ-TiAl 合金力学性能的影响

李海燕[1,2]，乔海洋[1]，冯瑞成[1,2]，王　麒[1]，王茂茂[1]，李建华[1,2]

(1. 兰州理工大学，甘肃 兰州 730050)

(2. 有色金属先进加工与再利用国家重点实验室，甘肃 兰州 730050)

摘　要：通过分子动力学模拟方法建立了单晶γ-TiAl合金的纳米切削模型和拉伸力学模型，研究了不同的切削深度对工件力学性能的影响。首先详细分析了切削过程中晶格转变和微观缺陷演化之间的关系；然后系统探讨了不同的切削深度对工件应力-应变曲线、位错形核位置和断口位置的影响。研究结果表明：在纳米切削过程中，晶格转变数量随着切削深度的增加而增加，并且与微观缺陷演化具有一致性；在一定切削深度范围内，切削后工件的屈服应力和弹性模量会有所提高。另外，切削深度对工件的位错形核位置和断口位置有较大的影响，切削后工件位错形核于工件的亚表面，而未经切削的工件其位错形核于边界处；工件的断口位置随着切削深度的增加向拉伸端靠近。

关键词：纳米切削；拉伸；分子动力学模拟；晶格转变；位错

作者简介：李海燕，女，1979 年生，讲师，兰州理工大学机电工程学院，甘肃 兰州 730050，电话：0931-7823072，E-mail: y5217@163.com