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ARTICLE

Molecular Dynamics Simulation of the Effect of Process Parameters on Ni/Fe Metal Thermal Spraying

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Abstract: Molecular dynamics simulations were performed to study the deposition of the thermal spraying material under different process parameters. The effects of temperatures, cluster size, and spraying speed on the deposition of Ni clusters on the Fe substrate were examined. The morphology of clusters and the subsurface damage of the substrate were analyzed. The results show that in the heating-up process of Ni cluster, the melting point becomes higher with the increase of cluster size, and the complete melting temperature of Ni cluster is about 1800 K. During the spraying process, the matrix shows a "mountain" shape due to the impact force to disordered atoms. Furthermore, it is also found that spraying speed plays an important role in the deposition process. At lower spraying speed, the flattening ratio decreases again, but at higher spraying speed, the substrate has defects, such as vacancy and atomic cluster after the impact of clusters. Thus, there is a critical spraying speed mechanism in thermal spraying.

Key words: thermal spray; cluster temperature; substrate defect; cluster morphology; molecular dynamics

With the rapid development of high-end equipment, thermal spraying technology has become the key to material surface protection and strengthening. The thermal spraying process can produce a thin layer on the surface that is superior to the the body material in performance, and can be endowed with the properties of high-temperature resistance, wear resistance, corrosion resistance, radiation protection and fatigue resistance[1-3].

Researchers have studied spraying technology. Sun et al[4] studied the oxidation behavior of thermal sprayed $MoSi_2$-based composite materials and found that the constituent phase, porosity, and residual stress are key factors affecting the performance of two-dimensional structural components. Bai et al[5] analyzed the particle flight behavior in the supersonic plasma spraying process and its effect on the microstructure and properties of nano-coating. The results showed that the influence of spray power on particle velocity is greater than that of temperature, and the temperature and velocity of particle determine the melting state of the particles and the content of the unmelted nanoparticles of as-sprayed coating. Zhang et al[6] researched the substrate materials, thermal interface contact resistance, grain size distribution and rapid solidification process in thermal spraying. It was found that the nucleation temperature and grain size distribution are closely related to contact angle. Singhal et al[7] simulated the critical speed of cold spraying under different turbulence models. The results showed that better coating quality and energy saving coating can be obtained at a lower critical speed. Chun et al[8] investigated the bonding mechanism of cold spraying in the deposition of metal particles and found that the adiabatic shear instability caused by plastic deformation near the interface between metal particles and substrate at the melting temperature is considered as the bonding mechanism of metal particles. However, Hassanigangaraj et al[9] proposed that when metal particles impact substrates at a sufficiently high velocity, the interaction of strong pressure waves with the free surface at the particle edge under natural dynamic effect may cause hydrodynamic plasticity that affects bonding, without shear instability.

In recent years, molecular dynamics simulation has proven

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to be an effective method to study the microscopic properties of materials, which can reveal phenomena that cannot be observed by traditional methods, and capture the position, velocity, stress of each atom as well as the microscopic mechanism and morphological evolution of particles[10]. Some scholars have conducted studies on spraying with molecular dynamics. Joshi et al[11,12] studied the deposition of Cu in the process of cold spraying by molecular dynamics simulation technology. The results showed that the bonding mechanism in the process of cold spraying can be attributed to adiabatic softening, adiabatic shear instability and a uniform coating formed by interfacial jetting of particle materials. Rahmati et al[13] used molecular dynamics simulation to predict the deformation behavior of solid copper particles against a copper substrate, and the results showed clear dislocation activity patterns associated with three different stages of deformation. Wang et al[14] researched the microstructure and micro simulation mechanism of high-temperature nano Cu particles sprayed on Cu substrate at room temperature. Two different types of microstructure formation mechanisms are observed through the establishment of a thermodynamic motivated model. Wang et al[15] performed molecular dynamics simulation to study the micro process of large palladium clusters impacting different hardness substrates at different initial speeds at room temperature. The results showed that with the increase of clusters, it is more favorable for the embedment and mixing of substrate atoms and clusters. At the same time, it is found that the deposition of the second cluster in a short time interval is more conducive to the combination of clusters and substrates. Wu et al[16] studied the effects of deposition conditions and annealing on the microstructure and morphology of NiAl thin films by molecular dynamics. Results showed that increasing the incident energy can roughen the surface of the unannealed films at 15 eV, enhance the bonding of the film and the substrate, and increase the damage of the incident atoms to the perfect crystal structure of the substrate. Nasim et al[17] investigated the influence of different particle sizes and impact velocities on the deposition of nano-scale graphite particles on the copper substrate. There is a critical impact velocity when the graphene flake and the massive graphite particles were separated, and the impact velocity of nano-scale graphite particles plays an important role in the successful deposition of graphene flake. Goel et al[18] studied the relationship between structure and performance of pure Cu particles during thermal spraying with molecular dynamics, and the quantitative results of the impacts at different velocities and temperatures were evaluated by a newly defined flattening aspect ratio. Shimizu et al[19] performed molecular dynamics to analyze the flattening process and the atomic behavior of droplets. The results showed that the transfer of atoms in the horizontal direction is in direct proportion to the horizontal distance from the central axis of the droplet, and the solidification of the droplet starts from the external source of the droplet. Zhang et al[20] analyzed mechanical properties and machinability of the Cu/Al nano-weldment and found that elastic modulus of the nano-weldment is between copper's and aluminum's; however, its yield strength is less than that of the two monocrystals. Meanwhile, Liu et al[21] studied the tension of Al_2Cu with voids. The results showed that the void greatly reduces the tensile strength and deformation ability of the material.

Molecular dynamics can be used to study thermal spraying at the molecular and atomic levels, and to get micro details that cannot be obtained in practical experiments, so it is a powerful supplement to the theory and experiments. In the past few years, there are many studies on cold spraying by molecular dynamics, but few on thermal spraying, especially the study on preheating cluster to melt temperature and the analysis of substrate after spraying with molecular dynamics. This study focuses on using molecular dynamics simulation to investigate the effect of melting temperature of clusters with different sizes and processing parameters on the morphology of clusters, the atomic structure of the substrate and the evolution of defects.

1 Model and Method

Thermal spraying is a series of substrate deposition process of melting clusters on the substrate. In order to study the melting temperature of clusters, the trace of cluster atoms, the evolution of substrate defects, and the deposition of a single Ni cluster on pure Fe substrate were simulated.

1.1 Simulation model

The schematic of the model used for thermal spraying process simulation is shown in Fig. 1. The simulation system consists of Fe atoms as a substrate, and a cluster made of Ni atoms. The crystals of Fe and Ni are bcc and fcc structures, respectively. The parameters of model and simulation are given in Table 1. The atoms of the Fe substrate are allocated in three different zones: the Newtonian layer, the thermal layer, and the fixed layer. The Newtonian layer contacts with thermal spraying particles to show the morphology changes of the thermal spraying particles. The thermal layer adopts Berendsen[22] temperature control method to absorb the heat generated in the spraying process. And the fixed layer

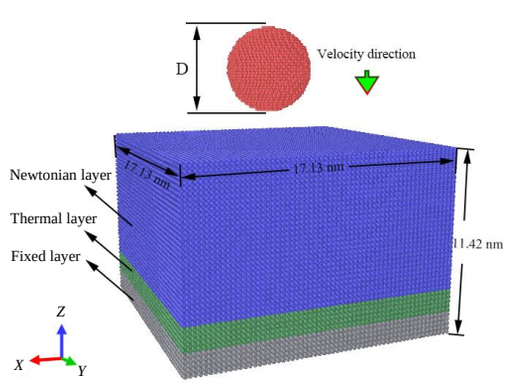

Fig.1 Three-dimensional physical model of thermal spraying based on molecular dynamics simulation

Table 1 Simulation parameters

Parameters	Value
a (lattice constant of Ni)/nm	0.352 nm
Clusters size, D/nm	5a, 10a, 15a, 20a
No. of atoms in clusters	261, 2109, 7070, 16755
Substrate size/nm	17.13×17.13×11.42
No. of atoms in substrate	291 600
Substrate temperature/K	293
Potential used	EAM
Time step/fs	1.0

prevents the substrate atoms from sliding during the spraying process. In order to avoid the size effect, the periodic boundary condition is adopted. Before the thermal spray simulation, the clusters and the substrate reach equilibrium at their respective specific temperatures.

The process of simulating thermal spraying is divided into two steps. Firstly, the model is fully relaxed, and then the cluster is sprayed along the Z-axis. Before spraying, in order to avoid interaction between cluster and substrate, Ni clusters are far enough above the surface of the Fe substrate. As mentioned in the previous literature[17,18], the spray parameters studied in this work are shown in Table 2.

1.2 Melting point analysis of Ni clusters

The interatomic potential determines the accuracy of molecular dynamics simulation. In this research, the interatomic potential of the Fe-Ni system is embedded atom model potential (EAM)[23], and the total atomic energy is given by the following equation:

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

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} represents the distance between atom i and atom j, $F_i(\rho_i)$ is the sum of electron cloud density produced by all other atoms, and extranuclear electron to atom i.

1.3 Analysis method

Lammps software was used for simulation in this work, and Ovito (Open Visualization Tool) [24] software was used for analysis and processing of simulation results. In order to study the melting state of thermal spraying clusters, the radial distribution function method in Ovito was selected to output data for analysis.

Table 2 Process parameters used in the thermal spraying simulation process

Group	Cluster size/nm	Spraying speed/m·s^{-1}	Cluster temperature/K
1	5a	2000	1000
2	5a	2000	1800
3	10a	2000	1800
4	15a	2000	1800
5	20a	2000	1800
6	20a	1000	1800
7	20a	1500	1800
8	20a	2500	1800

2 Simulation Results and Discussion

2.1 Melting point analysis of Ni clusters

Experiments cannot be used to determine the melting point of microscopic clusters, and only other physical parameters can be analyzed. In this work, the mean square displacement (MSD)[25] and the radial distribution function ($g(r)$) [26] were used to determine the melting point and melting situation of different sizes of Ni clusters. MSD values of different cluster sizes changing with temperature are shown in Fig.2.

When the MSD value is very small, it means that the clusters are solid. With increasing the MSD value, it means that the internal structure of clusters is disordered and clusters are melted. When the cluster size is 5a and 10a, the first transition of MSD occurs at 750 and 1500 K. Based on this observation, it can be concluded that the cluster atoms are disordered and the cluster is partially melted. Then MSD increases slowly with the increase of temperature. MSD start to increase sharply from 1800 K. When the cluster size is 15a and 20a, the MSD values show a steady trend as the temperature increases, which changes abruptly at 1700 and 1800 K, respectively. It can be found that the melting point of the cluster increases with the increase of the cluster size. Beyond 1800 K, all clusters atoms become completely disordered.

Meanwhile, the radial distribution function is shown in Fig. 3, which also proves the melting point variation of clusters. The decrease of the wave peaks and the increase of the wave width of the radial distribution function indicate that the disorder degree of the cluster becomes larger. For cluster sizes

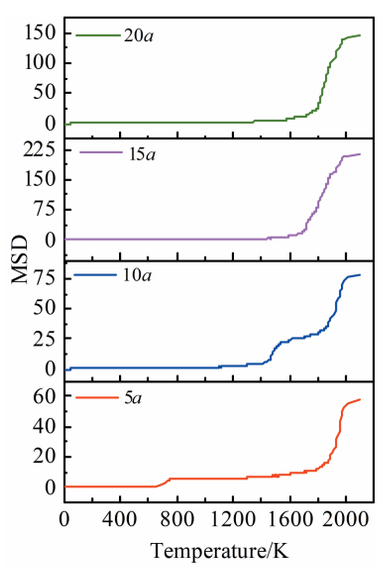

Fig.2 Change of MSD of Ni cluster with temperature under the cluster sizes of 5a, 10a, 15a, and 20a

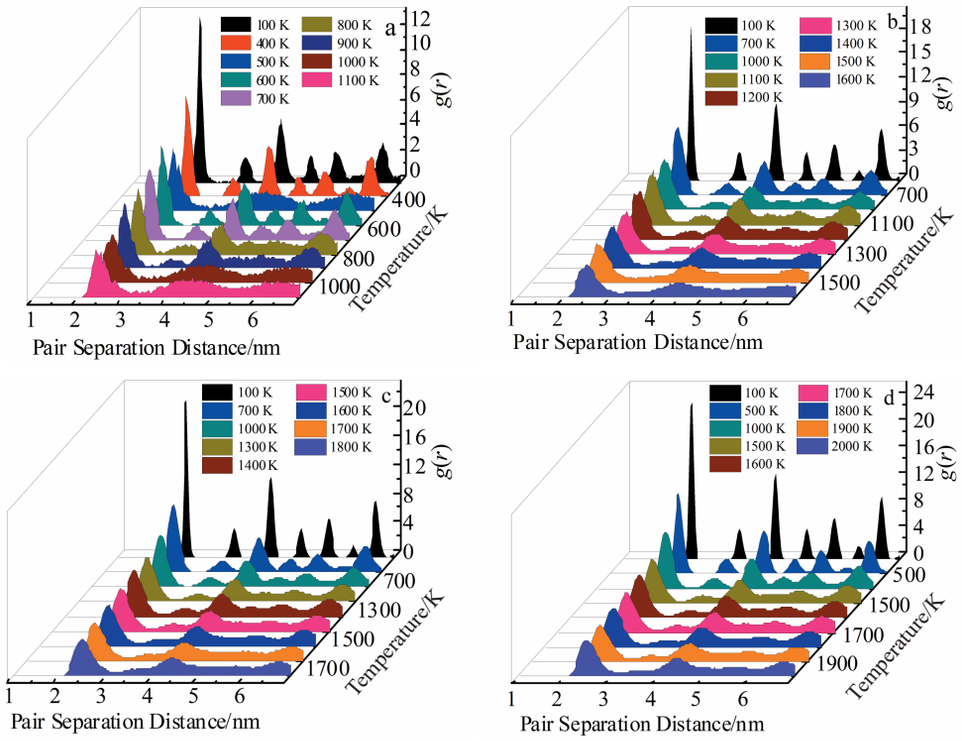

Fig.3 Radial distribution function of Ni clusters when the cluster sizes are 5*a* (a), 10*a* (b), 15*a* (c), and 20*a* (d)

of 5*a*, the observed second wave peaks disappear at 600 K, indicating partial melting of the cluster. With the increase of temperature, the wave peaks disappear gradually, indicating that the melting of clusters is intensified. For clusters size of 10*a*, the second peak, and the following peaks basically disappear at 1600 K. It may be noted that the second and later peaks of 15*a* and 20*a* disappear when the temperature is 1800 K.

Therefore, in the microscopic simulation, the melting points of Ni clusters with different sizes are different, and the melting points gradually increase as the size of clusters increases. The melting temperature of clusters is basically the same at 1800 K, and the experimental melting point of Ni is 1723 K[27], indicating that the melting temperature calculated by simulation is close to the experimental value.

2.2 Morphology analysis of thermal spray clusters under different process parameters

2.2.1 Thermal spraying process

In order to observe the impact process of clusters on the substrate, Fig. 4 and Fig. 5 show the morphology and cluster atom tracks of the third group of process parameters at different time when a single cluster impacts the substrate, respectively. The main body of Fig. 4 is the spray profile, the type of atoms is identified by CAN[28] technology, and the red clusters represent the morphology of clusters. When the time is 0 ps, the clusters have been heated to completely melt, droping in droplet shape, and placed at a certain distance above the surface of the surface. As time increases 0.5 ps, the cluster contacts the surface of the substrate. With the increase of collision time, the substrate and the cluster are squeezed seriously. The extruded atoms of the substrate are disordered and irregular, and take a shape of “mountain”. It happens because cluster atoms start to slip and spread around, and the outer atoms have great fluidity and impact force, so a significant amount of mass flow of the particle on the substrate takes place. In the subsequent 1.5 ps, when the maximum impact state is reached, the vertical impact has stopped. Then, due to the rebound phenomenon of the substrate, a flat liquid solid interface between the particle and substrate is formed and most of dislocations and other defects are absorbed. The elastic recovery of substrate atoms and lattice reconstruction occur, and clusters spread on the surface of the substrate, as shown at 2.5 ps. In the later stage, the diffusion morphology of clusters is basically determined, and only a few atoms change dynamically, no mass flow can be observed anymore and the lattice reconstruction of the substrate is obvious.

In order to expound the migration or flow of the atoms in the cluster, the trace lines of the atoms in the outer ring of the whole spray profile of the cluster are shown in Fig.5. Through these representative atoms, the process of the change of the cluster morphology can be seen clearly. In addition, it indicates that the outer atoms have strong mobility and diffusion.

2.2.2 Flattening ratio

The fluidity of thermal spray clusters can be used to evaluate the spray quality. The flattening ratio is widely used to describe the deformation ability of clusters in the spray process[29]. Therefore, the flattening ratio is divided into

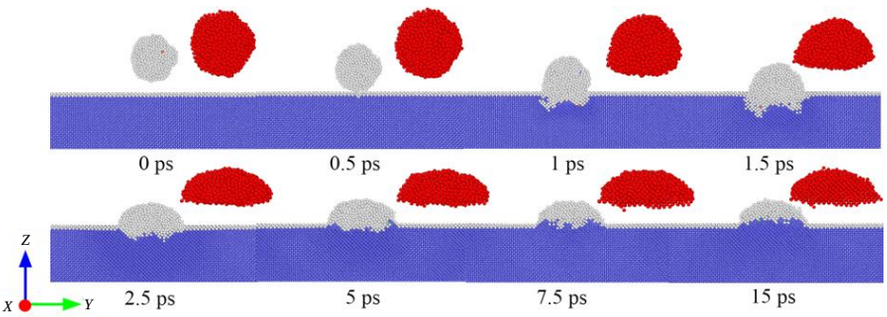

Fig. 4 Morphology snapshot of spraying the Fe substrate with fully melted Ni clusters at different time

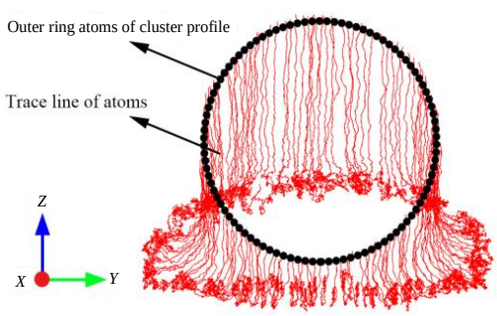

Fig.5 Trace line of atoms in the outer ring of Ni cluster profile

horizontal flattening ratio and vertical flattening ratio. As shown in Fig. 6, the horizontal flattening ratio (*L*/*D*) is the ratio of the maximum diameter *L* after spraying to the original diameter *D* of clusters, and the vertical flattening ratio (*H*/*D*) is the ratio of the maximum height *H* after spraying to the original diameter *D* of clusters. When the horizontal flattening ratio is larger and the vertical flattening ratio is smaller, the cluster has a larger extension range and better coating effect.

The effect of clusters temperature on the flattening ratio during thermal spraying process is shown in Fig. 7a. It should be noted that the coating effect of fully melted clusters is better, and it can also be concluded that thermal spraying is a better surface treatment process than cold spraying. The flattening ratio analysis at different speeds is shown in Fig. 7b. The results show that as the impact velocity increases, the deposition height decreases. It can be seen that the horizontal flattening ratio is proportional to the spraying speed. The horizontal fluidity is better as the spaying speed increases, and the effect of spraying speed on the vertical flattening ratio is relatively small. Therefore, with the increase of spraying speed, the flattening effect of clusters becomes better. Fig. 7c shows the result obtained by varying size of clusters at 2000 m/s and up to 1800 K temperature impact. Careful observation reveals that in all four cases, 20*a* has the best flattening effect.

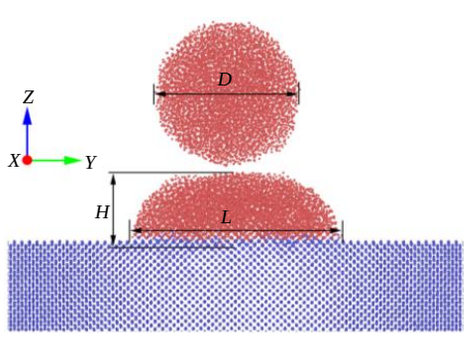

Fig.6 Example of spray flattening ratio (a spherical particle with diameter *D* is deformed into a disk-like shape with height *H* and diameter *L*)

2.3 Analysis of thermal spraying substrate under different process parameters

2.3.1 Atomic structure

The transformation of the substrate atomic structure is different under different process parameters. Fig. 8 shows the curve transformation of crystal structure under different process parameters. Fig. 8a and 8b show the crystal structure transition curves of fcc and other structures, where black and red are the temperatures of partial melting and complete melting, respectively. When the clusters are partial melting, there is a small amount of fcc atom transition, while for the complete melting, there is no fcc atom transition. At the same time, other atom transfer in complete melting is less than in partial melting. It can be seen that the melting state of the thermal spray cluster has a great effect on the substrate. The crystal structure transition curves of fcc and hcp structures can be clearly observed in Fig. 8c and 8d, in which the spraying speeds of black, red, blue and green are 2500, 2000, 1500 and 1000 m/s, respectively. At higher impact velocities, the number of the transition of fcc and hcp crystal structure increases rapidly and then decreases slowly during the impact process, because the higher the spraying speed of the cluster, the greater the impact force from cluster to the substrate, and the more the sliding system is activated. Subsequently, this trend is reduced due to elastic recovery and lattice reconstruction of the substrate atoms. However, only a small number of fcc and hcp crystal structures change during lower speed impact, which is due to the fact that the impact velocity of

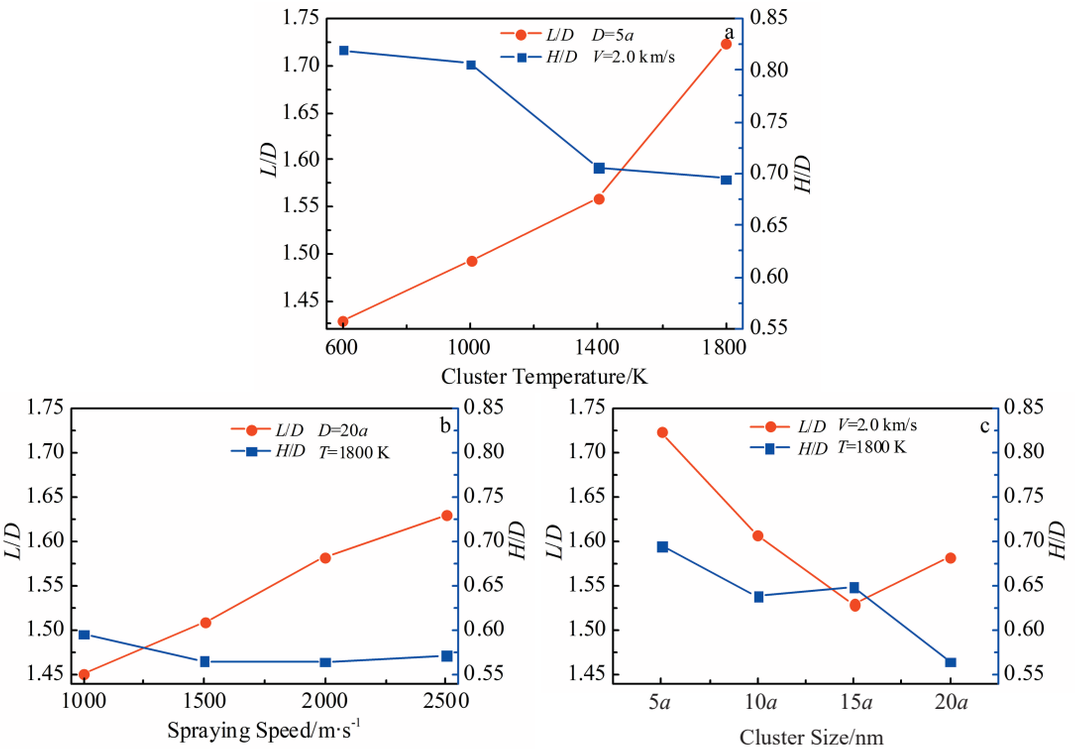

Fig.7 Flattening ratio under different cluster temperatures (a), spraying speeds (b), and cluster sizes (c)

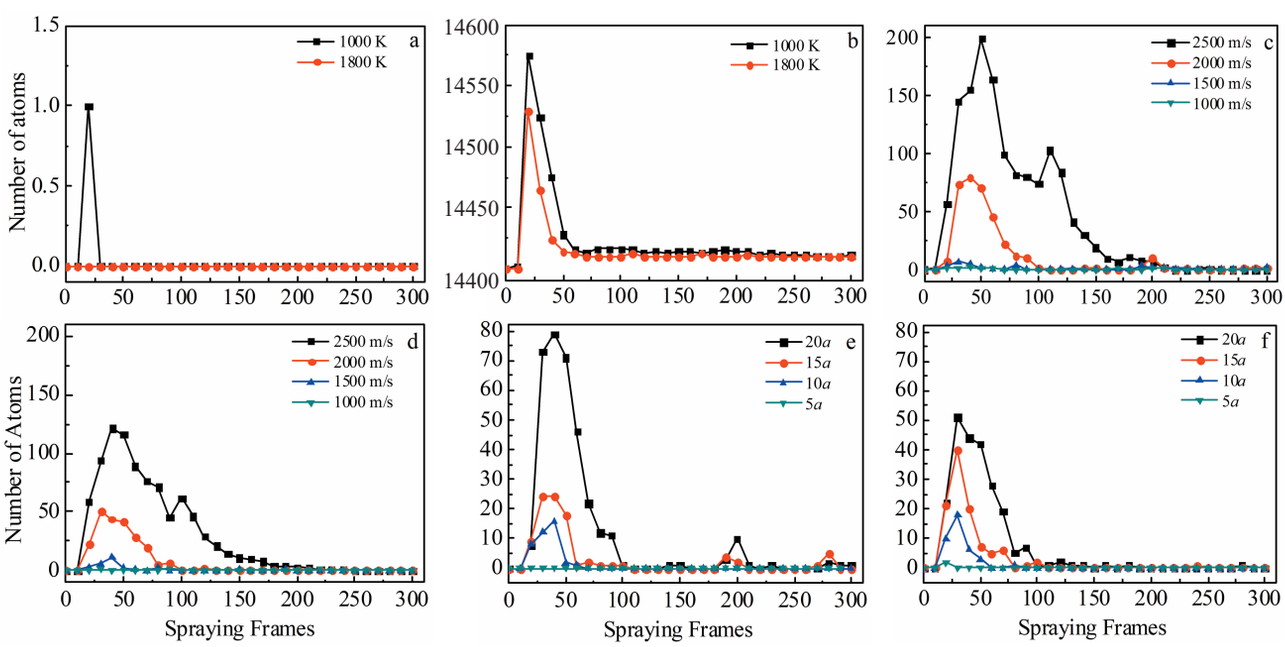

Fig.8 Crystal structure transition curves under different spraying parameters: (a, b) melting temperatures, (c, d) spraying speeds, and (e, f) cluster sizes

clusters on the substrate is lower and there is insufficient force to activate more slip systems. Therefore, there are only a small number of atom transitions. Fig. 8e and 8f show the crystal structure transition curves of fcc and hcp structures, in which the black, red, blue and green indicate that the cluster sizes are 20*a*, 15*a*, 10*a*, and 5*a*, respectively. During the spraying

process, with the increase of cluster size, the number of substrate atomic structure increases. At the same time, it takes longer for the substrate atoms to undergo elastic recovery and lattice reconstruction. It can be explained that the large size cluster itself contains a large number of atoms and has a wide contact area with the substrate during the spraying process, resulting in a large number of lattice structure transitions of the substrate atoms.

2.3.2 Subsurface

With different process parameters, the subsurface defects of the thermal spraying substrate are quite different. Fig.9 shows the distribution of subsurface defects under different process parameters, in which Fig.9a~9h correspond to 1~8 groups of process parameters, respectively. The defect atoms in Fig.9 are identified by CNA technology, in which the normal bcc is deleted, and the red, green and gray atoms are hcp, fcc and other atoms, respectively. Comparing Fig.9a with Fig.9b, it is found that the effect of completely molten cluster on the substrate is smaller than partially molten clusters. It is observed from Fig. 9b~9e that the subsurface damage of substrate increases with the increase of cluster size and a small number of defects are produced, such as vacancy and atomic cluster. From Fig. 9e~9h, it can be seen that the speed has a great influence on the subsurface of the substrate. A large number of vacancies and atom clusters are generated in the subsurface of the substrate at a spraying speed of 2500 m/s. Such a phenomenon indicates that the high spraying velocity activates more slip systems and causes more defects in the substrate, which has a great influence on the performance of the substrate itself. Impact velocity study reveals that a range of 2000 m/s of impact velocity is optimal for achieving uniform and dense coating for the conditions used in this simulation. Maintaining impact velocity within an optimal range is critical during the thermal spray process. Besides, the individual atoms in Fig.9 are left over from the evolution of the substrate structure during spaying.

2.4 Thermal spraying tensile testing

Tensile tests were performed to evaluate the quality of the specimen, and the stretch tests were performed along the *X*-axis with the perfect substrate, the crack substrate and the repaired substrate. The model is shown in Fig.10. Mechanical properties of nanoscale thermal spraying were further investigated by the substrate tension, and the tensile stress-strain curves are shown in Fig. 11. Specimens deform and experience the elastic and plastic deformation. All the three curves exhibit a quasi-linear stress-strain behavior up to their peak stress points where an abrupt stress drop is observed, which is aroused by the rapid crack propagation. The peak stress of perfect substrate, crack substrate and repaired substrate are 2.82, 2.43 and 2.71 GPa, respectively. It can be seen that thermal spraying can significantly repair the substrate, but it cannot reach the strength of perfect substrate, because the coating of thermal sprayed clusters on the substrate will produce a small amount of defects.

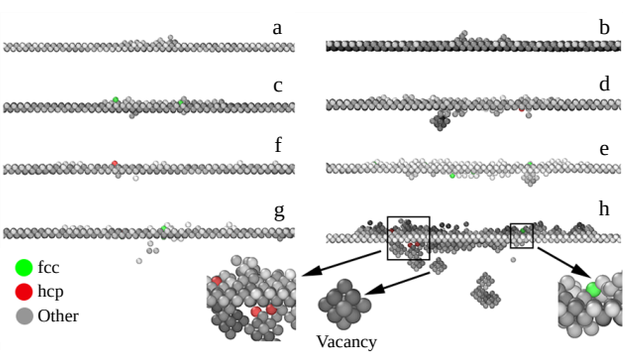

Fig.9 Defect distribution in subsurface of the substrate under different spraying parameters (9a~9h correspond to 1~8 groups of process parameters in Table 2, respectively)

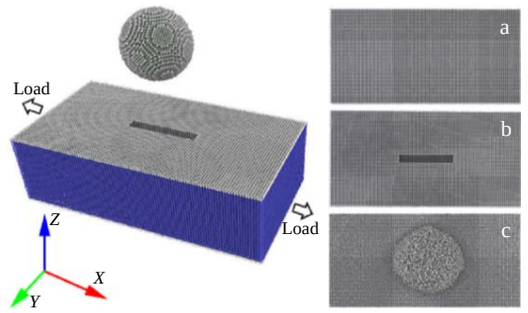

Fig.10 Simulation model of perfect substrate (a), crack substrate (b), and repaired substrate (c)

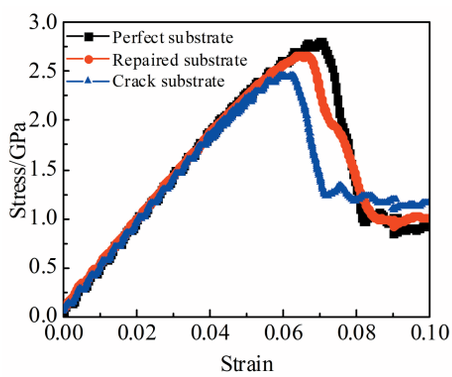

Fig.11 Tensile stress-strain curves for the substrate at three different states

3 Conclusions

1) On the nanoscale, the melting temperature of clusters with different sizes varies, and the outer layer of small clusters is more likely to reach the melting point firstly. With the increase of clusters, the melting point of the outer layer increases. The melting temperature of Ni clusters in molecular dynamics is about 1800 K.

2) During the whole process of impacting the substrate, the atoms in the outer layer of the cluster have good fluidity. Common neighbor analysis reveals that the extruded atoms in the substrate are in a shape of “mountain”. According to the analysis of the flattening ratio of clusters, the coating effect of fully melted clusters is good, and the spraying speed has a great influence on the flattening ratio of clusters.

3) The thermal spraying process has little damage to the substrate. Under different process parameters, with the increase of spraying speed and cluster size, the number of crystal structure transformation of fcc and hcp increases, and there are different point defects. Among them, the defect of the subsurface depends significantly on the impact velocity. At 2500 m/s, there are a large number of defects such as vacancy and cluster in the substrate. When the cluster is completely melted and the spray speed is 2000 m/s, the thermal spraying effect is the best. Therefore, there is a critical spraying speed mechanism in thermal spraying.

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工艺参数对Ni/Fe金属热喷涂影响的分子动力学模拟

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摘　要：采用分子动力学模拟方法研究不同工艺参数下热喷涂材料的沉积现象。模拟温度、团簇尺寸和喷涂速度对Fe基体上Ni团簇沉积的影响，分析团簇的形貌和基底的亚表面损伤。结果表明，在Ni团簇升温过程中，熔点随团簇尺寸增大而增高，Ni团簇在1800 K左右完全熔融。喷涂过程中，基体因冲击力至无序原子呈“山”型。此外，喷涂速度在沉积过程中起重要作用。在较低喷涂速度下，基体的展平比较低，但在较高喷涂速度下，基体受团簇冲击后会出现空位和原子团簇等缺陷。因此，热喷涂过程存在临界喷涂速度机制。

关键词：热喷涂；团簇温度；基体缺陷；团簇形貌；分子动力学

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