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Numerical Investigation on Effects of Interactions Between Particles on Coating Formation in Cold Spraying

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In this study, an investigation on the effects of interactions between copper particles on coating formation was conducted by using a finite element analysis method to clarify the bonding mechanism in cold spraying. The predicted results reveal that the interactions between particles significantly affect the particle deformation and thus coating formation. When the initial parallel distance between particles is short, particles compress with the generation of gap between them. For the vertical case, the initial distance between particles also has an important effect. Short vertical distance makes the subsequent incident particle deform so weakly that the bonding performance is probably not strong enough to form a coating. Furthermore, for successive impacting particles, the subsequent incident particles will tamp the former deposited particles, causing the coating to be little porous near the surface and denser inside the coating.

Keywords cold spraying, high-velocity impact, numerical simulation, particle interactions

1. Introduction

A broad variety of impact phenomena is observed in many cases both in micro- and macro-scales when an object impinges on another one, such as erosive particles colliding with a solid surface at a relatively low velocity ballistic impact and penetration of a macro-body at a higher velocity causing a destruction of the impacted surface (Ref 1-3). However, the metallic particles with a speed ranging from 300 to 1200 m/s can adhere to the impacted surface forming a coating. This process is termed as cold gas dynamic spray (Ref 4, 5). Spray particles (typically <50 μm) are accelerated to a high velocity (ranging from 300 to 1200 m/s) by using a supersonic gas flow from a Laval-type nozzle. A coating is formed through intensive plastic deformation of particles impacting on a substrate at a temperature well below the melting point of spray material. Therefore, cold spray represents a radical deviation from the conventional thermal spray in deposition process. On the other hand, with a lot of advantages, such as the wider choices of metals and alloys as coating materials, the capability of oxygen-free coating, and high deposition efficiency, cold spray has attracted more and more attention from the entire world.

Experimental studies have been intensively conducted to examine the bonding mechanism in cold spraying. The most prevailing hypothesis is that plastic deformation may disrupt thin surface films, such as oxides, and provide intimate conformal contact under high local pressure, thus permitting bonding to occur (Ref 6, 7). Moreover, the critical velocity and deposition efficiency in cold spraying was also studied through experiment by different investigators, and some meaningful conclusions have been obtained (Ref 8-11). Besides, a few studies also focused on the impacting process and deformation behavior of sprayed particles due to the importance of the particle deformation on successful deposition and thus bonding mechanism. Considering the extremely short impacting time scale, it is difficult to experimentally observe the whole deformation process of particles, only the formed coating can be observed through the experimental way. Therefore, the numerical method was always employed to study the particle deformation process as well as the bonding mechanism in cold spraying (Ref 6, 12-17). It has been reported that particle mechanical properties, particle size, incident velocity, and angle play an important role in the deformation behavior and coating formation (Ref 12-16). The effect of calculation settings concerning element type, ALE adaptive meshing, contact interaction, material damage, etc. was also systematically investigated in a recent study (Ref 17). However, most of the previous numerical studies were focused on the single particle impacting on a substrate. The detailed numerical investigations on multiple particles impacting process are still lacking. In actual spraying process, massive particles fall

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down simultaneously and impact on the substrate at a much higher velocity, the interaction between particles cannot be avoided. Hence, in this article, the investigation on the effects of interactions between particles on coating formation was conducted using numerical method.

2. Computational Descriptions

2.1 Numerical Methods

The impact behavior of particles on a substrate was modeled by using an explicit finite element analysis program LS-DYNA (Ref 18). Lagrange formulations were employed in solutions based on mass, momentum, and energy conservation equations. Simulations were solved in conjunction with appropriate boundary conditions and material constitutive model. Compared to the high inertial force from the high-speed carrying flow, all body forces, such as gravity, were neglected. Furthermore, owing to the axial symmetric feature of the impact process, the impacting process was simplified as a two-dimensional (2D) problem as shown in Fig. 1(a), the vertical impacting, and Fig. 1(b), the parallel impacting to save computational resources. All the contact processes were implemented by using an automatic 2D single-surface penalty formulation available in LS-DYNA. The radius and height of the substrate were chosen as 10 times of the particle diameter (20 μm) to ensure the computational accuracy. The meshing was conducted using quad elements with one-point integration, and the grid size for the particle is 1 μm. Nonuniform mesh with minimum grid size of 1 μm was adopted for the substrate domain as shown in Fig. 1. A fixed boundary condition was applied to the bottom plane and a free boundary condition for the others. The initial particle velocity was chosen as 500 m/s.

2.2 Material Model

As for the material model, both the particles and the substrate were described as a Johnson and Cook plasticity model which accounts for strain and strain rate hardening as well as thermal softening. The stresses were expressed according to the Von Mises plasticity model. The yield stress (σ_y) of this material is expressed as follows (Ref 18, 19):

$$\sigma_y = [A + B(\varepsilon_e^p)^N][1 + C \ln \dot{\varepsilon}^*][1 - (T^*)^M] \quad \text{(Eq 1)}$$

where A, B, N, C, and M are material-related constants dependent on materials; ε_e^p is effective plastic strain; and $\dot{\varepsilon}^*$ is effective plastic strain rate normalized with respect to a reference strain rate. T^* is a nondimensional temperature defined as (Ref 18, 19):

$$T^* = \frac{T - T_0}{T_m - T_0} \quad \text{(Eq 2)}$$

where T_m is the melting temperature and T_0 is the reference temperature. A linear Mie-Gruneisen equation of state was employed for the elastic behavior of copper (Ref 18). The mechanical and thermal material properties were assumed to be isotropic. The copper properties used in the simulations are shown in Table 1.

Table 1 Material properties of copper

Material	Copper
Density, kg/m^3	8960
Heat capacity, J/kg·K	383
Thermal conductivity, W/m·K	386
Young's modulus, GPa	124
Poisson's ratio	0.34
A, MPa	90
B, MPa	292
N	0.31
C	0.025
M	1.09
T_m, K	1356
T_0, K	298
Reference strain rate, s^{-1}	1

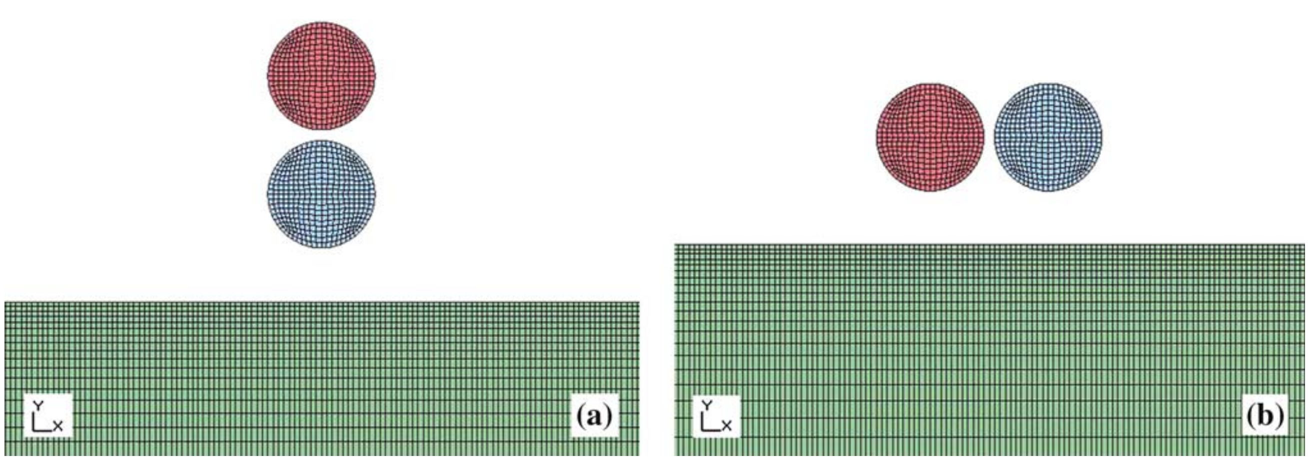

Fig. 1 Computational layouts and mesh: (a) vertical impacting and (b) parallel impacting

3. Results and Discussion

3.1 Effect of Interaction Between Parallel Particles on Coating Formation

Figure 2 shows the simulated results of two parallel copper particles impacting on a copper substrate with initial parallel distances of 0, 2, 4, 6, 8, and 10 μm at 65 ns. It is clear that all of the particles have flattened to form a lens-like shape, which is in good agreement with the experimental observation (Ref 13). However, for the case of the 0 μm initial parallel distance as shown in Fig. 2(a), although metal jets are formed at the surrounding region of the impacting area, an obvious separation is present between two particles. This type of gap is also observed with increasing the parallel distance till 10 μm as shown in Fig. 2(f).

For more examination, the gap width is employed to characterize the interaction between parallel particles. Figure 3 shows the effect of initial parallel distance on the gap width. It is easily found that with increasing the initial parallel distance, the gap width decreases gradually. The maximum value is obtained at the initial parallel distance of 0 μm, amounting to approximately 4.2 μm. When the distance is increased to more than 10 μm, the space between two particles is filled with the substrate material and thus the influence of the interaction between parallel particles can be neglected. The gap width at this circumstance is considered as 0 μm. The reason for this phenomenon can be attributed to the compressive force between particles. When the distance between two particles is so close, particles compress during the impacting process, which results in the generation of the X-axial velocities for both particles at the same time. The high X-axial velocity combines with the Y-axial velocity, causing the original normal incident velocity to deflect a low angle. Meanwhile, owing to the just reverse directions of the X-axial velocity for any group of particles, the deflect angle is also opposite and thus the gap is naturally generated. Figure 4 displays the simulated temporal development of X-axial velocities of two parallel copper particles with different initial distances between them. It is obviously found that the X-axial velocity indeed exists when particles interact with each other during the impacting process. For any group of interacting particles, the direction of X-axial velocity is just opposite. Moreover, it is necessary to notice that with increasing the initial parallel distance, the X-axial velocity declines gradually, which leads to the decrease in gap width.

Furthermore, according to the discussion above, it can be concluded that when the interaction occurs between parallel particles, the impacting process is similar to the low-angle incident process by a single particle. For the case of 0 μm initial parallel distance, the X-axial velocity is about 100 m/s and the equivalent incident angle can be considered as approximately 13°. This value decreases

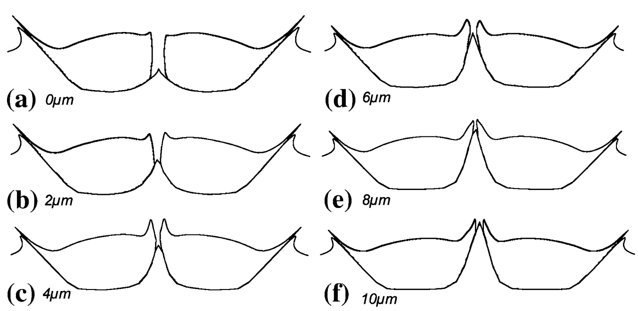

Fig. 2 Contours of two parallel copper particles impacting on a copper substrate with different initial distances at 65 ns

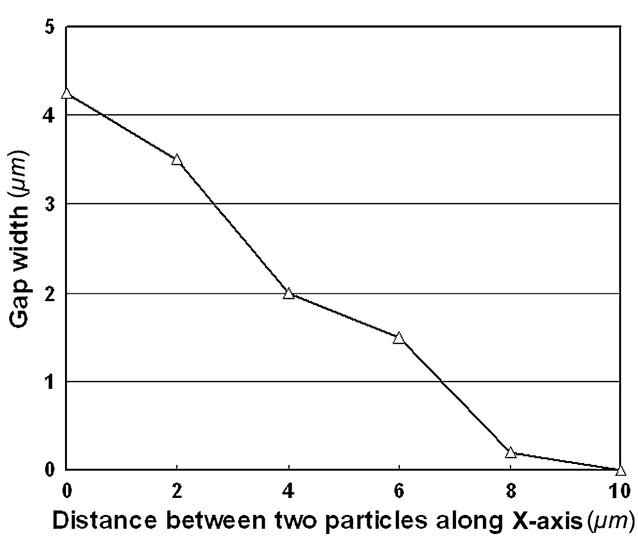

Fig. 3 Effect of initial parallel distance on the gap width between two parallel particles

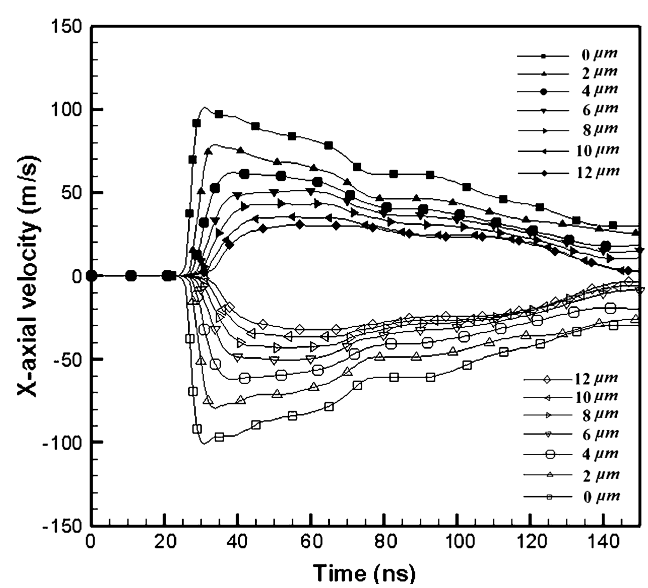

Fig. 4 Simulated temporal development of X-axial velocities of two parallel copper particles under different initial distances between them

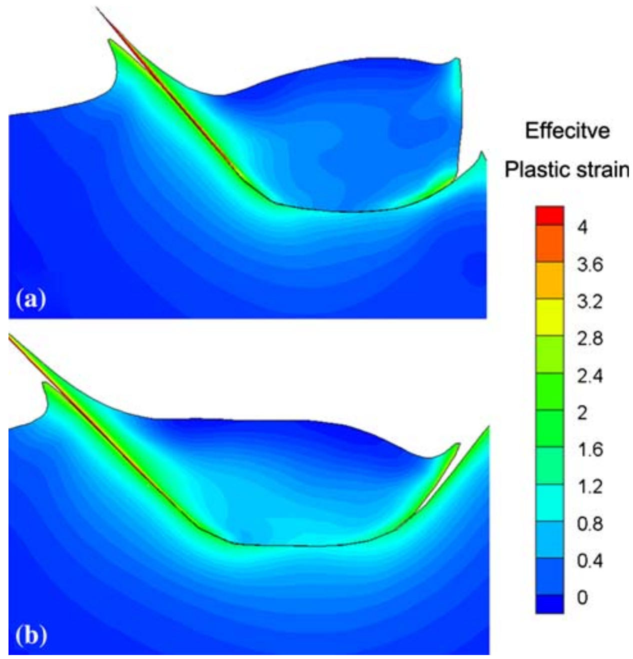

Fig. 5 Contours of the effective plastic strain of: (a) the copper particle with the initial parallel distance of 0 μm and (b) a single copper particle with the incident angle of 13°

with the increase of the initial parallel distance. Therefore, to further verify the correctness of the analysis described above, the contour of effective plastic strain of one copper particle with the initial parallel distance of 0 μm is displayed in Fig. 5. For comparison, the contour of effective plastic strain of a single copper particle impacting on a copper substrate with the incident angle of 13° is also given in Fig. 5. It is clearly seen that both the particles have a similar shape and distribution of effective plastic strain after impacting. The narrow contact zone experiences intensive deformation with the high value at the left side and low value at the right side as well as the bottom. Figure 6 shows the typical experimental result of cross-section morphology of a deformed copper particle impacting on a copper substrate at an incident angle of 20°, conducted by Li et al. (Ref 20). It is obvious that the particle deforms significantly and the jet can be found at left side of the deformed particle, which is consistent with the simulated results.

3.2 Effect of Interaction Between Vertical Particles on Coating Formation

The interaction between vertical particles is also important to the coating formation. In this study, as a first approximation, the initial vertical distance was set at 0 to 5 μm to reduce the calculation time. Figure 7 shows contours of the effective plastic strain of two vertical copper particles impacting on a copper substrate with the initial vertical distances of 0, 1, 2, 3, 4, and 5 μm at 65 ns to examine the effect of interaction between vertical particles on coating formation. It is clearly seen that all of the

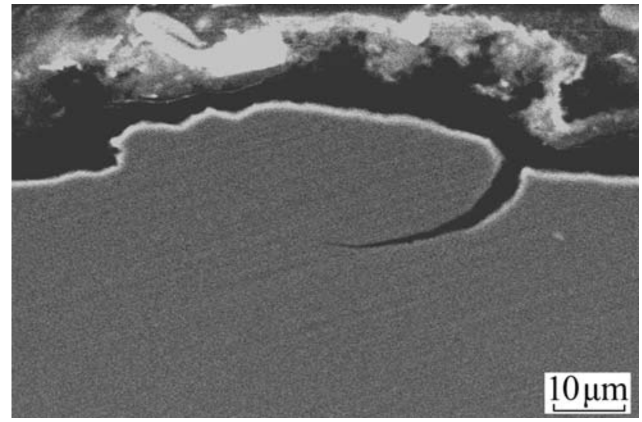

Fig. 6 Typical experimental result of cross-section morphology of a deformed copper particle impacting on a copper substrate at an incident angle of 20° (Ref 20)

former deposited particles experience an intensive deformation accompanying the generation of metal jets and flatten to form a band-like shape instead of a lens-like shape due to the impact of the subsequent incident particle. The maximum plastic strain is found at the lateral sides of each particle. However, for the subsequent deposited particle, the shape presents a significant discrepancy compared with the former one. The subsequent particle with a larger initial vertical distance deforms more intensively than that with a short distance. Figure 8 shows the simulated temporal development of effective plastic strain of the subsequent deposited particle. It is clearly found that the maximum effective plastic strain increases with the progression of impacting. Moreover, with increasing the initial vertical distance, the effective plastic strain also increases obviously, which means more intensive deformation with longer initial vertical distance.

In the previous study (Ref 13), it was found that it is easy to predict the deformation behavior of cold-sprayed particles by the compression ratio (R_c), which is defined as:

$$R_c = \frac{d_p - h_p}{d_p}$$

where h_p is the height of the flattened particle in the impact direction and d_p is the original particle diameter. Therefore, to provide a deep investigation on the effect of vertical interaction on particle deformation, the compression ratio is employed to characterize the plastic deformation of both particles. Figure 9 shows the variation of compression ratio with the initial vertical distance. It is clearly seen that with increasing the initial vertical distance, the compression ratio of the former deposited particle decreases gradually, while that of the subsequent deposited particle increases almost linearly. This fact indicates that short initial vertical distance has a positive effect on the deformation of the former deposited particle. However, for the subsequent deposited particle, the deformation is so weak that the bonding performance may

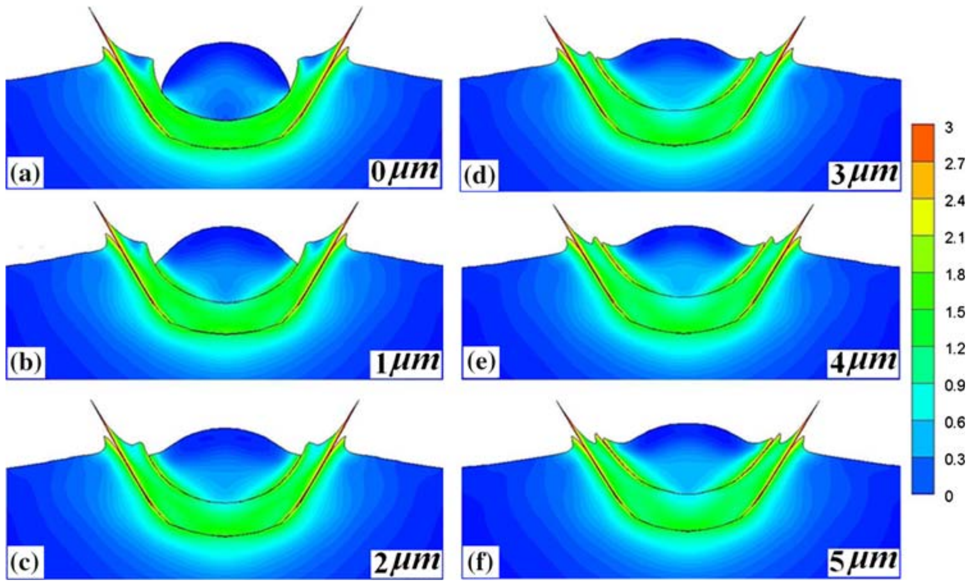

Fig. 7 Contours of the effective plastic strain of two vertical copper particles impacting on a copper substrate with different initial distances at 65 ns

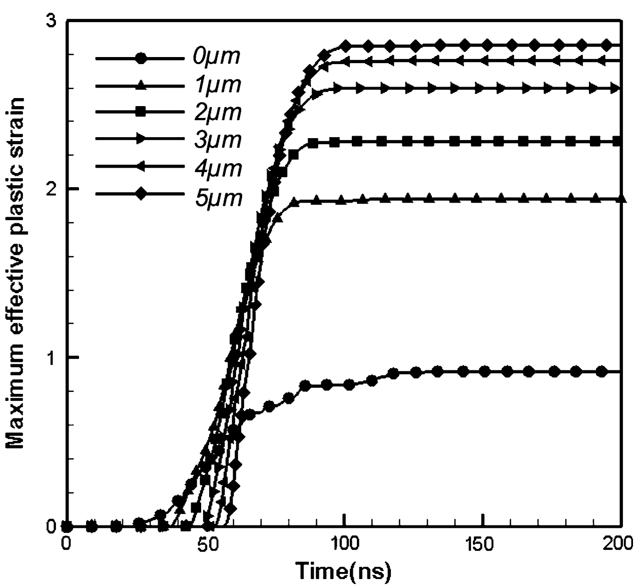

Fig. 8 Simulated temporal development of effective plastic strain of the subsequent deposited particle

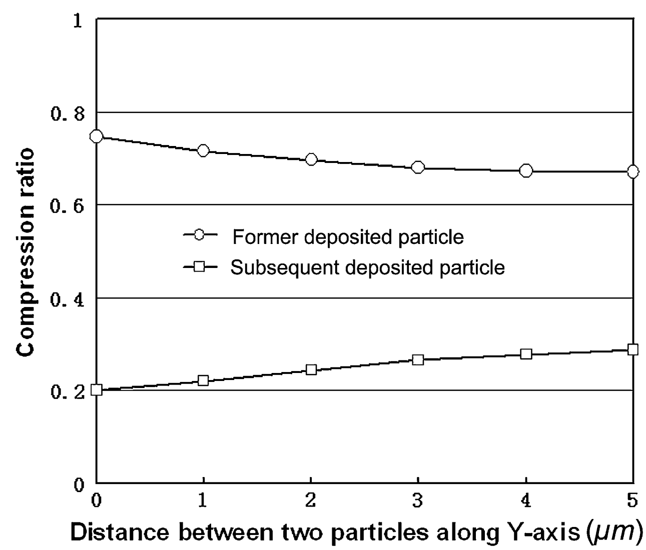

Fig. 9 Effect of initial vertical distance on the compression ratio of two vertical particles

not be strong enough to form a coating when the initial distance is less than a certain value. The reason for this phenomenon can be attributed to the cushioning action of the former deposited particle. Before the former particle completes the whole deformation process, the subsequent one approaches and impacts on it. Most kinetic energy of subsequent particle are buffered by the former one, which results in no sufficient energy available to complete the intensive deformation of the subsequent particle and hence a failure in the formation of a coating.

3.3 Effect of Tamping Action of Subsequent Particles on Coating Formation

Figure 10 shows the contour of the effective plastic strain of three successive impacting copper particles on a copper substrate with the initial vertical distance of 3 μm. For convenience, the particles are named as A, B, and C, respectively, according to the sequence of impacting on the substrate. It is clear that particle A has experienced the most intensive deformation, followed by particles B and C. The metal jets are formed at the surround region of each particle. For more detailed investigation on the particle deformation, the compression ratio is given in

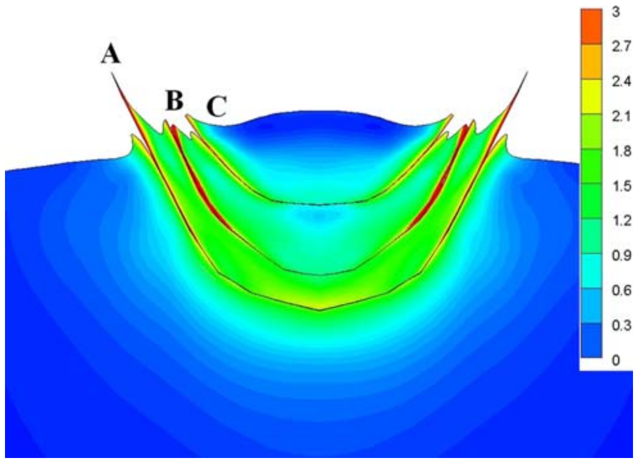

Fig. 10 Contour of the effective plastic strain of three successive impacting copper particles on a copper substrate with the initial vertical distance of 3 μm

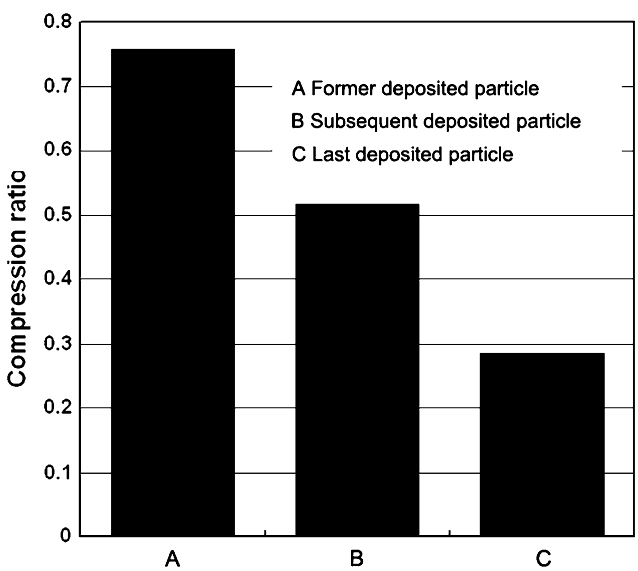

Fig. 11 Compression ratio of three successive impacting particles with the initial vertical distance of 3 μm

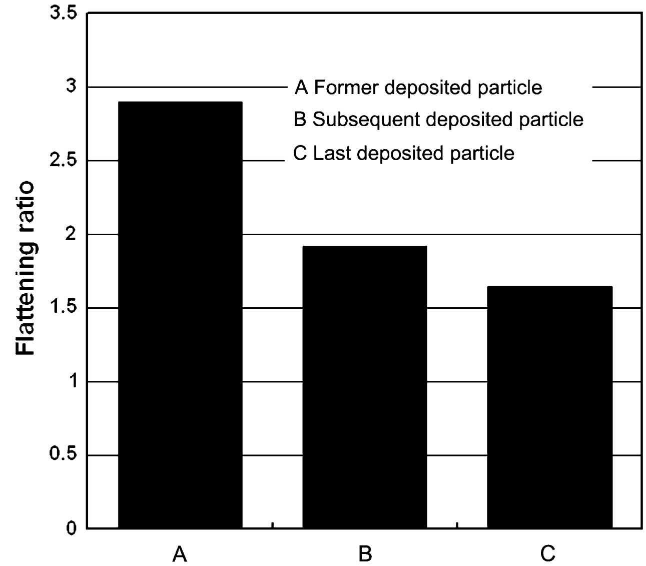

Fig. 12 Flattening ratio of three successive impacting particles with the initial vertical distance of 3 μm

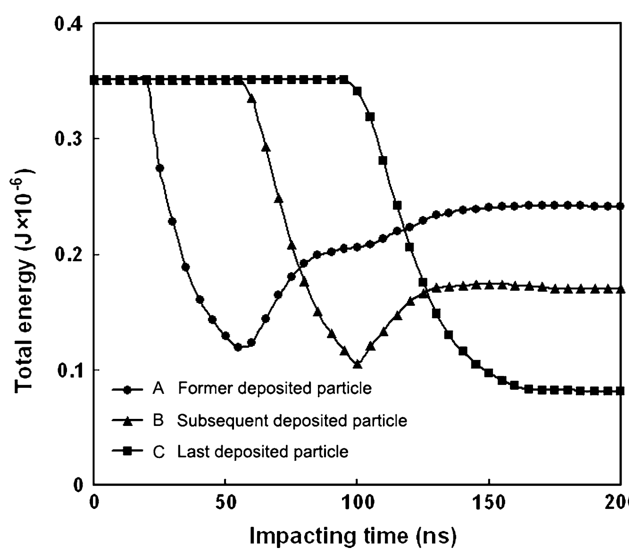

Fig. 13 Simulated temporal development of total energy of three successive impacting particles with the initial vertical distance of 3 μm

Fig. 11. At the same time, because the flattening ratio (R_f) is usually used to characterize the particle flattening extent, which is defined as

$$R_f = \frac{D}{d_p}$$

where D is the spreading diameter of the flattened particle and d_p is the original particle diameter, the flattening ratio is also given in Fig. 12 to characterize the particle deformation. It is obviously seen that the compression ratio of particle A has the highest value, reaching 0.75, followed by particle B and particle C, amounting to 0.51 and 0.29, respectively. The flattening ratio also has the same changing tendency as the compression ratio. The maximum value is obtained with particle A, reaching 2.90, followed by particle B and particle C, amounting to 1.92 and 1.64, respectively. This fact indicates that the deformation of the deposited particles will become increasingly intensive due to the impacting of the subsequent incident particles, which may cause the lower part of the coating to obtain a better bonding strength. This phenomenon can be reasonably explained by the theory of energy transfer and transformation. Figure 13 shows the simulated temporal development of total energy (kinetic plus internal) of three successive impacting copper particles. It is clear that the total energy of particle A reduces quickly at the beginning of the impact because the energy transfers to the substrate and part of which transforms into heat at the deformed zones. Subsequently, it begins to increase at 55 and 108 ns by gaining energy from the particle B and particle C. Eventually, particle A obtain the highest total energy and thus the most intensive deformation. Particle B follows the same changing patent as particle A due to the impact of particle C. However, no increase in the total energy was found for particle C owing to no further impacting on it, which leads to the weakest deformation of particle C in the three particles. Based on the simulated results above, it can be concluded that the subsequent incident particles have the capability to tamp the deposited particles and promote the bonding strength. Moreover, as a result of the tamping action of the subsequent particles, the coating will be little porous near the coating surface compared with the inside of the coating.

Figure 14 compares the contours of effective plastic strain of five copper particles impacting on a copper substrate with the initial distance of 1 and 10 μm. It is interesting to find that the effective plastic strain at the contact regions between particles marked by the squares in Fig. 14(a) is much lower than that in Fig. 14(b), which means better bonding performance when the initial distance is 10 μm. The result is in good agreement with the discussion in Section 3.1. Furthermore, it should be pointed out that owing to the further impacting by the subsequent incident particles, the deposited particles are tamped, which results in much higher effective plastic strain at the contact regions marked by the white square than that marked by the black squares. These results provide strong evidence that interactions between particles actually play an important role in coating formation.

Li et al. has also reported the same results through experimental method (Ref 20, 21). Figure 15 shows typical microstructures of the titanium coatings deposited by using nitrogen as the carrier gas at 540 K conducted in Xi'an Jiaotong University. From Fig. 15(a), the gaps

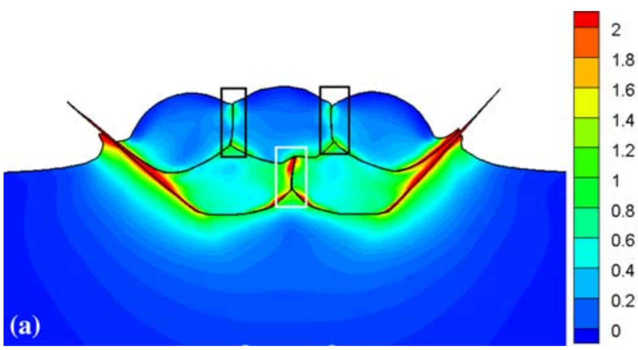

Fig. 14 Contours of the effective plastic strain of five copper particles impacting on a copper substrate: (a) with initial distance of 1 μm and (b) with initial distance of 10 μm

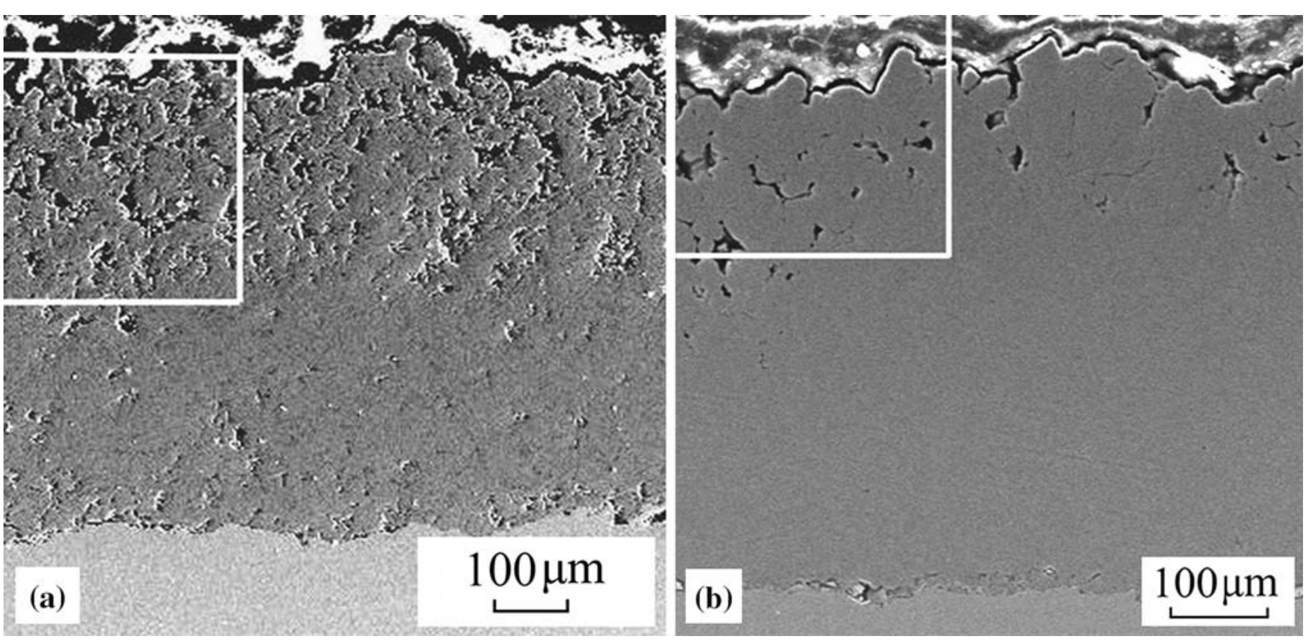

Fig. 15 Typical microstructures of the titanium coatings deposited by using nitrogen as the carrier gas at 540 K: (a) polygon titanium powder and (b) spherical titanium powder (Ref 20, 21)

marked by squares can be obviously observed at some regions, which probably arise from the interactions between particles. On the other hand, from Fig. 15(b), it can be clearly found that the top region close to the coating surface presents much porous microstructural features than the inner zone of the coating. Moreover, the density becomes larger with the increment of the depth from the substrate surface toward the coating surface. The experimental results agree well with the numerical investigations in this study and further add weight to our findings.

4. Conclusions

Numerical investigation on the effects of interactions between particles on coating formation was conducted by using a finite element analysis method. It is found that the interactions between particles play an important role in particle deformation and thus coating formation. When the initial parallel distance is short, particles compress with the generation of gap between them. This process is similar to the angle-incident process by single particle. For the vertical case, the initial distance also significantly affects the deformation of the sprayed particles. Small vertical distance makes the subsequent incident particles deform so weakly that the bonding performance is not probably strong enough to form a coating. Moreover, for successive impacting particles, the subsequent incident particles will tamp the former deposited particles, causing the coating to be little porous near the surface and denser inside the coating. Additionally, some experimental observations conducted by Li et al. (Ref 20, 21) agree well with the simulated results in this study.

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References

1. J.A. Zukas, *High Velocity Impact Dynamics*, John Wiley & Sons, New York, 1990
2. L.-L. Wang, T.-X. Yu, and Y.-C. Li, *Development on Impact Dynamics*, University of Science and Technology of China Press, Hefei, 1992 (in Chinese)
3. S.V. Klinkov, V.F. Kosarev, and M. Rein, Cold Spray Deposition: Significance of Particle Impact Phenomena, *Aerosp. Sci. Technol.*, 2005, **9**(7), p 582-591
4. A.P. Alkimov, V.F. Kosarev, and A.N. Papyrin, A Method of Cold Gas Dynamic Deposition, *Dokl. Akad. Nauk. SSSR*, 1990, **315**(5), p 1062-1065
5. A. Papyrin, Cold Spray Technology, *Adv. Mater. Process.*, 2001, **159**(9), p 49-51
6. H. Assadi, F. Gartner, T. Stoltenhoff, and H. Kreye, Bonding Mechanism in Cold Gas Spraying, *Acta Mater.*, 2003, **51**(15), p 4379-4394
7. R.C. Dykhuizen, M.F. Smith, D.L. Gilmore, R.A. Neiser, X. Jiang, and S. Sampath, Impact of High Velocity Cold Spray Particles, *J. Therm. Spray Technol.*, 1999, **8**(4), p 559-564
8. C.-J. Li, W.-Y. Li, and H.-L. Liao, Examination of the Critical Velocity for Deposition of Particles in Cold Spraying, *J. Therm. Spray Technol.*, 2006, **15**(2), p 212-222
9. S.V. Klinkov and V.F. Kosarev, Measurements of Cold Spray Deposition Efficiency, *J. Therm. Spray Technol.*, 2006, **15**(3), p 364-371
10. D.L. Gilmore, R.C. Dykhuizen, R.A. Neiser, T.J. Roemer, and M.F. Smith, Particle Velocity and Deposition Efficiency in the Cold Spray Process, *J. Therm. Spray Technol.*, 1999, **8**(4), p 576-582
11. T.H. Van Steenkiste, J.R. Smith, R.E. Teets, J.J. Moleski, D.W. Gorkiewicz, R.P. Tison, D.R. Marantz, K.A. Kowalsky, W.L. Riggs, P.H. Zajchowski, B. Pilsner, R.C. McCune, and K.J. Barnett, Kinetic Spray Coatings, *Surf. Coat. Technol.*, 1999, **111**(1), p 62-71
12. V.K. Champagne, Jr., D. Helfritch, P. Leyman, S. Grendahl, and B. Klotz, Interface Material Mixing Formed by the Deposition of Copper on Aluminum by Means of the Cold Spray Process, *J. Therm. Spray Technol.*, 2005, **14**(3), p 330-334
13. W.-Y. Li, H.-L. Liao, C.-J. Li, G. Li, C. Coddet, and X.-F. Wang, On High Velocity Impact of Micro-Sized Metallic Particles in Cold Spraying, *Appl. Surf. Sci.*, 2006, **253**(5), p 2852-2862
14. G. Li, X.-F. Wang, and W.-Y. Li, Effect of Different Incidence Angles on Bonding Performance in Cold Spraying, *Trans. Nonferr. Met. Soc. China*, 2007, **17**(1), p 116-121
15. W.-Y. Li, H.-L. Liao, C.-J. Li, H.-S. Bang, and C. Coddet, Numerical Simulation of Deformation Behavior of Al Particles Impacting on Al Substrate and Effect of Surface Oxide Films on Interfacial Bonding in Cold Spraying, *Appl. Surf. Sci.*, 2007, **253**(11), p 5084-5091
16. M. Grujicic, C.-L. Zhao, W.S. DeRosset, and D. Helfritch, Adiabatic Shear Instability Based Mechanism for Particles/Substrate Bonding in the Cold-Gas Dynamic-Spray Process, *Mater. Des.*, 2004, **25**(8), p 681-688
17. W.-Y. Li, C. Zhang, C.-J. Li, and H.-L. Liao, Modeling Aspects of High Velocity Impact of Particles in Cold Spraying by Explicit Finite Element Analysis, *J. Therm. Spray Technol.*, 2009, in press, doi:10.1007/s11666-009-9325-2
18. *LS-DYNA Theoretical Manual*, Livermore Software Technology Corporation, Livermore, CA, 1998
19. G.R. Johnson and W.H. Cook, Fracture Characteristics of Three Metals Subjected to Various Strains, Strain Rates, Temperatures, and Pressures, *Eng. Fract. Mech.*, 1985, **21**(1), p 31-48
20. W.-Y. Li, "Study on the Effect of Particle Parameters on Deposition Behavior, Microstructure Evolution and Properties in Cold Spraying," Ph.D. Thesis, Xi'an Jiaotong University, China, 2005
21. C.-J. Li and W.-Y. Li, Deposition Characteristics of Titanium Coating in Cold Spraying, *Surf. Coat. Technol.*, 2003, **167**(2-3), p 278-283