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Research paper



Numerical Calculation of Three Phase Flow (Gas – Solid – Liquid) of Thermal Spray Process

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Abstract

A new coupling method between the FVM (Finite Volume Method) - solution for compressible gas flows and the MPS (Moving Particle Semi-implicit) - solution for droplet deformation have been developed. This simulation of thermal spray processes covered from the acceleration until droplet substrate solidification. At the temperature of 300K, the trend of flatness result is proportional to $Re^{0.26}$, which agreed well with the experimental result. The adhesive efficiency and aspect ratio are also improved under FVM + MPS calculation as compared with the calculation of MPS only.

Keywords: *Thermal Spray, Finite Volume Method, Moving Particle Semi-implicit, Flatness of splat, Droplet deformation*

1. Introduction

Nowadays the development of thermal spray technology has been progressed, and many new technologies such as ultra-high temperature plasma jet and high-speed flame sprayed using fuel gas explosion energy have been introduced. In the thermal spraying method, thermal spraying particles are deposited on a substrate and surface treatment is performed. The process of film formation in thermal spraying can be divided into three elementary processes. The first is the heating acceleration process, where the sprayed droplets are ejected from the high temperature nozzle, with receive thermal energy and kinetic energy and fly in the atmosphere. Secondly, is a collision flattening solidification process. Sprayed droplets collide with the base material, so that it is flattened and solidified simultaneously by heat exchange. Third one is a lamination process, and flattened thermal spray particles are piled up by repeating the first two elementary processes. The sprayed droplet that collides, flattened and adhered with this base material is called splat.

The phenomenon in the elementary process of this splat is a very small scale, spatially range from several μmeter to approximate of 10 μmeters. Furthermore this process is under high speed conditioned, (in μsec), and it is impossible to measure the flattening behavior in time experimentally. Under these circumstances, clear analytical of micro phenomena is required. However, the flattening process of thermal sprayed particles is like splash, which is a complex phenomenon with sudden deformation of the interface, liquid splitting and coalescence [1].

This phenomenon is difficult to view under interface capture method such as the VOF method, which has been used in general multiphase flow analysis. This interface depends on the calculation grid, and if we want to perform the analysis of droplet particles collide on the base material, flying phenomenon and deformation, it is necessary to use the entire surface between the jet from the nozzle and the base material. This will increase the computational cost and it almost impossible due to very fine calculation grid is required.

The high speed droplets collide with the substrate to form a coating. The temperature different between the droplets and the substrate make the heated droplets to be cooled and solidified. Via experimental, the particles flatness was found proportional to $Re^{0.2\text{-}0.3}$[2]. CFD analysis on sprayed particles and base material has been successfully conducted by [3][4][5]. A research on temperature field for plasma jet has been conducted by [6]. As per described, due to the difficulty of interfacial resolution by using lattice, until now, CFD analysis of plasma jet and analysis of droplet collision near the substrate does not consider each interference accurately.

In this research, we propose a particle method (MPS method) which can analyze the large deformation, splitting and coalescence of liquid as a new calculation method and a gas-liquid coupling method of finite volume method which can stably solve the compressible flow. By doing this, we aim to solve the interface resolution problem in the interface capture method and to establish a complicated gas-liquid multiphase flow analysis method that can deal with large deformation case. In this way, by realizing simulation of the flattening process of the flying particles in the thermal spraying method, it is necessary to calculate a wide range scale simulating the heating acceleration process and the collision flattening solidification process at the same time to identify the controlling factor of the physical phenomenon and the controlling factor of the flattening.

2. Methodology

2.1 Gas flow calculation method

Fluid flows simulation has been achieved by Finite Volume Method. The unsteady Navier–Stokes equation is solved with third-order accuracy of MUSCL [7]. The air is assumed to be an ideal gas and the viscosity coefficient is evaluated by using Sutherland equation. The non-viscous flux is evaluated via SLAU method, and viscous flux is discretized using the central difference. Van

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Albada flux limiter is adapted and time integration is calculated by an explicit 3rd order TVD Runge-Kutta. [8][9]. Structured grid that has 154 × 154 × 330 (= 7.82 × 10^6) total grid points as show in Figure 1 is used in this study

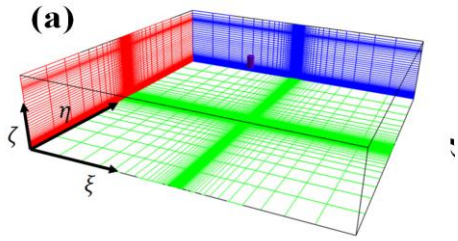


Fig.1: (a) Overall computational grid

The jet initial velocity distribution (without particles) is shown in Figure 2. Initial jet velocity is specified as 60m/s with the geometry of the nozzle are to be 5mm in diameter and 50mm nozzle distance to the substrate. In this calculation, the boundary-fitted grid has been applied for the flow around the droplet, so that the interface droplet boundary layer could be regenerated accurately.

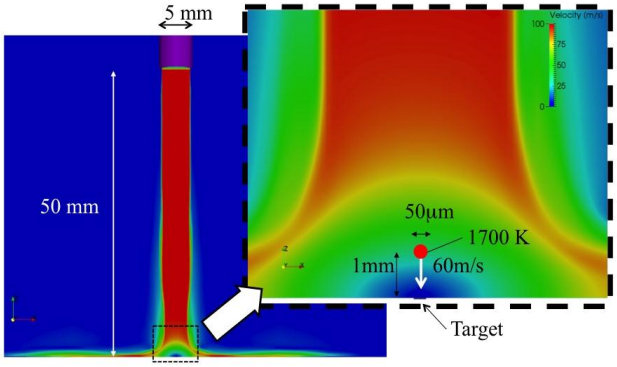


Fig.2: The jet initial conditions (velocity).

Figure 3 shows the droplet computational condition. The 7800 finite number of particles has been introduced with initial droplet temperature, T_1 is 1700K. The distance initial MPS particle, r_o is 2 μmeter and initial droplet diameter is 50 μmeter. Two different substrate temperatures, T_2 are tested, where 300K and 673K. In the droplet interface, the virtual boundary condition method is used which forms the plausible flow around the droplets [10]. The particle has formed into droplet.

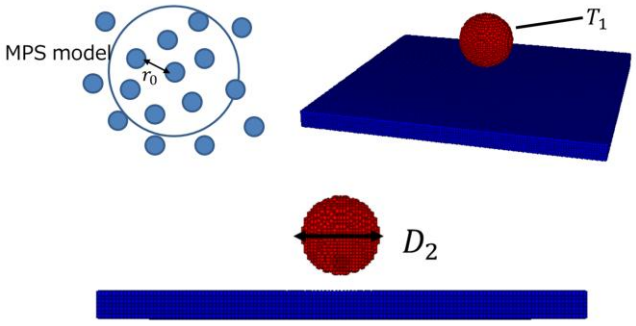


Fig.3: Computational condition for droplet

The Reynolds number equal to 133 is used in this study. The calculation divided into two steps, which are the convergence of the flow calculation (without any particles) and follow by the introduction of a droplet (together with velocity and temperature), as shown in Figure 2.

2.2. Particle calculation method

The three-dimensional incompressible Navier-Stokes equation has been discretized by using MPS (Moving Particle Semi-implicit) method, for simulating the droplet dynamics movement, where

$$\frac{D\rho}{Dt} = 0 \tag{1}$$

$$\frac{Du}{Dt} + \frac{1}{\rho}\nabla p - \upsilon\nabla^2 u - F_{ext} = 0 \tag{2}$$

Equation (1) is called conservation of mass (continues equation) where the MPS is adapted make the temporal change in density become zero (density constant respect to time). This approached contain the explicit velocity field integration and the implicit pressure equation integration, as similar as [11]. The Khayyer's model is used for solving the Laplace equation [12][13]. D/Dt is a Lagrangian differentiation, is a time differential term by a viewpoint moving with the fluid. When solving an equation discretized by particles, the convective particles are always been tracks while discrete points alway in motion. Since the convection term is included in the Navier-Stokes equations, and the particle convection tracking are in Lagrange differential, so the equation is considered as the raw time derivative. Thus, unlike the Euler method, there is no need to calculate the convection term.
For Equation (2), the left side is the Lagrangian derivative with respect to the velocity vector, the second term is the pressure gradient term, the third term is the viscosity term, and the last term is consist the gravity term and the surface tension term (aerodynamic term by gas). The simulation findings were compared with the experimental results [14][15][16].

2.3. Interface determination (Free Surface)

In MPS method, the condition of free surface has been determined by the density of particles number. Since the particles are not arranged outside the free surface, so the particles on the free surface is determined based on reduction of particle number density. Therefore, when the explicit calculation is completed in the semi implicit algorithm, the calculated particle number density should be larger than introductory of particle number density

$$n^* < \beta n^0 \tag{3}$$

The value of β should be less than 1, which we used 0.95 in this calculation. In addition, the determination condition based on the general particle number density has been calculated and the Gotoh ASA conditions are applied as the auxiliary determination in the determination of free surface particles [17].

2.4. F_{ext} term model

As explain in 2.2, the external force term, $\boldsymbol{F}_{ext}$ contains the gravity term and the surface tension term (aerodynamic term by gas). In most cases (VOF method), the surface tension of the particle is used CSF (Continuum Surface Force) model and this model using inter-particle force by potential energy [18]. Since the CSF model calculates the curvature from the normal vector of the interface, the calculation tends to become unstable. Furthermore, when particles separate from the interface, they are not returned to the interface and are easily diffused as they are. In the surface tension model, the calculation is performed only by the particle position, so it is not necessary to calculate the curvature of the interface and it can be calculated stably without suddenly entering a large value. Due to this condition, the Ishii method which eliminated parameter adjustment and improved internal pressure of droplet was adopted in present study [19].

The normal force F_p, and the shear force F_s are applied on the interface between the gas and the particles. The calculation of F_s is normally leads for highly time consumed due to air flow boundary layer resolved. Based on this circumstance, F_p and F_s are being simplified as

$$F_P = p_i S n_i \tag{4}$$

$$F_S = \frac{1}{2}\rho S C_d (u_i^{gas} - u_i)\left|u_i^{gas} - u_i\right| \tag{5}$$

Here, S is representing the particle cross-sectional area (a particle) and C_d is the drag coefficient (sphere). Subscript i is represent the respective particle, which n_i is the normal vector on the inter surface, u_i^{gas} is the atmospheric gas velocity vector and u_i is the velocity vector. As a result, the surface force and shear force due to pressure from the gas phase can summarize as

$$F_{air} = F_{air} + F_s \tag{6}$$

2.5. Heat conduction model

After the droplet in contacted with the substrate, the hot temperature from the droplet and lower temperature of the substrate has been experience the heat transfer. Since the heat transfer in contact between two surfaces, so the heat conduction mechanism being used. This cooling process can be achieved by:

$$\frac{Dh}{Dt} = \nabla j \tag{7}$$

h is the droplet particle enthalpy (each) while J is the heat flux from droplet to the substrate which can be obtained by,

$$J = \frac{2k_1k_2}{k_1 + k_2}\nabla j \tag{8}$$

Here, both k_1 and k_2 are the thermal conductivity of liquid droplet and substrate. Please be noticed that this calculation has assumed that the thermal resistance contact between the interface is negligible, as similar as the calculation in VOF method [20].

2.6. Phase transition (solidification) model

Solidification and melting are the phase changes between liquid phase and solid phase. Unlike the phase change between the gas phase and the liquid phase, the density change in the phase change between the liquid phase and the solid phase is negligibly small. Therefore, by changing solid phase particles by solidification from liquid phase particles to wall particles has been conversely being done. In the calculation, the heat conduction term is explicitly discretized by the Laplacian model. Each particle holds temperature (in a function of enthalpy) as a variable and calculates heat conduction. In actual calculation, the solid phase ratio γ is introduced as a variable for each particle as a measure of phase change

$$\gamma = \begin{cases} 1 & (h < h_{s0}) \\ \dfrac{h_{s1} - h}{h_{s1} - h_{s0}} & (h_{s0} \le h \le h_{s1}) \\ 0 & (h > h_{s1}) \end{cases} \tag{9}$$

where h_{s0} is the enthalpy at the initial of melting process and h_{s1} is the enthalpy at the end of the melting process. In this case, if the solid phase ratio is equal to 1, it is completely solid phase, while if 0, it is completely liquid phase, and if the value lies between this value, it consider mixed (solid phase + liquid phase). However, in order to simplify the calculation, solid phase ratio was treated as divided into solid phase and liquid phase on the basis of 0.5.

3. Result And Discussion

Figure 4 shows the time history of speed the z - x cross section of the sprayed droplet collision process at a droplet velocity of 50 m/s and an initial temperature of the substrate of 300 K.

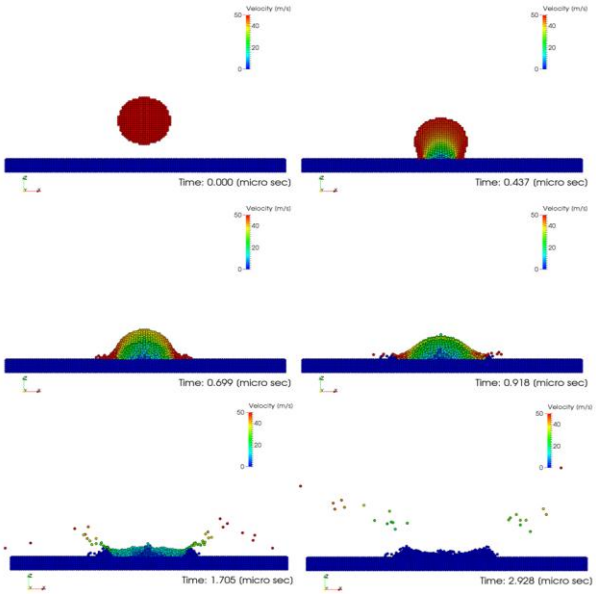


Fig.4: Time history of speed with base material temperature 300K.

Since it becomes easier to understand by visualization afterwards, we will look at the two-dimensional cross section. From the speed history in Figure 4, it can be seen that the collision of the droplet with the substrate causes the kinetic energy in the translational direction to be converted into the flattening direction. At this time, the droplet became a region of high velocity from the moment of collision to the outer edge part, and the region of low velocity was obtained at the center part. Thereby, the outer edge part of the droplet spreads in the direction of flattening, it can be said that it has almost no speed and is stationary. In other words, in the flattening process, the outer edge is moving most receiving the energy of the collision.

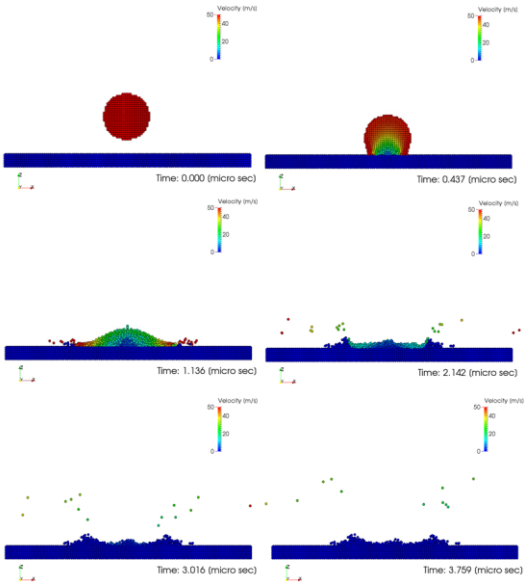


Fig.5: Time history of speed with base material temperature 675K.

Figures 5 show the velocity time history of state change of the sprayed droplet collision process at a droplet velocity of 50 m/s and an initial temperature of the substrate of 673 K. Even in the

flattening process of thermal spraying when the substrate temperature is high, the outer edge portion spreads flatly at a high rate as in the case where the substrate temperature is low, while being cooled from the outer edge portion and solidified. It turned out to be a result.

However, it can be seen that the angle formed by the outer edges after solidification is gentler than when the substrate temperature is low. This is thought to be due to the difference in cooling rate. When the substrate temperature is low, cooling occurs from the outer edge rapidly after the droplet collision. At this time, before the speed for flattening becomes sufficiently high, it is not possible to obtain a large velocity in the flat direction as the whole liquid due to solidification by cooling, and it cannot spread beyond the solidified portion and accumulates it can be said that it became a steep outer edge by having it. The phenomenon that the outer edge of the splat rises in this calculation shows the phenomenon similar to that seen in the actual sprayed splat and it is known that a dense splat can be obtained when the substrate temperature is high [2].

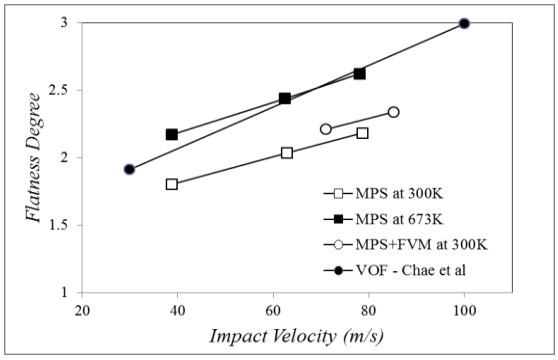


Fig.6: Flatness degree versus impact velocity.

The splat flatness degree as a function of the impact velocity of the droplet is shown in Figure 6. The flatness degree can be obtained as the ratio of the final splat diameter and the diameter of the particle just before impingement process. The figure shows the results of FVM + MPS coupled analysis and the uncoupled analysis (MPS) at two different temperatures of 300K and 673K. The result shows the flatness increases with the impact velocity, and as substrate temperature increased, the flatness degree also increases. For uncoupled MPS, at the initial temperature of 300K, the flatness degree is found to be proportional to Reynold number, $Re^{0.25}$, while in the case of 673K, the flatness degree is equivalent to $Re^{0.30}$. At 300K, the flatness degree of the FVM + MPS coupled analyses shows slightly higher than the results of the uncoupled analysis (MPS), where it proportional to the $Re^{0.26}$.

Table 1: Splat State

	Adhesion Efficiency (%)	Aspect Ratio
MPS	79.36	1.85
FVM + MPS	80.32	1.94

Table 1 shows the results of the MPS-only spraying analysis and the combined analysis of MPS method and FVM. The splat obtained by coupled calculation improved both adhesion efficiency and flatness compared with calculation of liquid alone. Although the adhesion efficiency improved by 1%, the flatness ratio improved nearly 10% on the basis of 1, and a very large difference was observed. This confirmed the influence of gas-liquid interference in flight and spraying droplet flight and collision flattening solidification process.

4. Conclusion

A new FVM and MPS coupling with virtual boundary method are successfully being established. The conclusions are;

(1) The plasma spray processes have successfully being observed, started with the acceleration and deformation of a droplet until the solidification process.
(2) The splat flatness for both temperature of 300K and 673K are agree well with the experimental result ($Re^{0.2\text{-}0.3}$).
(3) The virtual boundary method has worked well in simulating the full-scaled modeling calculation,
(4) Both adhesion efficiency and flatness has improved compared with calculation of liquid alone.

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