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Computer simulation of cold sprayed deposition using smoothed particle hydrodynamics

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Abstract

The smoothed particle hydrodynamics (SPH) method is applied to simulate the cold spray (CS) process by modeling the impact of a spherical powder particle on substrate. In this work, the adhesive interaction between the contacting surfaces is described by intersurface forces using the cohesive zone model. The application of the SPH method permits simulation of the impact process without the use of mesh and thus avoids the disadvantages of traditional numerical method in handling large deformations and tracing moving interfaces in the highly transient non-linear dynamic CS process. The simulated deformed particle shape evolution and estimated critical velocity from other sources were compared and good agreement was obtained. The analyses demonstrate the feasibility of the presented SPH methodology and the adhesive interaction model for simulating the deformation behavior of CS particles.

Keywords: Cold spray; Smoothed particle hydrodynamics; Critical velocity

1. Introduction

Cold spray (CS) is a materials deposition process in which relatively small particles of size range between 10 and 50 μm are accelerated in a supersonic inert gas flow and subsequently develop a coating on an appropriate substrate or a deposited layer of material by an impaction process. Upon impact above a critical velocity, the particles and substrate undergo intensive plastic deformation under high strain rate, and forms an interfacial bond [1-4]. The actual mechanism by which the particles deform and bond is still not well understood. This is because owing to the short duration of the impact process, it is impossible to observe the entire deformation process. Hence, it is difficult to investigate the particle/substrate interaction solely by experimental means. In this respect, numerical method is best suited for studying CS bonding mechanism. Past computational simulations [4-11] used mesh based Langrangian codes such as

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the finite element methods (FEM) and the Euler codes such as the finite difference methods (FDM) to investigate the bonding mechanism in CS. However, FEM is often associated with excessive distortion of mesh and FDM is difficult to trace free surfaces and moving interfaces, and deemed unsuitable for estimating the critical velocity [12-13]. Recent developments of the smoothed particle hydrodynamics (SPH) method and its applications in solving solid mechanic problems make it fairly attractive in simulating high velocity impact [12,14-15].

SPH is a mesh free, adaptive, Lagrangian particle method that uses smoothed particles as interpolation points to represent materials at discrete locations. This meshless nature allows it to handle problems with extremely large deformation and hence a better alternative to the traditional numerical methods in modelling the CS process. In a recent study Li et al. [12] successfully applied the SPH methodology to investigate the effect of oblique impact on particle deformation of CS particles. All particles from the simulation results were assumed to adhere onto the substrate. The paper demonstrates the feasibility of the SPH method for the simulation of the CS process but did not elaborate on the dominant bonding mechanism.

In this paper the application of SPH in simulating the CS process is presented. Dynamic strengthening of materials, generation of heat, heat conduction, thermal softening and adhesive interaction, are incorporated into the SPH model. The methodology adopted is mostly identical to that of Randles et al. [15], with minor alteration to facilitate interaction at the particle/substrate interface. The feasibility of the SPH method in predicting the deformation behaviour of CS particles was assessed through comparisons results using numerical and experimental results from other sources. The capability of SPH in modelling the CS process is discussed based on these findings.

2. SPH Methodology

SPH is a computational technique for problem solving in Computational Continuum Dynamics extended to treat the dynamics response of solids. Information is only known at discrete points (particles) and integrals are evaluated as sums over neighboring particles. Instead of a mesh SPH uses an interpolation kernel to evaluate these functions by obtaining the kernel estimates [14-15]. The kernel estimate of a function $f(x')$ at a certain position is given as

$$\langle f(x)\rangle = \int f(x')W\left(\frac{|x-x'|}{h}\right)dx' \tag{1}$$

where W is the smoothing kernel which has a width determined by the parameter h, the smoothing length. Identifying $\rho(x')\mathrm{d}x'$ as the differential mass dm and taking the summation of neighboring particles and the particle i itself, the discrete kernel estimate becomes

$$\langle f(x)\rangle \cong \sum_{i=1}^{N} m_i f_i W\left(\frac{|x-x'|}{h}\right)/p_i \tag{2}$$

In this framework the interpolation kernel is defined in terms of a cubic B-spline given in the following form:

$$W_4(v,h) = \frac{1}{\pi h^3}\begin{cases}\left(1-\frac{3}{2}v^2+\frac{3}{4}v^3\right) & 0<v<1\\ \frac{1}{4}(2-v)^3 & 1<v<2\\ 0 & \text{otherwise}\end{cases} \tag{3}$$

where $v = |x_j - x_i|/h$. The number of neighboring particles is limited within a distance of $2h$ from the kernel's peak, beyond which it goes to zero.

The continuum mechanical behavior of the model is described by the following conservation equations of continuum mechanics, written in the SPH framework, whereby the change in density, the acceleration, and the change in internal energy can be obtained from the equation of conservation of mass, conservation of momentum, and conservation of energy respectively.

$$\rho_i = \sum_j m_j W_{ij} \tag{4}$$

$$\frac{dU_i}{dt} = -\sum_j \frac{m_j}{\rho_i \rho_j}(\sigma_j - \sigma_i).\nabla W_{ij} \tag{5}$$

$$\frac{dE_i}{dt} = -\sum_j \frac{m_j}{\rho_i \rho_j}(U_j - U_i).\sigma_i.\nabla W_{ij} \tag{6}$$

where ρ is the scalar density, U is the velocity vector, E is the specific internal energy, σ is the stress tensor, and t is the time.

3. Particle/substrate Interaction Model

In the event of intimate contact between the particle and substrate surfaces, by assuming that bonding strengths arises as a result of secondary intermolecular forces at the interface, adhesive interaction between the contacting surfaces can be established using the cohesive zone model as illustrated in Fig.1. The constitutive relation of the model is specified in terms of the traction and separation distance across the contact interface. In this work, the Dugdale-Barenblatt cohesive zone model [16-17] was employed. The model assumes that the intersurface traction σ_o is constant when the separation distance δ is less than the critical separation distance δ_c. Typically, $\sigma_o \sim 10^7$ N/m^2 and $\delta_c \sim 10^{-8}$ m [18]. The work of adhesion of the interface is the area under the curve, i.e., $W = \sigma^* \delta_c$

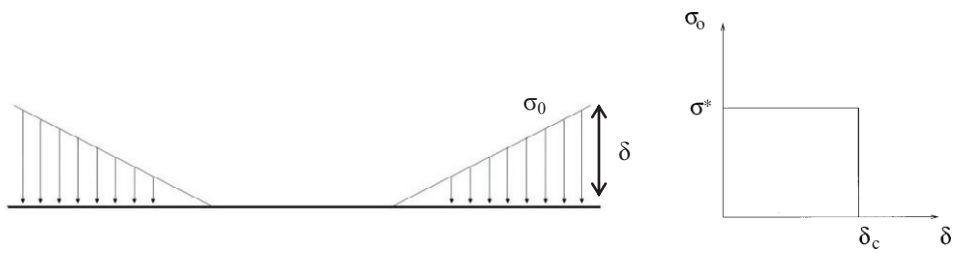

Fig. 1. Particle/substrate interaction due to intersurface traction, σ_o modeled by the Dugdale-Barenblatt cohesive zone model

Intersurface traction is activated only when contact between SPH particles of different bodies is established. Contact occurs when the distance between the particles are smaller than two times the smoothing length. The SPH particle from one body is treated as neighboring particle in another body, and the interaction between the two is solved automatically through the conservation of equations. The interface reaction model can be summarized as follows.

1. Driven by intersurface traction modeled by the Dugdale-Barenblatt cohesive zone model.
2. Limited to interaction of SPH particles from two different bodies.
3. Activated upon formation of mutually conforming contact surfaces.

4. Analysis

2D models were used to simulate the particle deformation behaviour. The width and height of the substrate were taken to be 6 times larger than the particle diameter. The particles were uniformly spaced in the x and y direction. The total number of powder and substrate particles varies depending on the inter-particle distance, which are determined according to the analysis. The distance between the powder particle and the substrate is 10 times the inter-particle distance so that there is no initial penetration. A fixed boundary condition was applied to the bottom plane and a free boundary condition for the others. The simulation was performed with initial particle velocity ranging from 500m/s to 1000m/s applied in the negative y-direction to all powder particles. The elastic behavior of the materials is described in terms of a linear Mie-Gruneisen equation of state [15]. The Johnson-Cook plasticity model [19] which accounts for strain, strain hardening and thermal softening, was employed to describe the plastic response of the materials. The model is an empirically based representation of the yield stress defined as

$$\sigma_Y = \left[A + B(\varepsilon_p)^n\right]\left[1 + C\ln(\dot{\varepsilon_p}/\dot{\varepsilon_0})\right]\left[1 - (T^*)^m\right] \tag{7}$$

where σ_Y is the yield stress, $\dot{\varepsilon}_p = (2/3)\sqrt{(3K_2)}$ is the equivalent plastic strain rate, K_2 is the second invariant of the plastic strain rate tensor, ε_p is the time integral of $\dot{\varepsilon}_p$, $\dot{\varepsilon}_0$ is the reference strain rate, usually normalized to 1.0/s, n is the work hardening exponent and A, B, C and m are constants. $T^* = (T - T_0)/(T_m - T_0)$, is the dimensionless temperature, where T is the temperature in Kelvin, T_m is the melting temperature of the material and T_0 is a reference temperature.

4.1 Defomation behaviour

The impact of a 25 μm copper powder particle on a steel substrate simulated using SPH was compared to the simulation results performed using the CTH code [11]. The CTH code implements the Eulerian method but mesh is allowed to distort together with the material. Remeshing is performed to overcome severe mesh distortion. Lund viscoplastic model and the Zerilli-Armstrong model was used to model the steel substrate and the copper powder particle respectively. The parameters of the Johnson Cook model and the state of equation for copper and steel used in the SPH model are obtained from the literatures [7,20]. The shape evolution of the deformed powder particle and substrate impacted at 700 m/s modelled by SPH and CTH is shown in Fig 2. Upon impact the powder particles and the substrate undergo plastic deformation. The spherical powder particle is flattened and a crater is generated in the flat substrate. Intensive deformation occurs at the contact zone between the powder particle and substrate indicated by the red region in Fig. 2a, where the effective plastic strain exceeds the rupture strain. There is a good agreement between the results obtained by SPH and CTH.

4.2 Particle velocity range for deposition

The impact of a 25 μm aluminium powder particle on a steel substrate simulated using SPH was compared to the analytical result obtained in literature [21]. Wu et al. calculated the adhesion energy and the rebound energy to estimate the particle/substrate interaction. The particles were assumed to deposit when the adhesion energy is above the rebound energy. The critical and maximum velocity is determined to be where A-R (adhesion energy minus rebound energy) equals to zero. The parameters of the Johnson Cook model and the state of equation for aluminium and steel used for the SPH model are obtained from the literatures [7,20,22]. The particle velocity range for deposition of a single aluminium powder particle impacting on a steel substrate at different particle velocities modelled by SPH and calculated using the

adhesion and rebound energy equation is depicted in Fig 3. From analyses of the SPH simulation, the critical and maximum velocity is obtained by analyzing the rebound distance of the powder particle. Rebound distance is defined as the average distance between the contact surface of the powder particle and the substrate after a certain impact time. When no rebound is observed, rebound distance is taken as 0 and the particle is assumed to have deposited onto the substrate. Powder particles were also observed to rebound at low and high velocities. Deposition range of the powder particle estimated using SPH and A-R equation is 450 m/s - 1000 m/s and 480 m/s - 1000 m/s respectively. The SPH results compare fairly well with the analytically obtained results.

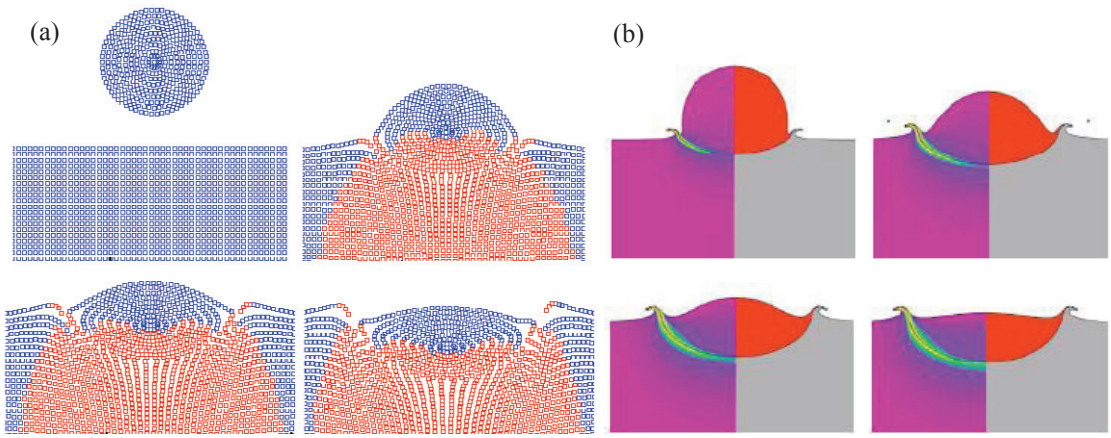

Fig. 2. (a) SPH and (b) CTH simulation of deformed copper particle on steel substrate impacted at 700 m/s from 0-250 ns

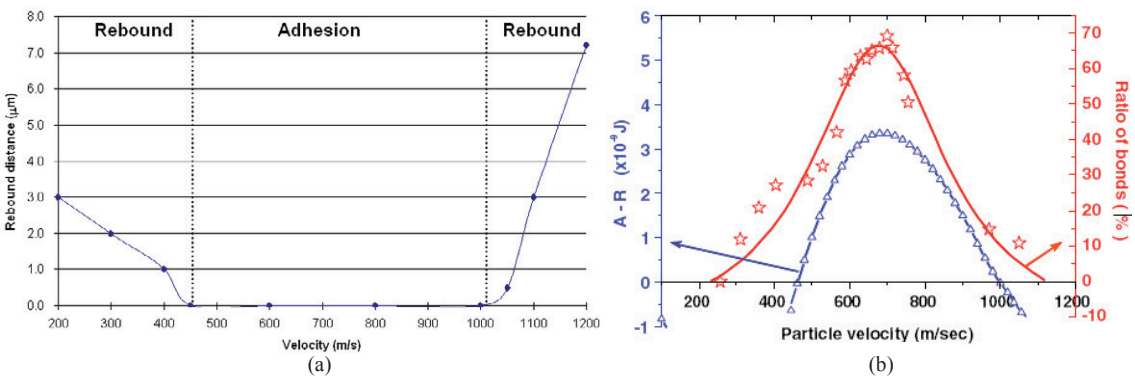

Fig. 3. Critical and maximum velocity calculated using (a) SPH and (b) adhesion and rebound energy equation

5. Conclusion

In this paper, the deposition mechanism of the high pressure type CS technique is investigated through numerical simulation using the SPH method by modelling the impact of spherical powder particles on substrate. Based on the results, the following conclusions can be drawn:

1. The particle deformation behavior modeled by the SPH method compares fairly well to that modeled by the Eulerian method which indicates the feasibility of the SPH method for simulating the impact behavior in cold spraying.
2. The cohesive zone model can be used to describe the particle/substrate interaction correctly.
3. A rebound phenomenon was observed in which there exists a particle velocity range where deposition occurs.
4. The SPH method can be used as a tool to predict particle velocity deposition range and optimize spray parameters for different materials.

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