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COMPUTATIONAL MODELLING OF COLD SPRAY PROCESS USING PARTICLE-BASED METHODS

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Abstract. Cold gas dynamic spraying (CGDS), as a high strain rate shearing and innovative solid-state technique enables to rapidly develop additive manufacturing and coating for metal deposition. This paper investigates the development and evolution of various interfacial bonding characteristics during high strain rate shearing process through Multiphysics numerical simulations of single particle impact. Two different particle-based modeling strategies such as smoothed particle hydrodynamics (SPH), molecular dynamics (MD) are investigated using commercial software ABAQUS/Explicit and LAMMPS, respectively. To separate the difficulties related to complex metallurgy of alloys, our first investigations focus on pure aluminum. The Johnson-Cook (J-C) constitutive model is used to describe the high strain rate self-consolidation process in SPH modeling. Embedded Atom Method (EAM) is used to describe the interactions between Aluminum atoms in MD modeling. The predictions from the different particle-based models are compared with each other and with experimental results. Through the investigations, SPH numerical approach has strong advantage in capturing the phenomena that occur during the cold spray process. It is able to describe the complex features of particle and substrate, especially in the interface vicinity. At the same time, MD numerical approach gives the fundamental understanding of the deposition behavior at the atomistic level. The key finding is the strong relationship between the un-uniform distribution of shear strain and jet formation during high-speed collision. Plastic strain along with an increase of temperature lead to thermal softening of pure Aluminum resulting in metallurgical bonding at the interface.

Keywords: Smoothed Particle Hydrodynamics, Molecular Dynamics, Impact Bonding, Cold Spray.

1 INTRODUCTION

The cold spray process is an additive method that uses the supersonic collision of micron sized powders. The powder is sprayed by the expansion of a gas throughout a convergent-divergent nozzle. This principle was development in the 1980s and today, it offers a perspective of eco-friendly additive route for diverse metals, in addition to diverse realisations in the field of the coating technology [1]. The spraying conditions use a gas compressed at high pressure with the possibility to work at low temperatures, and to cover thereby a wide variety of materials [2-4], for applications in aerospace, automotive, electronics, and other industrial sector, or for repair application as well [5, 6]. The computational analysis of the powder response during the high-speed collision is a particular topic of the cold spray technology because such collision process is governed by a high-strain rate regime. The computational approach has the capability to provide an in-situ, short scale, and real-time understanding of the particle response which can be difficult to track by means of an experimental observation [7, 8]. Basically, there are computational simulations at the scale of the powders up to the macroscopic scale of the deposit, using diverse methos such as Eulerian, Lagrangian, Coupled Eulerian Lagrangian (CEL), Arbitrary Lagrangian Eulerian (ALE) and SPH [9].

In this study, we focus on the application of particle-based methods to comprehensively model and simulate the cold spray process, especially for the single particle impact behaviour. The model consists of a smoothed particle hydrodynamics (SPH) method for the macroscopic analysis of the particle deformation, and a molecular dynamic (MD) method to highlight the complex microscopic phenomena within the particle at a very short scale. Each model is presented in this paper and applied to the cold spray deposition of a single Aluminium powder onto an Aluminium substrate, identified in the literature [16].

2 METHODOLOGIES

2.1 Smoothed Particle Hydrodynamics

The smoothed particle hydrodynamics (SPH) method is a kind of computational technique used for simulating and modelling fluid flows and other physical phenomena, especially to describe extreme plastic deformation behaviour. Unlike element-based methods, SPH represents fluid as a collection of discrete particles, where each particle could carry properties such as pressure, velocity, density and so on. The specific foundation of SPH method is the interpolation theory detailed in literature [10].

The single particle impact behaviour of pure Aluminium particles impacting on a pure Aluminium was investigated. 3D model was used to simulate the high strain rate self-consolidation as shown in Figure 1. The diameter of spherical particle of pure Aluminium was set to be 20 μm, which is corresponded to the average size of the Aluminium particles in the in-situ observation. The radius and the height of the substrate were taken to be 2.5 and 2.5 times larger than the particle radius. A fixed boundary condition was applied to the bottom of the substrate. Whereas free boundary condition for other areas. The impacting single particle was given a uniform velocity field of 800 m/s. The computational model was meshed using 8-node brick element that considers bilinear in displacement and linear in temperature. An extremely fine element size with 0.6 μm was adopt in both the particle the impact region to obtain the distribution of stress, strain and temperature accurately.

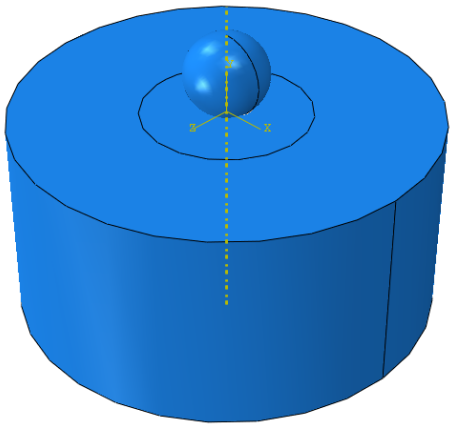

Figure 1: Schematic diagram of 3D model with SPH method.

In addition, to facilitate direct comparison with in-situ observations, all setup parameters and boundary conditions of the 3D model in ABAQUS / Explicit were kept the same as in the experiment. The impact behaviour between particle and substrate is assumed to be an adiabatic process. In the simulation, a linear Mie-Gruneisen equation of state (EOS) was employed for the elastic behaviour of Al 1050, The linear Hugoniot form ($U_S - U_P$) can be linearly described:

$$P = \frac{\rho_0 C_0^2 \eta}{(1 - S\eta)^2}\left(1 - \frac{\Gamma_0}{2}\eta\right) + \Gamma_0 \rho_0 E_m \tag{1}$$

η represents the nominal volumetric compressive strain;
ρ_0 represents is the initial density;
ρ represents the current density;
C_0 represents the bulk speed of sound;
Γ_0 represents the material constant;
S represents the linear Hugoniot slope coefficient;
E_m represents the internal energy per unit reference specific volume.

The microparticles always undergo severe deformation upon impact. High strain rate shearing needs to be modelled for capturing behaviours of impact particle during cold spray impact process. To describe the dynamic severe deformation behaviour, the Johnson-Cook plasticity model was used to determine the effects of plastic deformation, strain-rate hardening and thermal softening [11]. The specific equation of this model is defined as:

$$\sigma = (A + B\varepsilon^n)\left(1 + C\, ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\left[1 - \left(\frac{T - T_{reference}}{T_{melt} - T_{reference}}\right)^m\right] \tag{1}$$

Where *A, B, C, n* and *m* are the materials constants from experiment. σ is the equivalent plastic stress. ε^n is the equivalent plastic strain. $T_{reference}$ is the reference temperature. T_{melt} is the melting point. From various experiments and simulations, it can be concluded that the fraction of plastic deformation converted into heat energy is almost 0.9 due to the heat fraction. Due to the plastic dissipation, there will be an associated increase in temperature. Thus, 90% of the plastic strain energy is assumed to be dissipated during the simulation. In that case, all the material properties of pure Aluminium were taken from the literature [12].

2.2 Molecular Dynamics

Molecular dynamics is a versatile and widely used computational simulation method applicated in physics, chemistry, and materials science to investigate the dynamic behaviour of molecules and atoms by simulating their interactions over time. It provides insights into the motion, interactions, and thermodynamic properties of molecular systems. In our study, molecular dynamics simulations were performed based on LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code from the literature [13]. The interactions between pure Aluminium atoms were described by Embedded Atom Method (EAM). Based on the atomic scale, we considered establishing a model of single particle impact on the substrate with a diameter of 200 Å, and a cuboid single Aluminium substrate of size 400×400×600Å, as shown in Figure 2. In this study we only consider a pure single crystal Aluminium / Aluminium system without considering an oxide layer. The visualization tool (OVITO) is used to obtain the atomic stress, strain, temperature, dislocations and configurations during the molecular dynamic simulation [14].

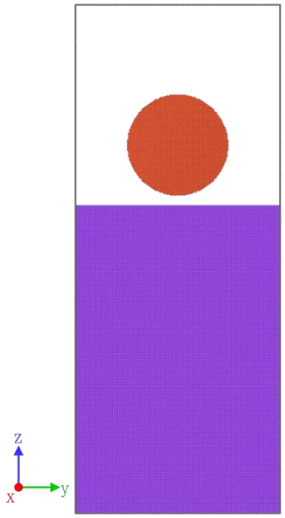

Figure 2: Schematic diagram of 3D model with SPH method.

3 RESULTS AND DISCUSSION

Figure 3 shows the contours of the Von Mises stress, effective plastic strain and temperature as pure Aluminum particle impacts on the substrate at 800 m/s. It is obvious that the single particle underwent severe plastic deformation forming crater on the flat substrate. The maximum plastic strain is located at the interface between the particle and the substrate. Whereas the maximum stress is located under the inner deflection of the impact particle. Since the temperature of the metal material is related to plastic deformation, and since the maximum strain is close to the surface due to the large deformation of the particle, it is obvious that the maximum temperature could be found near the interface. Both the particle and substrate participate in the formation of the jet.

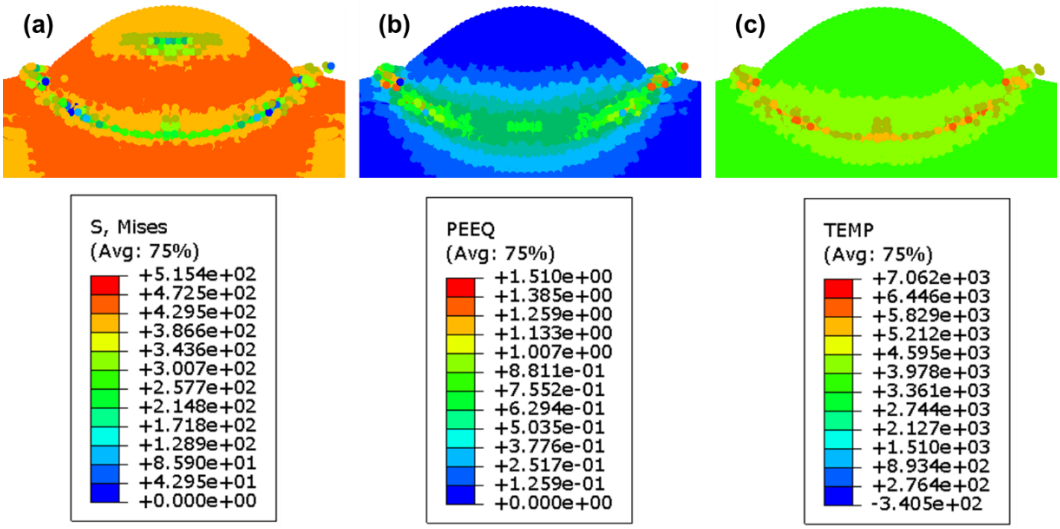

Figure 3: Snapshots of (a) stress, (b) shear strain and (c) temperature profiles after impact with SPH method.

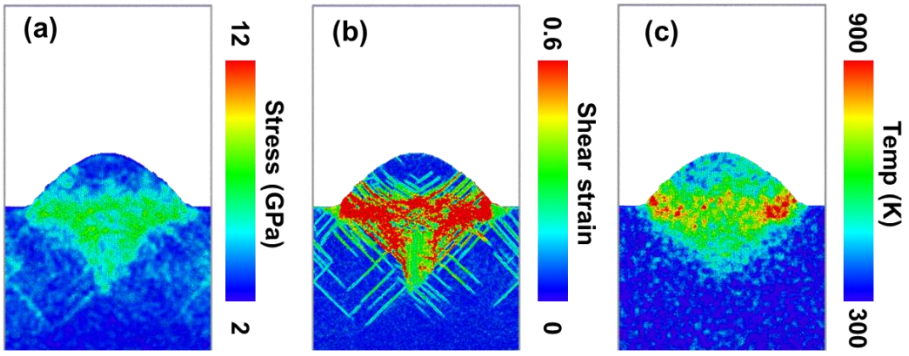

Figure 4: Snapshots of (a) stress, (b) shear strain and (c) temperature profiles after impact with MD method.

Figure 4 shows the snapshots of the Von Mises stress, effective plastic strain and temperature distribution after impact with MD method. The MD method predicts that at the given impact velocity of 800 m/s, the spherical Aluminum particle is also flatten and a crater is generated on the flat substrate. Temperature contour reveals that localized heating near the impact region. But it is difficult to obtain the jet generation from MD simulation.

The microstructural snapshot of the pure Aluminum splat region coated on the pure Aluminum substrate at the impact velocity of 800 m/s. Then the local atomic microstructure is colored based on common neighbor analysis (CNA) approach [15] as shown in Figure 5. The colors in Figure 5 show the specific atomic microstructures: grey means atoms which do not have any crystalline structure, green is FCC, red is HCP, blue is BCC. The particles form shallow craters on the substrate and create a thicker melted region along the interface during the high strain rate shearing. At this interface, most of the atoms form a thicker amorphous structure. The interface across the amorphous structure shows the onset of metallurgical bonding at this shearing strain rate.

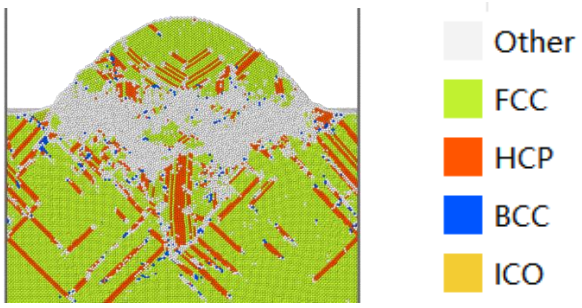

Figure 5: Microstructural snapshot after the impact with MD method. FCC (green), HCP (red), BCC (blue) and grey (atoms without crystalline structure).

As can be seen in Figure 6, when plastic deformation proceeding at a very high strain rate and causes a single particle to reach metallurgical bonding with the substrate, most of the crystals in the lower half of the particle undergo severe plastic deformation and form a dense dislocation network structure.

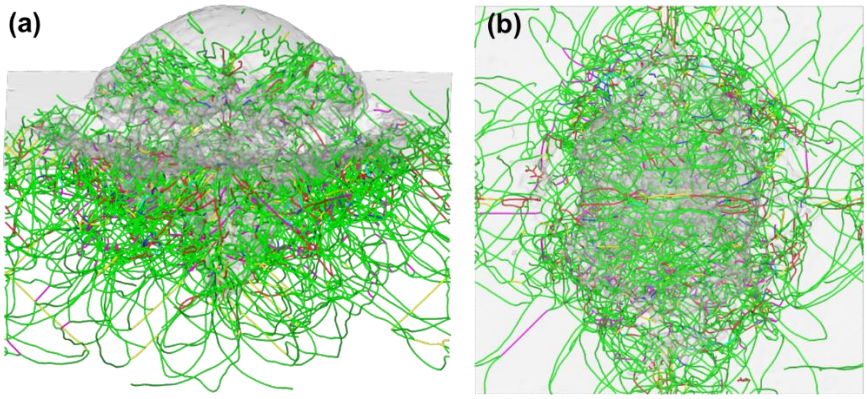

Figure 6: Dislocation network after the impact with MD method. (a) side view; (b) top view.

Figure 7 shows the scanning electron microscope (SEM) images obtained from the in-situ experiment for the bonded splats of a 20 μm Aluminium powder particle impacted onto a flat Aluminium substrate at 700 m/s, 800 m/s, respectively. From the in-situ results it can be seen as the particle velocity increases, the plastic deformation of the particles and substrate increases. Compared to the in-situ observations, the SPH method and MD method have strong advantage in capturing the phenomena especially the plastic deformation in the Cold spray process. It can describe the complex features of particle and substrate, especially in the interface.

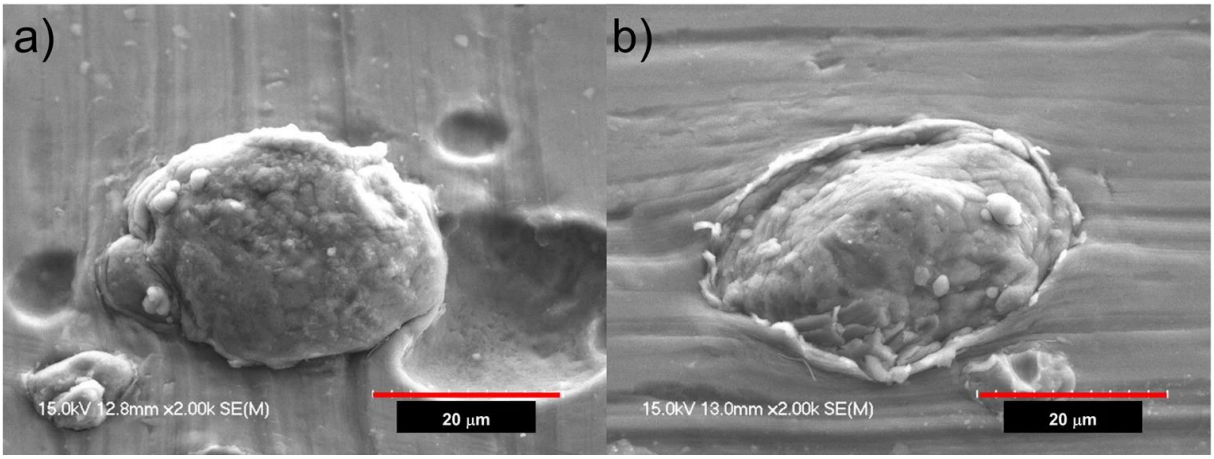

Figure 7: SEM images obtained from the experiments for the bonded splats of a 20 μm powder particle impacted onto the surface of a flat Aluminum substrate at particle velocities: (a) 700 m/s; (b) 800 m/s. [16]

4 CONCLUSIONS

This paper investigates the computational analysis of cold spray deposition of an Al particle onto an Al substrate using two particle-based method: a SPH method for the macroscopic deformation of the powder due to the high-speed collision, and a MD method for the subscale phenomena at the atomic scale. The major conclusions can be depicted as following.

- The simulations showed that while there is some localized heating during impact, the overall temperature rise in the system remained relatively low, supporting the cold spray's characteristic minimal thermal impact. High-velocity particle exhibited significant deformation as they approached the substrate.
- In particular, SPH method is suitable for simulating extreme deformation while low computational accuracy in this study. MD method gives a good understanding of atomic level mechanism and has the capability of modelling microstructure transformation and dislocation movement during high strain rate shearing.

In conclusion, this study has demonstrated the significant potential of particle-based methods, namely SPH and MD simulations to understand the complex multiscale phenomena during the cold spray process.

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Conflicts of Interest: The authors declare no conflict of interest.

REFERENCES

[1] Koithara, L. L., Raoelison, R. N., Costil, S. Flow phenomenon of micron-sized particles during cold spray additive manufacturing: High-speed optic observation and characterization. *Adv. Powder. Technol.* (2020) **31**(3): 1060-1079.

[2] Raoelison, R. N., Koithara, L. L., Costil, S. Cold spray coating of PEEK surface by copper deposition: Interfacial adhesion at high deposition efficiency and bonding strength. *CIRP J Manuf. Sci. Tec.* (2021) **35**: 63-68.

[3] Raoelison, R. N., Aubignat, E., Planche, M. P., et al. Low-pressure cold spraying under 6bar pressure deposition: Exploration of high deposition efficiency solutions using a mathematical modelling. *Surf. Coat. Technol*. (2016) **302**: 47-55.

[4] Koithara, L. L., Raoelison, R. N., Costil, S., et al. High deposition efficiency and delamination issues during high-pressure cold spraying metallization of PEEK using spherical copper powders. *Int. J. Adv. Manuf.* (2020) **107**: 4427-4436.

[5] Raoelison, R. N., Xie, Y., Sapanathan, T., et al. Cold gas dynamic spray technology: a comprehensive review of processing conditions for various technological developments till to date. *Addit. Manuf.* (2017) **19**: 134-159.

[6] Raoelison R N, Verdy C, Liao H. Cold gas dynamic spray additive manufacturing today: Deposit possibilities, technological solutions and viable applications. *Mater. Des.* (2017) **133**: 266-287.

[7] Raoelison R N. Analytical description of solid particles kinematics due to a fluid flow and application to the depiction of characteristic kinematics in cold spraying. *Powder. Technol.* (2017) **319**: 191-203.

[8] Raoelison R N, Koithara L L, Costil S, et al. Turbulences of the supersonic gas flow during cold spraying and their negative effects: A DNS CFD analysis coupled with experimental observation and laser impulse high-speed shadowgraphs of the particles in-flight flow. *Int. J. Heat. Mass. Tran.* (2020) **147**: 118894.

[9] Adaan-Nyiak, M. A., Tiamiyu, A. A. Recent advances on bonding mechanism in cold spray process: A review of single-particle impact methods. *J. Mater. Res.* (2023) **38**(1): 69-95.

[10] Li, W. Y., Yin, S., Wang, X. F. Numerical investigations of the effect of oblique impact on particle deformation in cold spraying by the SPH method. *Appl. Surf. Sci.* (2010) **256**(12): 3725-3734.

[11] Henao, J., Bolelli, G., Concustell, A., et al. Deposition behavior of cold-sprayed metallic glass particles onto different substrates. *Surf. Coat. Technol.* (2018) **349**: 13-23.

[12] King, P. C., Bae, G., Zahiri, S. H., et al. An experimental and finite element study of cold spray copper impact onto two aluminum substrates. *J. Therm. Spray Technol*. (2010) **19**: 620-634.

[13] Thompson, A. P., Aktulga, H. M., Berger, R., et al. LAMMPS-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Comput. Phys. Commun.* (2022) **271**: 108171.

[14] Stukowski, A. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. Modelling Simul. *Mater. Sci. Eng.* (2009) **18**(1): 015012.

[15] Reddy, C. D., Zhang, Z. Q., Msolli, S., et al. Impact velocity-dependent bonding mechanisms in metal cold spray. *Surf. Coat. Technol.* (2022) **433**: 128085.

[16] Manap, A., Okabe, T., Ogawa, K., et al. Experimental and smoothed particle

hydrodynamics analysis of interfacial bonding between aluminum powder particles and aluminum substrate by cold spray technique. *Int. J. Adv. Manuf.* (2019) **103**: 4519-4527.