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PARTICLE BONDING MECHANISM IN CGDS-A THREE-DIMENSIONAL APPROACH

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ABSTRACT

Cold gas dynamics spray (CGDS) is a surface coating process using highly accelerated particles to form the surface coating by high speed impact of the particles. In the CGDS process, metal particles of generally 1-50 µm diameter is carried by a gas stream in high pressure (typically 20-30 atm) through a DE Laval type nozzle to achieve supersonic flying so as to impact on the substrate. Typically, the impact velocity ranges between 300 and 1200 m/s in the CGDS process. When the particle gains its critical velocity, the minimum in-flight speed at which it can deposit, adiabatic shear instabilities will occur. Herein, to ascertain the critical velocities of different particle sizes on the bonding efficiency in CGDS process, three-dimensional numerical simulations of single particle deposition process were performed. In the CGDS process, one of the most important parameters which determine the bonding strength with the substrate is particle impact temperature. Bonding will occur when the particle's impacting velocity surpass the critical velocity, at which the interface can achieve 60 % of melting temperature of particle material (Ref 1). Therefore, critical velocity should be a main parameter on the coating quality. The particle critical velocity is determined not only by its size, but also by its material properties. This study numerically investigate the critical velocity for the particle deposition process in CGDS. In the present numerical analysis, copper (Cu) was chosen as particle material and aluminum (Al) as substrate material for this study. The impacting velocities were selected between 300 m/s and 800 m/s increasing in steps of 100 m/s. The simulation result reveals temporal and spatial interfacial temperature distribution and deformation between particle(s) and substrate. Finally, comparison is carried out between the computed results and experimental data.

Keywords: CGDS, bonding, critical velocity, particle impact

NOMENCLATURE

C_d	Wave speed of the material
c	Specific heat (J/tonne·°C)
E	Young's modulus (Mpa)
k	Thermal conductivity (W/(mm·°C))
L_{min}	Smallest element dimension in the mesh
p	Contact pressure between two surfaces (Mpa)

t	Time (s)
u	Velocity (mm/s)
G_f	Facture energy per unit area

Greek symbols

θ	Current temperature (℃)
θ_{melt}	Melting temperature (℃)
$\theta_{transition}$	Transition temperature (℃)
$\bar{\varepsilon}_{pl_f}$	Strain at failure
$\dot{\varepsilon}_0$	Relative strain rate (s^{-1})
$\Delta\bar{\varepsilon}_{pl}$	The equivalent plastic strain increment
μ	Coefficient of friction
ρ	Mass density (tonne/mm^3)
ν	Poisson's ratio
ω	Damage parameter

1. INTRODUCTION

Cold Gas Dynamic Spray (CGDS) is a promising coating technique which is accelerating particles by aerodynamics to high-speed and impact onto the substrate. In the process, spray particles (usually 1-50μm) are accelerated to high velocity (typically 300~1200 m/s) by a high-speed and high pressure (generally 20-30 atm) gas flow before impact on the substrate. In order to reach such a supersonic velocity, spray particles are carried by the high pressure gas through a convergent-divergent De Laval type nozzle. Figure 1 shows the schematic of CGDS process. The adiabatic shear instabilities will occur when the particle exceeds its critical velocity, the minimal deposition speed in CGDS process. The critical velocity is dependent on both the to-be–deposited and substrate material properties and the particle size. CGDS has been extensively investigated numerically and experimentally due to the inherent advantages comparing to the traditional thermal spray processes. It has been proven that CGDS could become the next generation of commercially viable surface coating process for various industries, such as aerospace, automobile, chemical etc._In this research, the three-dimensional numerical simulations of the behavior of single particle deposition on the substrate was carried out to study the effect of various particle sizes on critical velocities during the bonding process.

Figure 1.Cold gas dynamic spraying process

For conventional spray coating process, for example, Arc Spray, High Velocity Air Fuel (HVAF), High Velocity Oxygen Fuel (HVOF), and Plasma Spray etc., high temperature is required to pre-heat the coating material, thermal spraying even demands 2000°C or more. In these processes, excessive oxidation,

evaporation, phase transformation, and significant residual stresses etc. may occur causing unsuccessful coating. Since CGDS operates at low temperature, all thermal related problems due to high temperature listed above could be minimized. Here is a list making CGDS process an advantaged technique (Ref 2):

A. A low level of residual stresses compared to thermal spray processing.

B. The un-deposited particle can be collected and reused more efficiently than thermal spray technologies.

C. CGDS is performed at both low noise level (around 70-80db) and low temperature which is safer compared to HVOF (123db).

D. Temperature sensitive materials can be suitable for CGDS.

E. It can create Thick coatings allowing for free standing structures or even rapid prototyping.

F. High electrical and thermal conductivity of coatings could be produced by CGDS.

Even though the CGDS has many advantages to apply in industry, but it still have some limitation. The disadvantages will be listed as follow (Ref 3):

a. In as-sprayed condition only near-zero ductility can be attained in the cold-sprayed coating.

b. Although composites can be sprayed, it can't work well for pure ceramics and some alloys (such as work-hardening alloys).

c. For coatings over ceramic substrates only limited bond strength can be obtained by CGDS process.

d. Expensive helium is generally adopted for high quality coatings to achieve necessary velocities for deposition.

e. It is difficult to spray internal surfaces and complicated shapes as CGDS is also a line-of-sight process like many other coating techniques.

Literature Review

As reported by Irissou et al. (Ref 4), Thurston (Ref 5) proposed a method to apply metal upon another material in 1900. He used a blast of pressurized gas force to make the metal particles embed on the metal surface and form a permanent coating. Rocheville used the same method but using a de Laval type nozzle in 1985 (Ref 6). After changed the type of the nozzle, the high pressure air stream carried metal particles pass through the nozzle and reach a higher velocity in order to form a coating on the substrate. In mid-1980s, Papyrin (Ref 7) and his colleagues conducted a research on the interaction of supersonic two-phase flow (gas

+ solid particles) with the surface of immersed bodies in a wind tunnel. They discovered a new phenomenon called “cold spray” (Ref 7). They studied supersonic two-phase flow around different shapes of body by using new gas dynamics diagnostic tools, and_successfully deposited a wide range of pure metals, metal alloys and composites onto a variety of substrate materials, and also confirmed that the cold spray process was suitable for various applications.

Another similar deposition called aerosol deposition (AD) was developed nearly at the same time. Akedo et al. (Ref 8) developed jet molding system in the late 1990s, which worked under vacuum conditions, enabling deposition of various materials as planar films and also three-dimensional structures by masking (Akedo, et al. (Ref 8) and Akedo and Lebedev (Ref 9)). Later, the term “Aerosol Deposition Method” (AD) was used instead of “gas deposition” since the aerosol is usually not generated by vaporization of the material (Akedo (Ref 10), Hanft et al. (Ref 11)). For AD, the bonding mechanism for brittle particles is likely different than for CGDS metals. Particle deformation and cracking due to a hammering effect of subsequent bombarding particles is the main deposition mechanism for AD (Hanft et al. (Ref 11)), while up till now the most predominant bonding theory is based on adiabatic shear instability in CGDS (Grujicic et al. (Ref 12)). The velocity reached of AD is lower than that of CGDS in general, AD process significantly reduces the presence of the bow shock effect, representing shockwave, before the substrate, making it possible to successfully deposit very small particles (Moridi et al.(Ref 13), Akedo et al., (Ref 14)).

After the CGDS invented by Papyrin (Ref 7) and his colleagues, the number of research papers and the technologies which are related to cold spray has grown exponentially in the current decade. Assadi et al. (Ref 15) used numerical method to simulate the behavior of the particle deposition during the cold spray process. The simulation results were used to compare and estimate the experimentally evaluated critical velocity, strengths of coating etc. From the previous studies, it is believed that the adiabatic shear instability and the resultant plastic-flow localization are the major mechanisms responsible for the particle/substrate bonding during the CGDS process. Grujicic et al. (Ref 12) studied adiabatic shear instability of the cold spray process. He used dynamic axisymmetric thermal mechanical finite element method coupled with a one-dimensional thermo-mechanical model for adiabatic strain softening and accompanying adiabatic shear localization in his analysis. M. Grujicic found that different materials will come with different critical velocity which is the minimum impact velocity to generate adiabatic shear instability at the particle/substrate interface of

deposition. Li et al. (Ref 16) used numerical method to simulate the particle deposition phenomena in cold spray process. They tested various numerical settings to analyze the particle impact model such as material damage, Arbitrary Lagrangian Eulerian (ALE) adaptive meshing, and distortion control and contact interaction. He found that the setting of material damage can deal with the element excessive distortion problem. It is worth noting that Li et al. (Ref 17) found the influence of meshing size and heat conduction must be taken into consideration for a deeper understanding of the ability of numerical modeling on cold spray particle impacting. The results show that the denser meshing size is required for better output resolution. Yen (Ref 18) numerically investigated the effects of the distance between nozzle and substrate in CGDS process. In his research, different carrier gas, such as Nitrogen and Helium, carried different size of material particle from range 1μm to 50μm through the De Lavel type supersonic nozzle. He found that different carrier gas and different spray distance will have different accelerating features of the result in flow structures of the carrier gas. Yen indicated that carrier gas with smaller molecular weight has better accelerating ability for particles acceleration. It is worth noting that he also mentioned the shorter distance from nozzle exit to the substrate would extend the low velocity zone in the bow-shaped shock wave, which could be detrimental to particles acceleration. Schmidt et al. (Ref 19) assumed the particle will be coating on the substrate when the temperature of the monitor area around the particle reach 60% of the material melting point. Wong (Ref 20) numerically simulate the particle impact behavior in two-dimensional analysis. He tested different sizes and velocities to analyze the temperature variation of the particle. He used this assumption and found the particle will reach 60% melting points when it reached the velocity. In this paper, the point is also adopted, and will referred as minimum bonding temperature.

Wu et al. (Ref 21) also used numerical simulation to simulate the energy dissipation of the particle impact behavior. They analyzed the effect of particle's kinetic energy dissipation between the particle and substrate from the impact velocity and material properties. They found that the partition coefficient of energy will affect the deposition efficiency. The materials properties will also affect when it has significant differ between particle and substrate. In the work of Yildirim et al. (Ref 22), they tested various setting in numerical analysis to simulate the particle impact behavior. A three-dimensional model was used to run the simulation and compare to the two-dimensional model. Their results indicate that the temperature of two-dimensional model will raise too high because of the element distortion. It was concluded that the Lagrangian approach with

material failure was found effective in describing material behavior under high deformations and preventing excessive distortion of the mesh.

2. RESEARCH OBJECTIVE

There are several commercial FEM codes can be used to analysis the behavior of particle impact on substrate, such as ABAQUS/Explicit, CTH code, SPH code and ANSYS/LS-DYNA, etc. It can be known there are some factors will affect the deposition efficiency in the coating process. The factors include the different size of particle, material properties and velocity of the particle which will change the coating conditions. Besides, there are many difficulties to experimentally analysis the deformation of particle impact process and temperature distribution in this short duration. Hence, the numerical simulation is used to predict the distribution of the temperature and deformation of different size of particles in different velocities. Herein, the materials of the particle and the substrate are copper and aluminum, respectively. In order to get a fine coating on substrate, the cold gas coating process requires small size of the particles. Therefore, the particle size in 5μm and 10μm were chosen to be the model we tried to observe. From the previous study, the heat conduction and deformation of particle collision were investigated by using ABAQUS/Explicit couple with Johnson-cook model. Therefore, ABAQUS/Explicit was chosen to analyze the critical velocities of different sized particles in three-dimensional within this paper.

3. NUMERICAL METHOD

ABAQUS will be used as the finite element simulation environment to simulate the behavior when the particle impacts into substrate. This paper uses Central difference time integration which is known as Explicit method to integrate time of the dynamic problem. In this method, the current step's displacement only relates to the previous step's acceleration and displacement. For this research, the total time for the contact calculation is around 60 ns. Because of some influence of physical characteristics of waves, the particle impact behavior uses explicit method to solve will be more accurate. In this paper, ABAQUS/Explicit will be utilized as the solver and will be discussed below.

4. MATHEMATICAL MODEL

The particle impact behavior is a nonlinear dynamic process which the simulation uses the explicit dynamic analysis in ABAQUS/Explicit. As it was directed that the explicit dynamics analysis ideally suits

for investigating high-speed dynamic effects, while many advantages of the procedure also be applied to analyze slower processes (Ref 23).

4.1. Explicit dynamic procedure

In ABAQUS/Explicit, the explicit dynamics analysis is based on the introduction of an integration rule and diagonal or "lumped" element mass matrices (Ref 23). The explicit algorithm can be shown briefly as below:

a) Nodal calculations

Equation of dynamic

$$\{\ddot{u}\}_t = [M]^{-1} \cdot \left([P]_t - [I]_t\right)$$

Explicitly integration through time

$$\dot{u}^{i+\frac{1}{2}} = \dot{u}^{i-\frac{1}{2}} + \frac{\Delta t^{(i+1)} + \Delta t^{(i)}}{2} \ddot{u}^{(i)}$$

$$u^{i+1} = u^{(i)} + \Delta t^{(i+1)} \dot{u}^{(i+\frac{1}{2})}$$

b) Calculations on element

1) Derive increments of element strain, $d\varepsilon$, from the strain rate, $\dot{\varepsilon}$.

$$\dot{\varepsilon} = \frac{1}{2}\left(L + L^T\right) = \frac{1}{2}\left(\left[\frac{\partial v}{\partial x}\right] + \left[\frac{\partial v}{\partial x}\right]^T\right), \quad v = \frac{\partial x}{\partial t}$$

2) Derive stresses, σ, from following constitutive equations.

$$\sigma_{t+\Delta t} = f\left(\sigma_t, d\varepsilon\right)$$

3) Assemble nodal internal forces, $I_{(t+\Delta t)}$.

4) Set $(t + \Delta t)$ to t and return to step 1).

By using numerous limited time increments the computing procedure can integrate through the time domain.

4.2. The Definition of Stability

However, the central-difference operator used in explicit is not always stable, but conditionally. The stability limit for the operator without damping can be defined in terms of the system highest frequency, expressed as:

$$\Delta t \leq \frac{2}{\omega_{max}}$$

While the stable time increment with damping is given by

$$\Delta t \leq \frac{2}{\omega_{max}}\left(\sqrt{1+\xi_{max}^2}-\xi_{max}\right)$$

Where ξ_{max} represents the fraction of critical damping in the mode with the system highest frequency. Interestingly it counters to ordinary engineering intuition that it reduces the stable time increment to introduce damping into the solution. So a small amount of damping is introduced in the form of bulk viscosity to control high frequency oscillations in ABAQUS/Explicit.

To determine conservative bounds for the highest element frequency, adaptive algorithm is adopted in ABAQUS/Explicit. A global estimation algorithm determines the highest frequency of the entire model by continuously updating the estimate for the highest frequency. ABAQUS/Explicit starts from the element by element estimates. And as the step proceeds, the stability limit will be determined from the global estimator once the global estimation accuracy is acceptable. The smallest transit time of a dilatational wave across any of the elements in the mesh can approximate the stability limit, as shown below.

$$\Delta t \approx \frac{L_{min}}{c_d}$$

Where L_{min} is the minimum element dimension in the mesh and c_d means the dilatational wave speed. It is not clear how the element length should be determined, the equation is an estimation of the actual element-by-element stability limit. Even though the approximation can be taken, the resulting estimate is not always conservative. This model will be meshed by a given size of the element but not exactly the values. It depends on the features and seeds on the model. The dilatational wave speed is related to the properties of material. For a linear elastic material with Poisson's ratio equal to zero, the dilatational wave speed could be defined as following.

$$c_d = \sqrt{\frac{E}{\rho}}$$

Where E is the Young's modulus and ρ represents the mass density. It means that for the material the stiffer, it will come with higher wave speed and smaller stability limit. If the density is higher, the wave speed will be lower and come with the larger stability limit.

4.3. Energy Balance

To evaluate analysis of response, comparisons between various energy components can be made. Energy is balance for the entire model, expressing as

$$E_I + E_V + E_{FD} + E_{IHE} + E_{KE} - E_W - E_{PW} - E_{CW} - E_{MW} - E_{HF} = E_{total} = constant$$

where E_I represents internal energy, E_V refers to the dissipated viscous energy, E_{FD} means the dissipated frictional energy, while E_{IHE} means the internal heat energy, E_W represents the work done by externally applied forces, E_{KE} represents the kinetic energy, and E_{CW}, E_{PW}, and E_{MW} refer to the work done by constraint penalties, by contact penalties, and by propelling added mass, respectively. E_{HF} means the external heat energy. These energy components above sum as E_{total}, which ought to be constant. But in the calculation it's impossible, for approximation E_{total} is generally limited an error in 1%.

In the above components, the internal energy is more complex, can be expressed as the sum of sub components: the energy dissipated through inelastic processes such as plasticity, E_P, the recoverable elastic strain energy, E_E, the energy dissipated through damage, E_{DMD}; the energy dissipated through viscoelasticity or creep, E_{CD}; the artificial strain energy, E_A, and the energy dissipated through distortion control, E_{DC}:

$$E_I = E_E + E_P + E_{CD} + E_A + E_{DMD} + E_{DC}$$

The artificial strain energy is sum of energy stored in hourglass resistances and transverse shear in shell and beam elements. Noting of its large values, which indicates that it's necessary to refine mesh or make other changes to the mesh.

4.4. Coulomb Friction

The Coulomb friction model expresses relationship of the maximum allowable shear stress across an interface and the contact pressure between the contacting bodies. In the basic form, two contacting surfaces are able to stay relatively static when shear stress is under a certain value, the state is called sticking, once over the value they will start sliding over each other. And the critical shear stress is defined by Coulomb

friction model, τ_{crit}, at which the two surfaces starts sliding relatively under a fraction along interface of the contact pressure, p, the value can be calculated from $\tau_{crit} = \mu p$, where μ refers to the friction coefficient.

4.5. Johnson-Cook Model

In order to describe the behavior of the particle impact, the Johnson-cook model should be applied into the simulation. There are two settings applied in this numerical simulation. One is Johnson-cook Plasticity Model and another is Johnson-cook damage.

4.5.1. Johnson-Cook (JC) Plasticity Model

For the collision in between particles and the substrate, Johnson-cook plasticity model is adopted to describe deformation of material. The main advantages of the JC model is that it is a coupled material model can be used to capture viscoplasticity and ductile damage due to ballistic impact and penetration. JC model is perfect for CGDS since it allows large plastic strains, high strain rate and adiabatic heating. These are the major bonding mechanisms for CGDS.

For nonzero strain rate, the following equation can express the yield stress, $\bar{\sigma}$:

$$\bar{\sigma} = \left[A + B\left(\bar{\varepsilon}_{pl}\right)^n\right]\left[1 + Cln\left(\frac{\dot{\bar{\varepsilon}}_{pl}}{\dot{\varepsilon}_0}\right)\right]\left(1 - \hat{\theta}^m\right)$$

In the equation, $\dot{\varepsilon}_0$ means the reference strain rate, A, B, C, m and n represent material parameters while measuring at or under transition temperature, while $\dot{\bar{\varepsilon}}_{pl}$ represents PEEQ, the equivalent plastic strain rate. Specify the non-dimensional temperature, $\hat{\theta}$, as follow:

$$\hat{\boldsymbol{\theta}} \equiv \begin{cases} \mathbf{0} & \text{for } \boldsymbol{\theta} < \boldsymbol{\theta}_{\mathbf{transition}} \\ (\boldsymbol{\theta} - \boldsymbol{\theta}_{\mathbf{transition}})/(\boldsymbol{\theta}_{\mathbf{melt}} - \boldsymbol{\theta}_{\mathbf{transition}}) & \text{for } \boldsymbol{\theta}_{\mathbf{transition}} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}_{\mathbf{melt}} \\ \mathbf{1} & \text{for } \boldsymbol{\theta} > \boldsymbol{\theta}_{\mathbf{melt}} \end{cases}$$

Where θ represents the current temperature, θ_{melt} represents the melting temperature, while $\theta_{\text{transition}}$ refers to the transition temperature at or below which yield stress is not dependent on temperature.

4.5.2. Johnson-Cook Damage

In ABAQUS/Explicit, Johnson-cook failure model is suggested as more general for implementing materials' progressive damage and failure. The core concept of the model is the damage parameter, ω, which is described in the following:

$$\omega = \sum \left(\frac{\Delta \bar{\varepsilon}_{pl}}{\bar{\varepsilon}_{pl_f}} \right)$$

Where $\Delta \bar{\varepsilon}_{pl}$ means an addition of the equivalent plastic strain, and $\bar{\varepsilon}_{pl_f}$ refers to the strain at failure, then the summation can be executed over all the increments in the simulation. When the damage parameter exceeds 1, failure is presumed to occur.

Three parameters is relative to the strain at failure $\bar{\varepsilon}_{pl_f}$: the non-dimensional temperature, $\hat{\theta}$, defined in the Johnson-cook plasticity model; non-dimensional pressure-deviatory stress ratio, p/q (p for the pressure stress and q refers to the Von Mises stress); and plastic strain rate, $\dot{\bar{\varepsilon}}_{pl}/\dot{\varepsilon}_0$. The reliance is divisible and described as:

$$\bar{\varepsilon}_{pl_f} = \left[d_1 + d_2 exp\left(d_3 \frac{p}{q} \right) \right] \left[1 + d_4 ln\left(\frac{\dot{\bar{\varepsilon}}_{pl}}{\dot{\varepsilon}_0} \right) \right] \left(1 + d_5 \hat{\theta} \right)$$

Herein $d_1 \sim d_5$ refer to failure parameters metered at or below $\theta_{\text{transition}}$. Once the calculation met the failure criterion, it sets the deviatory stress components to remain zero for the rest simulation. Pressure stress for the rest of calculation can be treated two ways. It may be set to remain zero and you must choose element deletion during the element type assignment. It may also needed to keep compressive for the rest analysis by choosing not to activate the element deletion. The fracture energy mean area, G_f, will dissipate directly during the damage procedure. When set G_f as 0, instantaneous failure will occur. In this research, the exponential form is adopted for material damage evolution.

4.6. Assumption

In this research, some assumptions will be defined and shown to simplify the impact behavior as follow:

- The impact direction of particle is perpendicular to the substrate.
- Ignore the effect of gravity.
- 90% of plastic work is assumed empirically transforming to heat.

- 100% of friction work transfers to heat, rising temperature.
- The time of impact behavior between particle and substrate is about nanosecond (ns). Therefore, the total step time is assumed 60 nanosecond (6×10^{-8}seconds).

4.7. Geometric Model

This study used three-dimensional model to simulate the impact behavior and compare to two-dimensional model, taking particle as solid ball, and substrate as cylinder. Because of the axisymmetric characteristics of typical impact behavior, a quarter three-dimensional model was created, as in Figure 2. Where the height and radius of the cylindered substrate are four times radius of the particle. Both particle and substrate were separated into distinct sectors to get high quality mesh.

Figure 2. Computational model with meshing arrangement and the setting diagram of contact pair

4.8. Material Property

Copper was chosen as the material of the particle and aluminum alloy of the substrate. Both thermal and mechanic properties of the materials were taken as isotropic. Table 1 below illustrates properties of both materials.

Table 1. Copper (Ref 24) and aluminum alloy (Ref 25) properties input in computations.

Material	Cu	Al
Density, kg/m^3	8960	2700
Thermal Conductivity	386	220
Specific heat, J/(kg °C)	383	920
Melting Point, °C	1083	643
Elastic modulus, Gpa	124	65.762
Poisson's ratio	0.34	0.3
JC plasticity: A (Mpa), B (Mpa), n, C, m	90, 292, 0.31, 0.025, 1.09	148.361, 345.513, 0.183, 0.001, 0.859
JC damage: d_1, d_2, d_3, d_4, d_5	0.54, 4.89, -3.03, 0.014, 1.12	0.071, 1.248, -1.142, 0.147, 1
Reference temperature, °C	25	25
Reference strain rate, s^{-1}	1	1

4.9. Analysis Procedure

From the previous studies (Ref 12,15), the heat conduction was not considered due to simplified estimation. They applied adiabatic heating boundary condition during the particle bonding process. Schmidt et al. (Ref 19) demonstrated that the conduction heat transfer should be accounted for the temperature simulation. A. Moridi, H. Assadi et.al. (Ref 12,15) used the dynamic explicit process by Dynamic-Explicit simulation. In this process, it can set an adiabatic stress analysis in the material to generate heat by inelastic dissipation. T. Schmidt et.al. (Ref 19) adopted the other procedure, called coupled thermal stress analysis (Dynamic, Temp-Disp, Explicit). For this procedure, it can perform the thermal and mechanical solutions strongly affect each other. The heat conduction effect in this procedure which proposed by Schmidt et al. (Ref 19) is considered. Hence, the fully coupled thermal stress model is adopted for this investigation.

4.10. Contact Property

During the particle impact process, particle and substrate get in touch with one another. Therefore a particle-to-substrate contact model is used to define the contact pair between particle and substrate. The setting diagram of contact pair is shown as Figure 2. The normal behavior of the interaction was implemented as “Hard” contact. In previous study, the coefficient of friction between the impact interface of particle and substrate is assigned as 0.2.

In numerical analysis, some regions may need to be considered as fixed during the simulation time or may need to be specified non-zero displacements and rotations. The labels used in the simulation code for both displacement and rotational degrees of freedom (DOFs) are shown in Figure 3. In this study, the bottom of substrate is considered as fixed and symmetry on both x-axis and z-axis. Room temperature condition is assumed at 273 K as an initial condition for the comoutation.

4.11. Boundary, Initial Conditions and Mesh

Figure 3. Displacement and rotational DOFs

The mesh size between particle and substrate’s contact area are the same to guarantee high simulating precision. And the side mesh was four times size of the mesh in particle and substrate’s contact area. The mesh was quad structure type and arranged in 8-node (C3D8RT). The nominal meshing size for particle and contact area was used 1/50 of the particle’s diameter.

5. NUMERICAL SIMULATION RESULT

A typical particle impact behavior will be illustrated in Figure 4. The particle size is 5 μm and the impacting velocity is assigned as 600 m/s. The deformation behavior and temperature of the particle play an important role in CGDS process which can indicate the particle deposition is successful or not. Note that the average temperature was calculated by averaging the temperatures of all the adjacent element of the interface during the plastic shearing process.

Figure 4. The 5 μm sized particle impacting evolution at 600 m/s illustrated by ABAQUS/Explicit

As the particle impact process is starting, the shear stress of the plastic deformation causes local shear strain near the contact area between the particle and the substrate. And the adiabatic shear instabilities is caused by the localized shear straining when significant stress and plastic deformation occur (Ref 26). These instabilities will cause discontinuity in temperature and strain on the interface. It will lead to an material jetting which can be observed in Figure 4 (C).

5.1. The Particles Velocities Analysis

As mentioned earlier, the critical velocity is only one of the critical factors in determining the bonding effect, while of equal importance is the particle deposition temperature. Both impact velocity and deposition temperature determine whether a successful bonding could occur. However, it is worth noting that velocity dictates the deposition process since the total available energy is from the inherent kinetic from the particle. The bonding temperature, which was resulted from the shear plastic deformation, will determine the likelihood of the two adjacent materials (particle-particle or particle-substrate) could be bonded. Velocities from 300~800 m/s were chosen in simulation. This section will discuss the temperature of interface for the particle sizes of 5μm and 10μm impact on the substrate. The temperature contours result for 5μm and 10μm sized particles at 800m/s as representative velocity as Figure 5.

Figure 5. Simulated temperature contours for 5μm and 10 μm single particle impact at 800m/s.

The contour of Figures indicate the deformation of size 5μm and 10μm copper particle after collision. The highest localized temperature for each size particle is 882℃ for 5μm and 935℃ for 10μm at 800 m/s.

Although Figure 5 can show the localized temperature at different size of particles in 800m/s, to make clearer it is necessary to do a more quantitative analysis for the elemental temperature in high strain which may results in adiabatic shear instability. Hence temperature history, extreme temperature in particles impacting will be further discussed. Figure 6 illustrates the elemental temperature of the particle in highly strained contact area. The interface temperature of particle size of 1, 5 and 10μm are shown in Figure 7. And contours illustrate the average temperature will vary with different size of particles in different velocities. Figure 8 depicts the maximum surface average temperature at various velocities for 1, 5 and 10 μm particles. It is worth noting that the material of particle will become soften enough to coating on substrate when the temperature reaches minimum bonding temperature, which is 650°C for copper. From the Figure 8, it can be seen that the temperature of size 5μm and 10μm of particle will reach the temperature when the particle's velocity reaches 800 m/s, while 1 μm particle can't. Compare to previous study (Ref 18) of the in-flight velocity of 5μm in Table 2, 5 μm particle will reach this hypothesis when the velocity is 751 m/s as shown in Figure 8.

Table 2. Particles Impact velocities carried by N_2 gas (Ref 18).

Particle size (μm)	Velocity (m/s)
1	618.94
5	751.43
15	522.02
25	418.33
50	306.04

Figure 6. The monitor area of 1/4 three-dimensional symmetric model. (A) Pre-deform; (B) deformed states.

Figure 7. The chart of average temperature for 1 μm, 5 μm and 10 μm particle

Figure 8. The peak temperature evolution with velocity of 1, 5 and 10μm particle

5.2. Analysis of Velocities with Different Size Particles

As discussed above, the particle critical velocity can be estimated from the criterion that the interfacial temperature reaches the minimum bonding temperature during the particle impacting process. The influence of interface temperature in different size of particles with same velocity will be discussed. Figure 9 show the impact temperature comparison 1 μm, 5 μm with 10 μm at the velocities between 300 m/s and 800m/s. To

interpret the trends of these comparisons, temperature evolution at 300 m/s (Figure 9 A) and 800 m/s (Figure 9 F) were selected for the bonding effect discussions of different sized particles. As seen from Figure 9 A, 1 μm particle reaches its highest temperature 170℃ at 2 nanosecond, 5μm particle reaches its highest temperature 190℃ at 11 nanosecond and 10μm particle reaches its highest temperature 195℃ at 22 nanosecond when the velocity of particle is 300 m/s. On the other hand, 1 μm particle obtains its peak temperature 592℃ at 1 nanosecond, 5μm particle obtains its peak temperature 722℃ at 10 nanosecond and 10μm particle reaches its peak temperature 777℃ at 22 nanosecond when the velocity of particle is 800 m/s (see Figure 9 F). The reason for difference is the size of particle will affect the initial kinetic energy which is related to the energy dissipation. From these observations, it can be concluded that for smaller particles the interface temperature increases faster initially than the larger ones, and followed by a sharper temperature decrease, while the peak temperature is lower than the corresponding larger ones. Meanwhile temperature of larger particles increase and decrease slower, but can reach higher maximum temperature. Therefore the particle size affects significantly on the interface temperature characteristics.

Figure 9. The average temperature contour of 1, 5 and 10 μm particle at the velocity of 300~800 m/s

6. NUMERICAL SIMULATION AND EXPERIMENT RESULTS COMPARISON

6.1. Previous Study Combination

The CGDS process consist of two dynamic processes. One process is the carrier gas carrying particle and the other is the deposition process due to particle impacting on the substrate surface (see

Figure *10* (B) and (C)). As reported by Yen (Ref 18), nitrogen was used as carrier gas, copper as particle material, and the in-flight process of 1μm to 50μm size particle was analyzed by using ANSYS/FLUENT. As a result, pressure contour between DE Laval nozzle and the substrate was depicted in Figure 11, in front of the substrate bow shock can be observed generating high pressure region and reducing velocity of particles.

Figure 10. (A) Sketch of CGDS process. (B) The flow pattern of nozzle exit (Ref 18). (C) The CGDS deposition process

Figure 11. The N_2 carrier gas pressure distribution of the CGDS process [18]

Meanwhile, Wong (Ref 20) used 2D axisymmetric model to do the simulation and concluded the particle of size 5μm and 15μm particle can reach the hypothesis while the particle velocity gains 600 m/s. Although the particle bonding process is a multi-particle impact behavior. While it is worth noting that he also found out the first particle will have second jump or even the third jump of the temperature due to the second and third particle impact on it.

6.2. 2D and 3D model comparison

Most prior researches concentrated in the issue of two-dimensional numerical analysis, only few on the three-dimensional Lagrangian model. Nevertheless, it's worth pointing out that two-dimensional and three-dimensional analysis are significantly different. For example, from the previous study, Wong (Ref 20) found out the 5μm and 15μm will reach minimum bonding temperature of copper (Cu), at 600 m/s which is 657 ℃ and 722 ℃, respectively, and the particle of size 1μm at the velocity 800 m/s can reach copper's minimum bonding temperature 650 °C. Compare to this study, 5μm and 10μm can reach minimum bonding temperature of copper (Cu) at 800 m/s which is 722 ℃ and 777 ℃, respectively, while even 1 μm particle can only reach its peak temperature 592 °C at the velocity 800 m/s, lower than 650 °C, the copper's minimum bonding temperature. The reason for the discrepancy may relate to the fact that comparing to the 2D shell element only with 4 nodes and 6 degrees of freedom, the three dimensional solid element with 8 nodes and 48 degrees of freedom would result in more precise deformation and heat conduction.

6.3. Experiment Comparison

The cold spray dynamic spray experiment facility is depicted in Figure 12 (A) which is in focus of the De Laval nozzle and the substrate displaying as close-up look of Figure 12 (B). To protect particles from oxidized, the experiment utilized nitrogen to transport copper particles in 5μm to high velocity, yielding particles impacting and coating on an aluminum substrate.

As is proposed by Yen (Ref 18), the impact velocities of particles sized between 1μm and 50μm are listed in Table 2, which will be used as prediction of particle impact velocities. The impact velocity for 5μm particle will be taken to compare with experiment effect.

Figure 12. (A) Experimental setup of CGDS. (B) Detail of the de-laval nozzle and substrate.

From Table 2, an impact velocity of 751 m/s for the 5μm copper particle on aluminum substrate was predicted by Yen [18]. From 3D simulation analysis, the impacting temperature is shown in Figure 13(A), displaying that the minimum bonding temperature (650°C) could be reached at the 751 m/s impacting velocity. Note that the velocity was simulated from the exact experimental conditions from the experimental set-up shown in Figure 12 (Ref 18). Figure 13(B) illustrates the surface coating experimental result. It can be clearly observed that 5 μm particles can coat well on the aluminum substrate. This simulation result is implicitly in agreement with the experimental results, which could provide evidence that the current three-dimensional simulation could be used to predict the bonding process.

Figure 13. The diagram of comparison between numerical and experimental result for 5 μm particles. (A) The maximum temperature at different velocities. (B) The CGDS deposition result of nitrogen gas carried 5 μm particles.

For 1 μm sized particle, comparison diagram is shown in Figure 14, from Figure 14(A), maximum temperature of the particle increases as velocity, but at simulated highest velocity 800 m/s still doesn't reach minimum bonding temperature, that means poor or even failure impact deposition. And the inference is confirmed by the experimental result (Figure 14(B)), some significant scraping of the surface coatings can be observed. However, deposited particles can still be observed in Figure 14(B), it can be explained that the CGDS process is actually multi-particle phenomenon(Ref 1), and in the process particle/particle, particle/substrate interaction also significantly influence the deposition effect.

Figure 14 . The diagram of comparison between numerical and experimental result for 1 μm particles. (A) The maximum temperature at different velocities. (B) The CGDS deposition result of nitrogen gas carried 1μm particles.

7. CONCLUSION

A three-dimensional FEM model was developed to calculate the interface temperature between copper particle and aluminum substrate with different size of particles at different velocities. As the critical bonding velocity of different sized particles can be estimated from such temperature. From both numerical simulation and experimental results, conclusions can be stated that 1μm particle need initial velocity more than 800 m/s and temperature can't reach the 60% of copper melting temperature compare to the present paper. The reason leads to this difference is because of the using elements in two-dimension and three-dimension. Although the initial acceleration of the 10μm sized particle carried in the nitrogen gas is slower, it is easier than smaller

particles to obtain its critical velocity. From the results, it can be clear seen that 5μm and 10μm can reach 60% copper melting temperature when the velocity is higher than 700 m/s which means the hypothesis of 60% copper melting temperature could be used as a criteria in the future study. The result from numerical simulation of 5 μm has been used to compare with the experiment with reasonable agreement. The numerical simulation of CGDS in particle impact behavior can be adopted to estimate the critical velocity for specific sized particle in three-dimension. It has been revealed that the model applied in three-dimensional simulation would be more reasonable than in two-dimensional simulation due to more degree of freedom calculation and the additional dimensional effect of heat conduction.

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