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SIMULATING MULTI-PARTICLE DEPOSITION BASED ON CEL METHOD: STUDING THE EFFECTS OF PARTICLE AND SUBSTRATE TEMPERATURE ON DEPOSITION

The **subject matter** of this study is to use numerical simulation methods to study the influence of the temperature of particles and substrates on the post-deposition coating during the multi-particle deposition process of cold spray. The **goal** is to study the temperature of Al6061 particles and the temperature of the substrate, which are factors that have a greater impact on the deposited coating, and to observe the shape of the coating and the temperature distribution of the cross-section of the substrate after deposition. The tasks to be solved are as follows: use Python scripts to model multi-particles, generate and randomly assign positions according to particle size distribution in the Euler domain, and establish a cold spray multi-particle collision model to simulate the process of cold spray deposition. The **following methods were used**: The influence of temperature and substrate temperature on the deposited coating was studied through a single variable method; the Coupled Eulerian Lagrangian (CEL) method was used to simulate the collision process of cold-sprayed Al6061 multi-particles. The following **results** were obtained: changing the temperature of Al6061 particles has a more obvious control effect on the porosity of the deposited coating; after particles of different temperatures impact the constant-temperature substrate, the high-temperature area on the surface of the substrate is mainly located at the junction of pits; after the particle temperature reaches 650K, the coating changes after deposition are no longer significant, indicating an optimal temperature range for Al6061 particle deposition; increasing the temperature of the substrate can increase the depth of particle deposition on the substrate; at the same time, it serves as a reference basis for further using the CEL method to predict the porosity of the Al6061 coating. **Conclusions**. The scientific novelty of the results obtained is as follows: 1) powder preheating can effectively reduce the porosity of Al6061 coating; 2) the CEL method has good robustness and is used to simulate cold spray multi-particle deposition to monitor the porosity of the coating, which cannot be achieved by the SPH and ALE methods.

Keywords: cold spraying technology; CEL; Al6061; temperature; multi-particle deposition; substrate.

1. Introduction

Cold spray technology is a solid-state deposition technology that originated in the 1980s [1]; the particles accelerate to 400-1200 m/s in the Laval nozzle and then directly impact the surface of the substrate, eventually forming a layer on the surface of the substrate uniform thin coating [2, 3]. What happens to particles during the deposition process is physical reaction, which is mainly the plastic deformation of the particles during the deposition process [4, 5]. During the deposition process, the residual stress is the result of particle/substrate and particle/particle interaction, and finally in the substrate a dense coating is formed on the material; during this process, the interaction between particles continuously compresses the residual stress. This process helps to improve the fatigue resistance and high strength properties of the coating, thereby improving the performance of the part surface [6,7].

Cold spray technology is often used as the main way to repair surface damage and improve performance of materials in the aviation field [8-10]; In the actual spraying process, the inevitable defect is the porosity of the coating. Studying the influencing factors of coating porosity has always been the focus of researchers. Using numerical simulation methods to study coatings can satisfy the prediction of coating performance and is more economical. The current mainstream methods for simulating the cold spray deposition process include the SPH method, the ALE method and the Coupled Eulerian Lagrangian (CEL) method. The SPH method is a meshless adaptive Lagrangian calculation method, which is mostly used to simulate ultra-high-speed collisions. The ALE method combines the characteristics of pure Lagrangian analysis and Eulerian analysis. It is often used to simulate solids and fluids; However, it cannot well characterize the results after spraying when the particles are extremely deformed during the cold spraying process. The CEL

method has higher accuracy and robustness than the above two methods, and is currently a better method for simulating the multi-particle deposition process of cold spray. Especially for the situation where particles undergo large deformation, large displacement and large strain during deposition; The advantage is that the particles are wrapped in an Eulerian domain, which avoids the need for remeshing and highly distorted elements. Saleh [11] used the SPH method to simulate the impact model of single-particle and multi-particle Al6061 particles on the Al6061 substrate, and further analyzed the residual stress distribution by studying the deposition process of Al6061 particles on the Al6061 substrate. Lin [12] used ALE to simulate the evolution of residual stress during cold spraying of Al6061 particles on an Al6061 substrate. Interfacial bonding is one of the important factors in the numerical simulation of residual stress evolution in cold spraying. Song [13] used the CEL method to simulate the deposition process of Ti6Al4V particles on the Ti6Al4V substrate to study the effects of the temperature and speed of the particles on the porosity of the coating. MacDonald [14] used the CEL method to study the effect of temperature on the flattening rate of a single particle after it hits the substrate. Xie [15] used the CEL method to simulate and study the deformation level of the substrate surface after different particle temperatures hit the substrate. Zahiri [16] simulates the impact of a single Cu particle on an Al substrate through the CEL method, and studies the deformation effect after particle temperature and velocity collision; The above are all simulations based on single particle collisions; Single particle collision cannot fully express the structure of the entire coating; Therefore, the multi-particle collision model is the closest to the cold spray process; thus enabling numerical simulation methods to predict the performance of new coatings.

This article proposes a multi-particle deposition model to simulate the deposition process of Al6061 particles on the Al6061 substrate; Modeling of Al6061 multi-particle model through Python script; Use the CEL method to establish a multi-particle deposition model, embed the multi-particle model into the multi-particle deposition model, and simulate the cold spray process; Single factor analysis was used to further observe the shape of the coating and the temperature distribution on the surface of the substrate after deposition by changing the temperatures of the particles and the substrate, as well as the effect of temperature on porosity.

2. Experimental/Theoretical Details

2.1. Particles Model and Euler domain

A typical particle size distribution measured using a microvolume laser powder analyzer is shown in Figure 1.

The cumulative probability distribution of the particle sizes shown is estimated by a lognormal function.

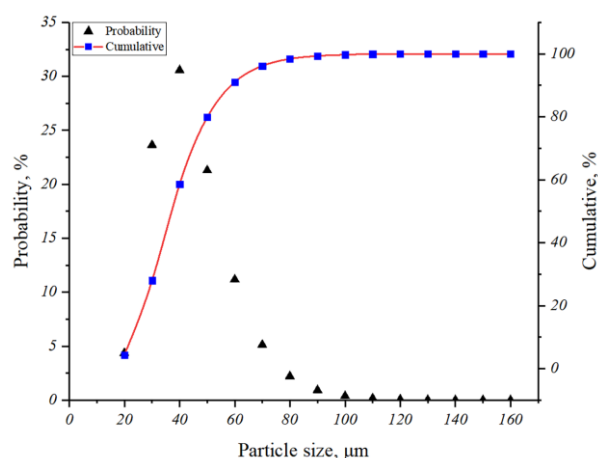


Fig. 1. Particle size distribution and cumulative distributions

In order to accurately represent the actual cold spray process, this article generates particles by uniformly sampling mass fraction parameters; The position coordinates of each particle are randomly assigned within the Euler domain; 200 Al6061 particles with a diameter of 20-70 microns are modeled through a Python script. It is necessary to ensure that each particle is distributed independently and there is no contact between particles to meet the conditions for simulated spraying. The Euler domain must wrap all particles. The Euler domain is set to the long method. The advantage is that it can generate a uniform hexahedral structure mesh [15]. Some scholars set the Euler domain as a cylinder [17]. The mesh generated by the cylinder is mainly a tetrahedral mesh. It is difficult to converge during the calculation process.

2.2. Material model

Simulate the multi-particle deposition process through the CEL method. Assuming that the material is isotropic, an inelastic heat share parameter needs to be set, and its properties are shown in Table 1. Plastic hardening uses the Johnson-Cook plasticity model to describe the dependence of material behavior on rate and temperature [18], and adds a hardening Johnson-Cook model representation.

The parameters of the Johnson-Cook plasticity model are obtained by least squares curve fitting of the deformed particle shapes measured in the ALIPIT test [19]. The ratio of plastic energy converted into heat is 0.9 [20]. The corresponding thermal response of a material is defined by its temperature-dependent thermal properties, such as Specific heat, Thermal conductivity and Thermal conductivity coefficient [21].

Table 1
Material properties for Al6061

Properties	Parameters	Value
General	Density, $\rho/(\text{kg} \cdot \text{m}^{-3})$	2700
	Specific heat C_p , $(\text{J/kg} \cdot \text{K})$	1009
	Thermal conductivity coefficient λ , $(\text{W/m} \cdot \text{K})$	155
	Melting temperature, K	925
	Inelastic heat fraction	0.9
	Elastic modulus, GPa	69.11
	Poisson's ratio, ν	0.331
	Shear modulus, GPa	25.9
Johnson-Cook model	A (Mpa), B (Mpa), n, m	270, 154.3, 0.239, 1.42
	Reference strain rate	1
	Reference temperature, K	298
	C_1, C_2, ϵ_c	0.002, 0.0029, 597.2
Failure initiation	d_1, d_2, d_3, d_4, d_5	-0.57, 1.45, 0.47, 0.011, 1.6

2.3. Particle velocity, temperature and predefined fields

The work of this article investigates the effect of particle and substrate temperature on post-deposition coatings. Reference [4] gives all Al6061 particles velocity value of 585 m/s in this article to ensure that all Al6061 particles can be uniformly ordered particles/substrates, and particle/particles deposit. As stated above, all particles are included in the Euler domain, so the essence is that all particles flow in the Euler domain, and the deposition process will be completed in the Euler domain.

This article controls the temperature range of Al6061 particles and Al6061 substrate to 400K-700K, and increases the temperature by 50K for each working condition, and studies the effects of different temperature working conditions on the post-deposition coating. A coupled temperature-displacement dynamic step with an appropriate time period is assigned to track the entire multi-particle impact process from the start of the simulation to the complete stop of all particles, with a total range of 970 ns to 1000 ns; where the contact model

adopts dynamic, temperature-displacement, Explicit model; define tangential and normal behavior as well as friction coefficient. Assign materials to all particles in the predefined field; use the discrete field volume fraction tool to set parameters for all particles in the Euler domain, and calculate the volume fraction of all particles in the Euler domain through field data to ensure that later the calculation proceeds smoothly.

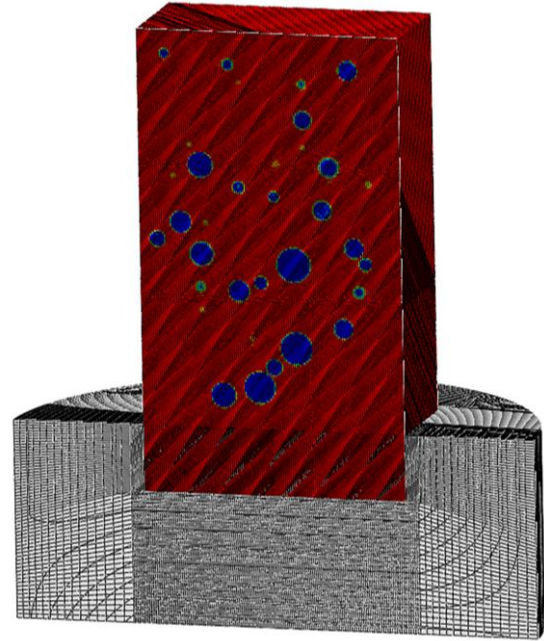
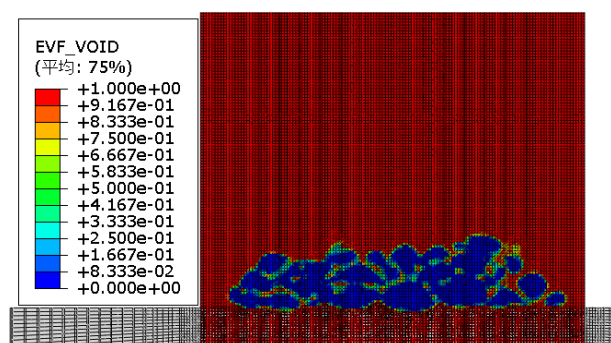


Fig. 2. Half-section view of model assembly and meshing

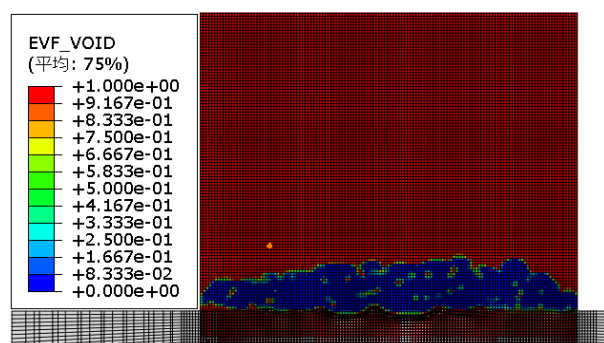
3. Results and Discussion

Single factor influence was used to study the influence of the temperature of Al6061 particles and substrate on the deposited coating. Figure 3 shows a cross-sectional view of the Euler volume fraction of the coating after deposition of particles and substrates in the temperature range of 400K-700K; EVF void value, the red EVF void has a value of 1, indicating the void area, the value of blue EVF void is 0, which means that the element is filled with material; observing the value of EVF void can characterize the porosity of the coating.

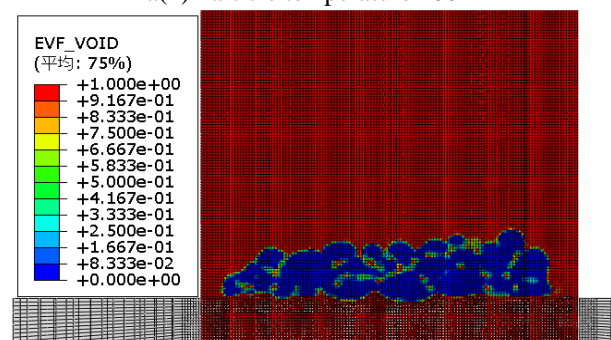
Observing the thickness of the coating, it can be seen that changing the particle temperature has a more obvious control effect on the porosity of the coating. Increasing the temperature of the particles is beneficial to the deposition process; the substrate temperature is constant, and increasing the temperature of the particles can reduce the porosity of the coating increases the density of the deposited coating. By simulating the deposition of multiple particles on a substrate using the CEL method, the porosity of the coating after deposition can be monitored.



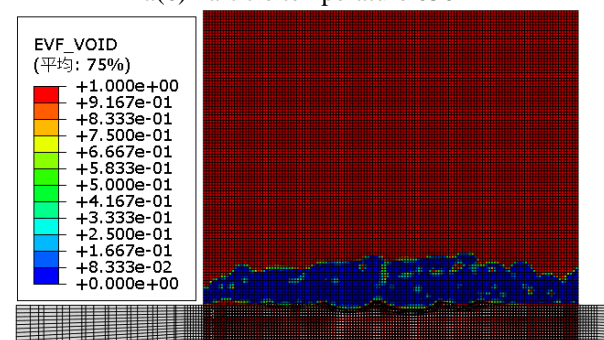
a(1) Particle temperature 400K



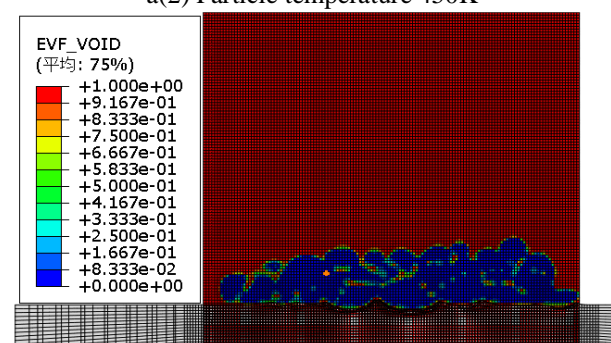
a(6) Particle temperature 650K



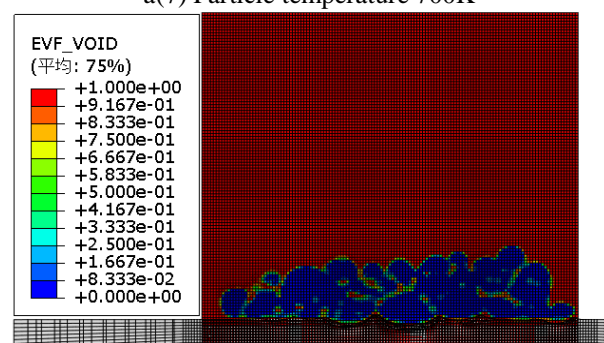
a(2) Particle temperature 450K



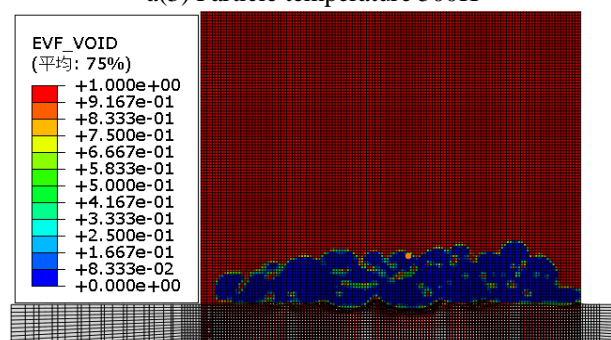
a(7) Particle temperature 700K



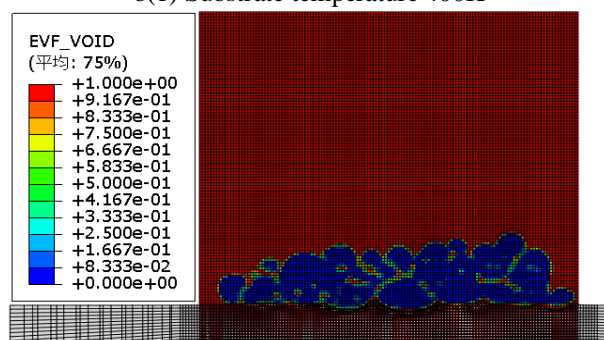
a(3) Particle temperature 500K



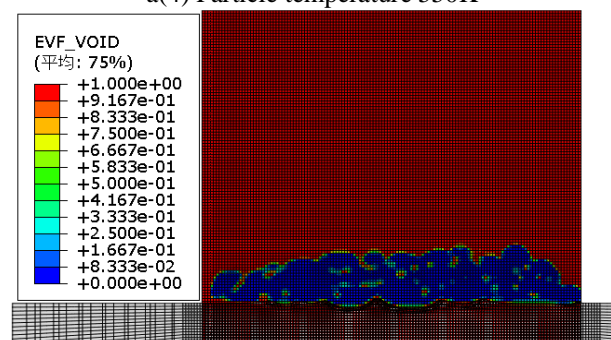
b(1) Substrate temperature 400K



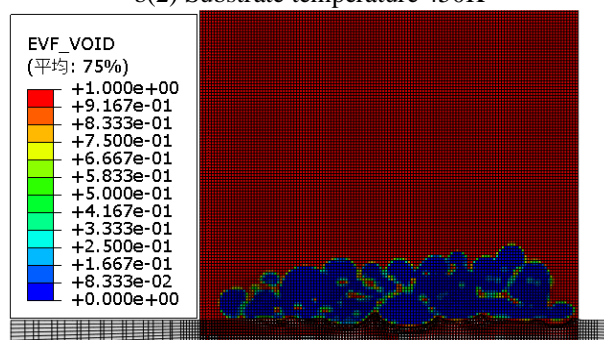
a(4) Particle temperature 550K



b(2) Substrate temperature 450K



a(5) Particle temperature 600K



b(3) Substrate temperature 500K

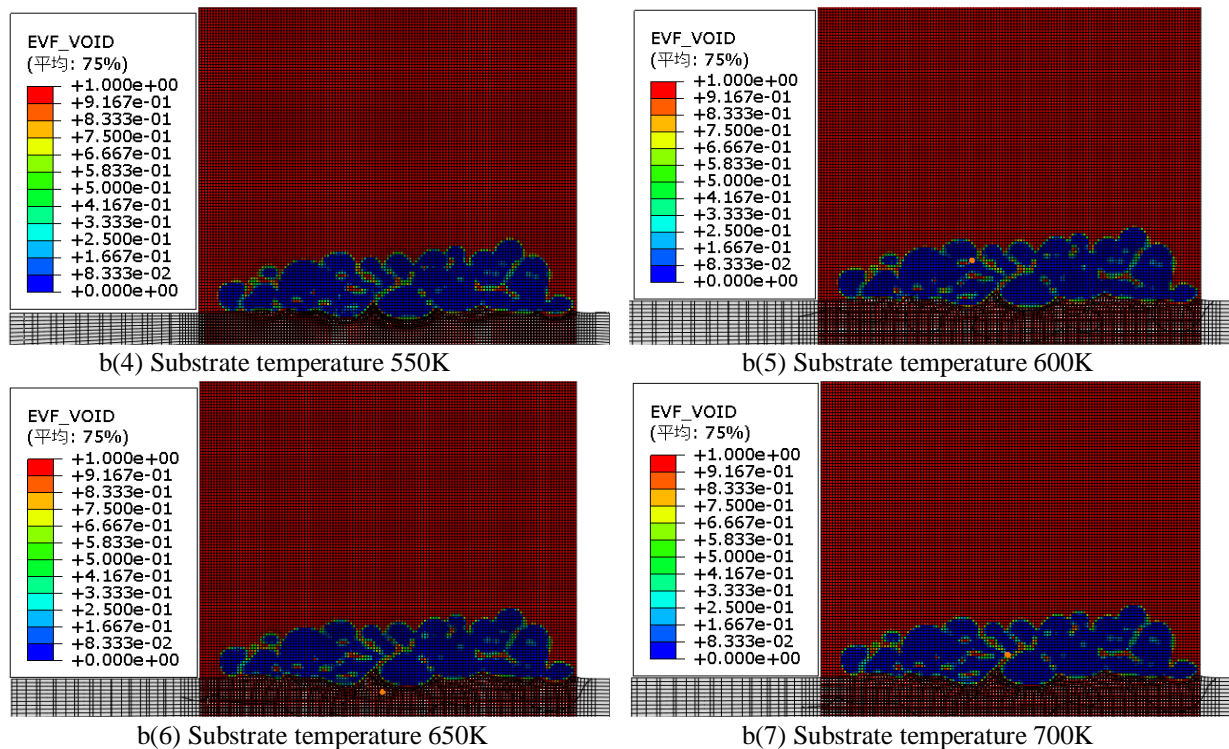


Fig. 3. Cross-sectional view of the Euler volume fraction of the coating after deposition of particles and substrate in the temperature range of 400K-700K;

(a1-a7): Substrate constant temperature 400K;

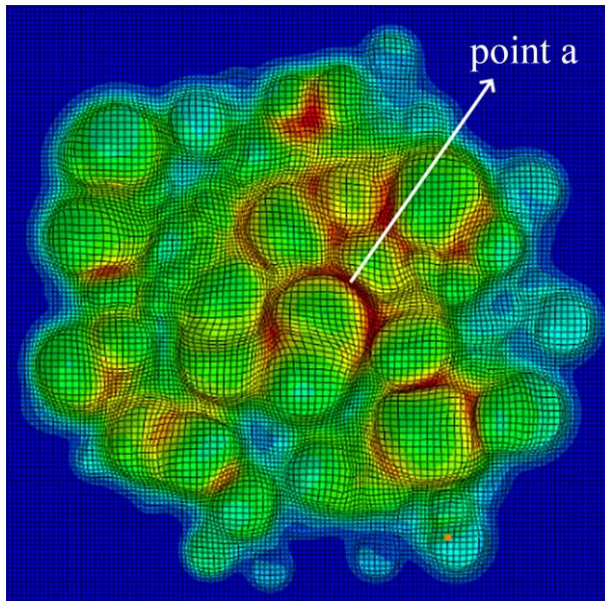
(b1-b7): Particle constant temperature 400K

Figure 4 shows the temperature distribution on the surface of the substrate after particles of different temperatures impact the constant-temperature substrate. Figure 4 shows that there are many pits on the surface of the substrate. The high-temperature areas of the substrate after the deposition are mainly distributed in pits and pits. The junction can also be explained as: the high temperature zone is mainly located at the extrusion part between particles; during the deposition process, the particles impact the surface of the substrate to form pits, and the junction of the pits generates a large amount of heat due to the high-speed extrusion of the particles, causing the substrate to heat up rapidly, and the temperature is higher than the initial temperature of the substrate, which is conducive to the mechanical interlocking between the particles and the substrate.

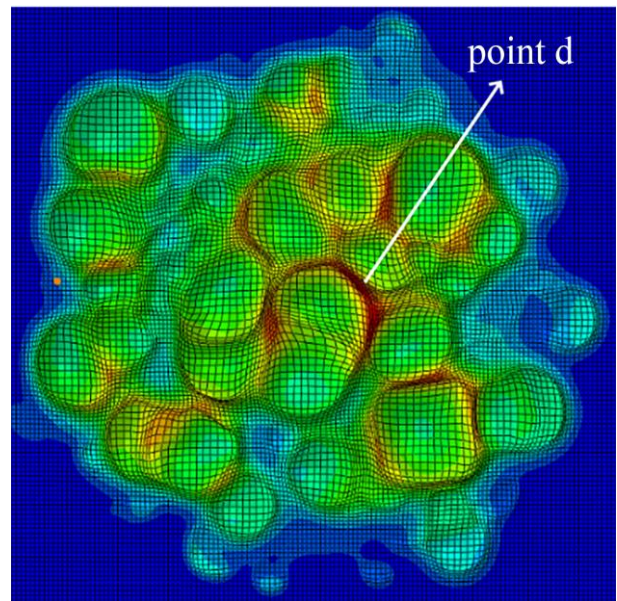
In Figure 4, select seven points a, b, c, d, e, f, and g on the same part of the substrate surface, and observe the temperature changes of these five points during the deposition process under different temperature conditions are shown in Figure 5; from the temperature curve of the substrate surface, it can be seen that the temperature of the substrate surface dropped briefly, then rose sharply and then dropped again. Due to a large number of particles continuously hit the surface of the substrate, causing the surface of the substrate to heat up rapidly. This process

is a deposition between the particles and the substrate, and the temperature of the substrate reaches a peak during this process; when some particles complete the deposition on the substrate, the subsequent particles continue to hit the particles that have completed the deposition. This process is a deposition between particles. This process transfers less heat to the substrate, so the temperature of the substrate decreases. During the temperature drop of the substrate, the temperature of the substrate decreases. An oscillation curve appears, because the subsequently deposited particles continue to deposit with the previous coating. And a small part of the heat generated during the deposition is transferred to the substrate, causing the temperature drop rate of the substrate to change. When the thickness of the coating reaches a certain value, the particles very little temperature is transferred to the substrate, so the surface temperature of the substrate decreases steadily.

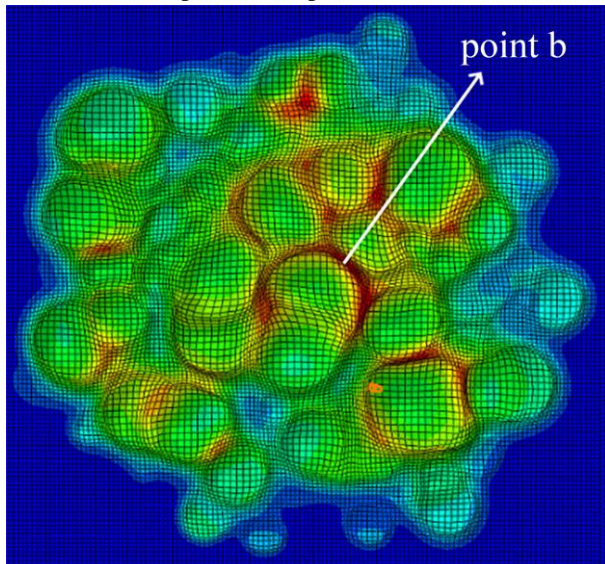
Figure 6 shows Cross-sectional view of coating temperature after deposition of particles and substrate in the temperature range of 400K-700K; (a): Substrate constant temperature 400K; (b): Particle constant temperature 400K. It can be seen from Figure 6 that the high-temperature area of the coating after the deposition of the particles is mainly located at the contact area between the particles and the substrate.



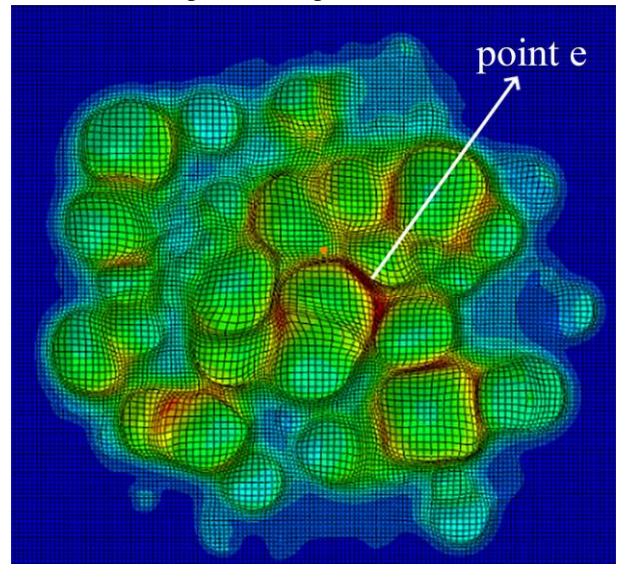
a: particle temperature 400K



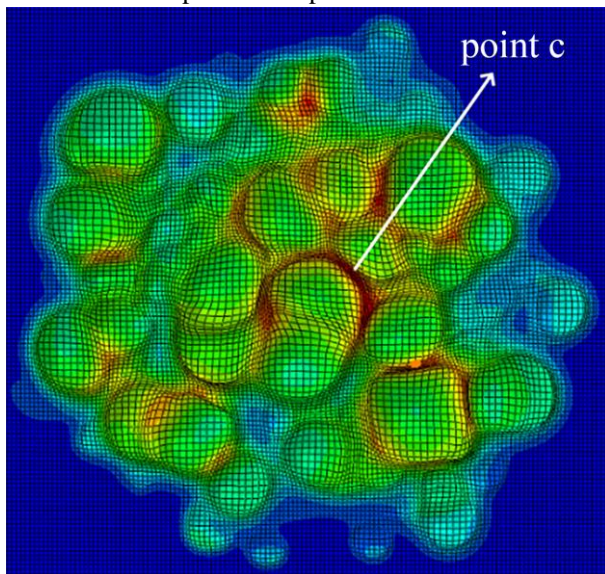
d: particle temperature 550K



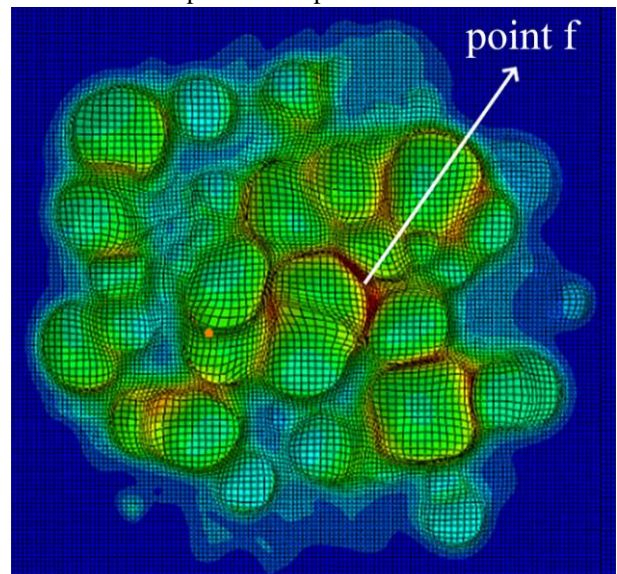
b: particle temperature 450K



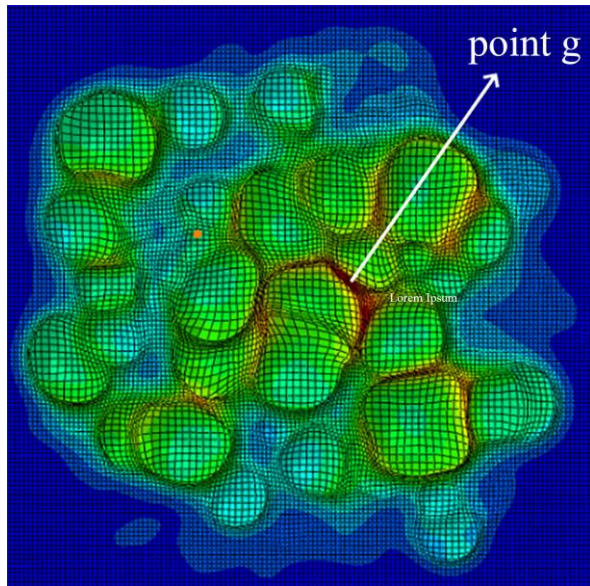
e: particle temperature 600K



c: particle temperature 500K



f: particle temperature 650K



g: particle temperature 700K

Fig. 4. Temperature distribution on the surface of the substrate after Al6061 particles of different temperatures impact the constant-temperature substrate 400K

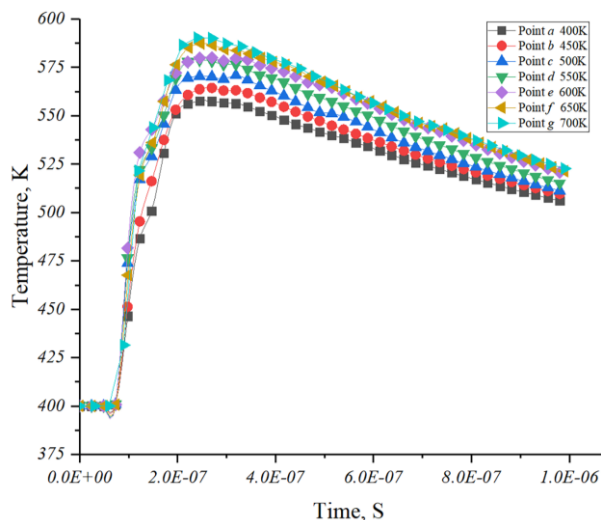


Fig. 5. Temperature changes over time at selected 7 points on the substrate surface

As the temperature of the particles increases, the high-temperature area also increases; by observing the thickness of the coating after deposition, it is better to change the temperature of the particles than to change the temperature of the substrate. When the substrate temperature is constant, after the particle temperature reaches 650K, the coating changes after deposition are no longer significant, which shows that there is an optimal temperature range for Al6061 particle deposition. Observing the temperature cross section of the substrate, it can be seen that

the temperature of the particles does not have a significant impact on the surface of the substrate after deposition; during the deposition process, it shows that the temperature generated by the deposition between particles mainly acts between particles. As can be seen from Figure 6, the temperature of the substrate has no obvious effect on the coating. Because during the deposition process, most of the mechanical bite between particles occurs; The changes that affect the temperature of the substrate are mainly particles that deposit with the substrate.

Figure 7 shows Temperature cross-section of the substrate after deposition of particles and substrate in the temperature range of 400K-700K; (a): Substrate constant temperature 400K; (b): Particle constant temperature 400K. It can be seen from Figure 7 that the temperature of the substrate is constant, Increasing the temperature of the particles does not have a significant effect on the temperature of the substrate after deposition. Based on the analysis of Figure 5, the rapid heating stage of the substrate is caused by the direct impact of particles on the substrate. When the subsequent particles deposit with the particles, the heating of the substrate is not significant. The results are the same as shown in Figure 6. The temperature of the particles is constant. Increasing the temperature of the substrate can increase the deposition depth of the particles on the substrate, which is beneficial to the combination of the substrate and the coating after deposition. when the substrate temperature exceeds 650K, sputtering occurs on the surface of the substrate. Excessive temperature of the substrate causes the material to soften, and the high temperature zone is mainly located at the connection of the pits, which is the same as the result in Figure 4.

Conclusions

This article uses the CEL method to simulate the process of cold spraying to simulate the deposition of multiple particles on the Al6061 substrate. By studying the effects of Al6061 particles and substrates at different temperatures on the deposition results, the shapes of the coating and substrate after deposition are observed, as well as the coating and the temperature distribution of the substrate cross section; Currently the CEL method can accurately simulate the multi-particle deposition method of cold spray deposition.

1. Changing the particle temperature has a more obvious control effect on the porosity of the deposited coating, thereby improving the density of the deposited coating; preheating the particles can effectively reduce the porosity; simulate multi-particles on the base through the CEL method the deposition on the material allows monitoring of the porosity of the coating after deposition, which is not possible with the ALE method.

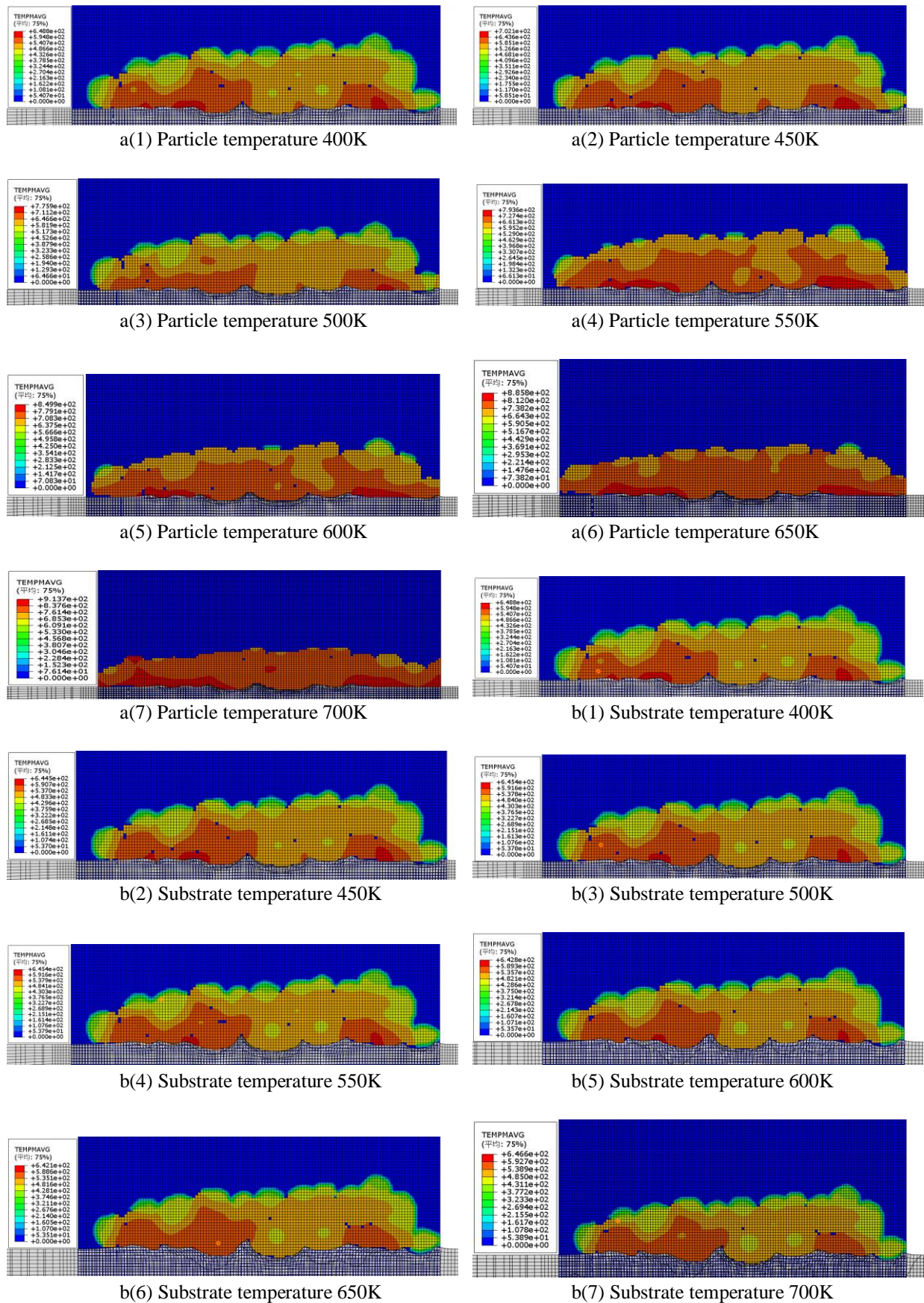


Fig. 6. Temperature cross-section of the coating surface after deposition of particles and substrate in the temperature range of 400K-700K. (a1-a7): Substrate constant temperature 400K; (b1-b7): Particle constant temperature 400K

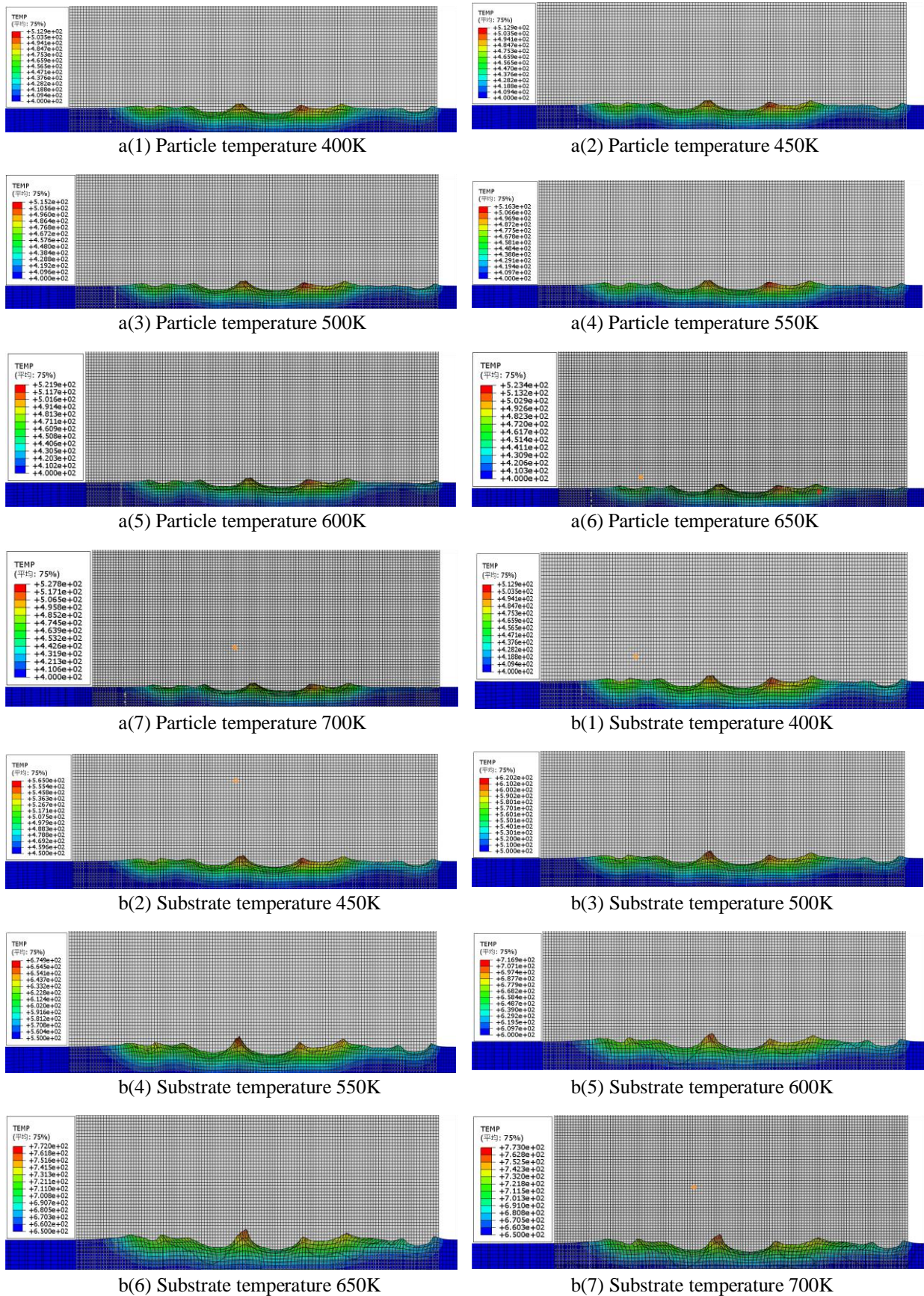


Fig. 7. Temperature cross-section of the substrate after deposition of particles and substrate in the temperature range of 400K-700K. (a1-a7): Substrate constant temperature 400K; (b1-b7): Particle constant temperature 400K

2. After particles of different temperatures impact the constant-temperature substrate, the high-temperature area on the surface of the substrate is mainly located at the junction of pits; this is the result of high-speed extrusion between particle depositions. The latter particles have little effect on the temperature change of the substrate.

3. When the particle temperature reaches 650K, the coating changes after deposition are no longer significant, indicating that there is an optimal temperature range for Al6061 particle deposition; therefore, excessively increasing the temperature of the particles is not the best solution.

4: Increasing the temperature of the substrate can increase the depth of particle deposition on the substrate, which is beneficial to the combination of the substrate and the coating after deposition.

5. It is recommended to use the CEL method to simulate the multi-particle deposition process in the later stage, so as to calculate and predict the porosity of the Al6061 coating. Multi-parameter coupling effects were used to study the porosity of Al6061 coating.

Contribution of authors: conceptualization – **Kun Tan, Wenjie Hu; Oleksandr Shorinov; Yurong Wang;** Material parameter model – **Yurong Wang;** Multi-particle model – **Oleksandr Shorinov;** Multi-particle deposition model – **Kun Tan, Wenjie Hu;** Numerical simulation work – **Kun Tan;** analysis of results – **Kun Tan.**

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, author ship or otherwise, that could affect the research and its results presented in this paper.

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The research was conducted with financial support.

Data availability

The work has associated data in the data repository.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence methods while creating the presented work.

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All the authors have read and agreed to the published version of this manuscript.

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МОДЕЛЮВАННЯ ОСАДЖЕННЯ БАГАТЬОХ ЧАСТИНОК НА ОСНОВІ МЕТОДУ CEL: ВИВЧЕННЯ ВПЛИВУ ТЕМПЕРАТУРИ ЧАСТИНОК І ПІДКЛАДКИ НА ОСАДЖЕННЯ

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Предметом статті є використання методів чисельного моделювання для вивчення впливу температури частинок і підкладок на покриття після осадження під час процесу осадження багатьох частинок холодним розпиленням. **Мета** полягає в тому, щоб вивчити температуру частинок Al6061 і температуру підкладки, який фактор має більший вплив на нанесене покриття, а також спостерігати за формою покриття та розподілом температури в поперечному перерізі підкладки після нанесення. **Завдання**, які необхідно вирішити: використовувати сценарії Python для моделювання багатьох частинок, генерувати та випадково призначати позиції відповідно до розподілу частинок за розмірами в області Ейлера; створити модель зіткнення багатьох частинок холодного розпилення для імітації процесу осадження холодного розпилення. Використані методи: Вплив температури та температури підкладки на нанесене покриття вивчався за допомогою методу однієї змінної; метод CEL був використаний для моделювання процесу зіткнення холодно розпилених багато частинок Al6061. Було отримано наступні результати: зміна температури частинок Al6061 має більш очевидний контрольний вплив на пористість нанесеного покриття; після того, як частинки з різною температурою впливають на підкладку з постійною температурою, високотемпературна область на поверхні підкладки в основному розташована на стику ямок; Коли після того, як температура частинок досягне 650 K, зміни покриття після осадження більше не є значними, що вказує на те, що існує оптимальний діапазон температур для осадження частинок Al6061; підвищення температури підкладки може збільшити глибину осадження частинок на підкладці; Водночас він служить еталонною базою для подальшого використання методу CEL для прогнозування

пористості покриття Al6061. **Висновки.** Наукова новизна отриманих результатів полягає в наступному: 1) попереднє нагрівання порошку може ефективно зменшити пористість покриття Al6061; 2) метод CEL має добру надійність і використовується для імітації осадження багатьох частинок холодним розпиленням для моніторингу пористості покриття, чого неможливо досягти методами SPH і ALE.

Ключові слова: технологія холодного напилення; CEL; Al6061; температура; багаточастинкове осадження; підкладка.

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