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Numerical Modelling and Application Potential of the Cold Spray Method

Abstract: The article presents the theoretical and practical aspects of the Cold Spray method numerical modelling, indicates the main numerical analysis research areas (particle speed modelling and particle deformation modelling), determines the major parameters considered during simulation, demonstrates analysis-based correlations as well as presents recommended software, modelling examples and their major problems, modelling result verification methods and their practical usability. The article also evaluates the usability of numerical analyses by demonstrating the application potential of Cold Spray method.

Keywords: Cold Spray method, numerical analysis

Introduction

Works related to modelling of the Cold Spray powder spraying process cover two major research areas, i.e. modelling of powder particle velocity and modelling of powder particle deformation. The numerical simulation of gas/powder velocity enables the determination of the gas state parameters both inside the nozzle and once the gas has left it as well as the distribution of powder particle velocity and temperature. Results are verified using experimental measurements performed usually by means of a quick-capture camera. The use of numerical methods for modelling particle deformation enables tracking the course of deformations, particle and substrate temperature as well as determining critical gas/powder velocity. These quantities help understand the layer formation mechanism as the experimental tracking of the joint formation process during cold spraying is difficult due to the short process duration (amounting to a few nanoseconds) and

its non-linear course. Metallographic analyses following the spraying process, in spite of being very useful, are not able to precisely determine the course of the process.

Modelling of Powder Particle Velocity

Due to the low molecular mass, the gas used as the working gas in the Cold Spray method is usually air, nitrogen, helium and their mixtures [2]. According to the one-dimensional isentropic approximation [5], gas velocity in the de Laval nozzle contraction is the product of the adiabatic curve exponent, gas temperature and individual gas constant (equal to the universal gas constant divided by the gas molecular mass). Due to the differences in the molecular mass and adiabatic curve exponent, it is more convenient to use helium and not nitrogen as the working gas. However, due to its high cost, helium is rarely used in practice. During spraying, the gas velocity increases also along with the temperature increase. In turn, pressure

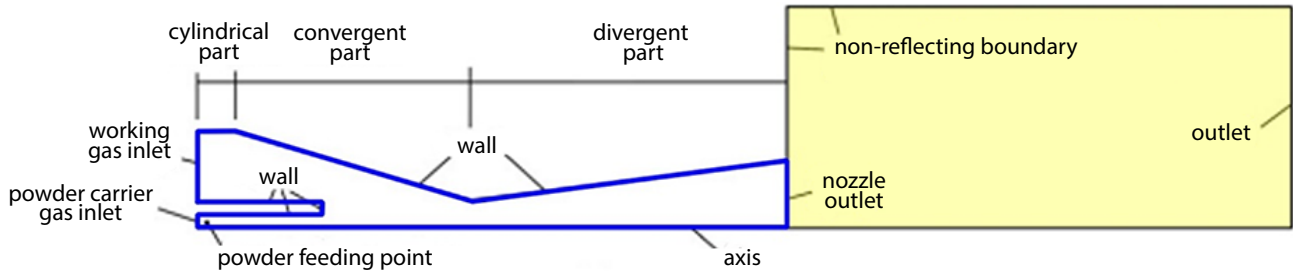


Fig. 1. Nozzle scheme used in the simulation [11]

causes the increase in gas density and, as a result, the increase in force affecting powder particles [3]. The simulation calculations for copper particles having a diameter of 22 μm at a temperature of 200°C and a pressure of 2.1 MPa revealed that powder particles in the helium stream reached 42% of the gas velocity, whereas in air they reached 62% of the working gas velocity [4]. This divergence is mainly due to the 2.5-fold difference between the gas velocities.

For the purpose of more precise representation of process-accompanying conditions analyses involve the use of numerical simulation packages, e.g. in Ansys Fluent software, solving the time-related Navier-Stokes equation [6,7]. The simulation primary variables are nozzle geometry, gas parameters (mainly temperature and pressure) and powder properties [8,9]. The most commonly used nozzle is the de Laval nozzle having a circular cross-section, yet also rectangular cross-section nozzles are used [10]. The nozzle geometry is described by the length of the convergent part and that of the divergent part as well as by the diameter of contraction and that of the outlet (Fig. 1) [3,11]. The optimum particle acceleration is that for the nozzle having a Mach number of approximately 4 or 6.25 for the nozzle divergent part length of 100 and 40 mm respectively. The Mach number is the quantity strictly dependent on the nozzle geometry and is calculated from the nozzle outlet area - contraction area ratio. In simulation tests, the nozzle geometry is optimised depending on the material sprayed, e.g. for the 316L stainless steel [9]. Behind the nozzle outlet, a cylindrical element is usually modelled, the purpose of which is to simulate the atmosphere

(air) where powder particles move after leaving the nozzle [11,12]. It is also necessary to model the substrate on which the layer is to be applied as this enables the observation of gas and particle trajectory after contact with the substrate material [13].

In the model, powder particles are treated as a discrete phase dispersed in a continuous phase and introduced by means of appropriate modules, e.g. in Ansys Fluent by means of the DPM module [14]. The particle motion equation is described by means of the Langrange equation.

As need may be, the simulation can be performed as 2D or 3D. In order to save computational time, only two dimensions are usually used [9,12]. The numerical simulation enables the determination of gas state parameters both inside the nozzle and after leaving it by gas, as well as the powder particle velocity and temperature distribution, where, depending on the gas used the particle velocity is increased by 50 m/s and 200 m/s for nitrogen and helium respectively [12]. In addition, modelling the gas stream interaction with the substrate surface

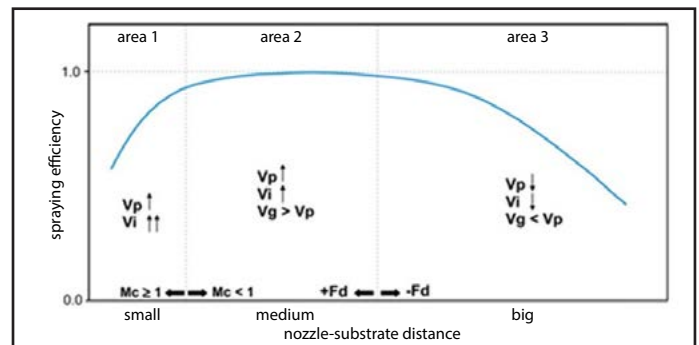


Fig. 2. Effect of the nozzle-substrate distance on spraying efficiency, F_d – resisting force, M_c – Mach number along the nozzle axis, V_g – gas velocity, V_i – velocity of impact into the substrate, V_p – velocity of the oncoming particle [15]

enables the determination of the substrate temperature during spraying, as well as the observation of shock wave formation in front of the substrate surface. Depending on the material and powder particle sizes, after leaving the nozzle, particles can accelerate over a certain distance or their velocity can instantly become lower. For this reason the distance between the nozzle and the substrate has a significant effect on spraying efficiency (Fig. 2) [15].

In low-pressure spraying, due to the characteristic structure of the nozzle, which does not widen continuously but by the stepped diameter change, in the divergent part it is possible to observe the change of gas velocity (Fig. 3).

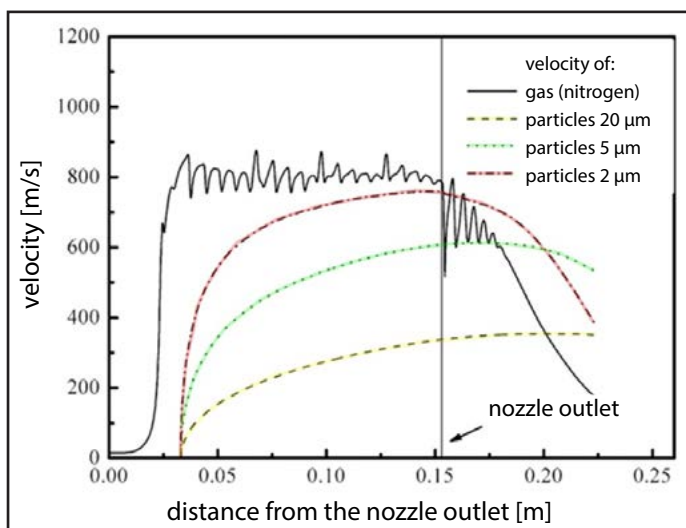


Fig. 3. Change of gas velocity in the function of process parameters for the spherical copper particles in nitrogen having a pressure of 0.7 MPa and a temperature of 573 K during low-pressure spraying [11]

Presently, devices for measuring gas/particle velocity in the Cold Spray method, verifying numerical simulation results, are manufactured by two companies, i.e. Canadian Tecnar (DPV200 and AccuraSpray) and Finnish Oseir (Spray Watch). Initially the devices were intended for plasma spraying processes, hence velocity measurements were possible for particles having a temperature of $1000^{\circ}\text{C} \div 2000^{\circ}\text{C}$. In the Cold Spray method, due to the lack of particle radiation it is necessary to add laser beam backlighting [16,17]. To satisfy this need the companies offer additional measurement device accessories such as a diode laser. The

scheme of particle velocity measurement using the DPV2000 device is presented in Figure 4 [18]. The device is composed of a CCD camera and a diode laser enabling the backlighting of powder particles. It is important that the camera sensor should cover the whole particle flux width. When the shutter is open (for approximately $100 \mu\text{s}$) the particle flux is backlit by the laser. The distance between the successive light points on the camera matrix is measured and processed using image processing algorithms. The powder particle velocity is determined by dividing the distance measured between the points by the time between the successive laser impulses. This method is characterised by very high accuracy [19,20].

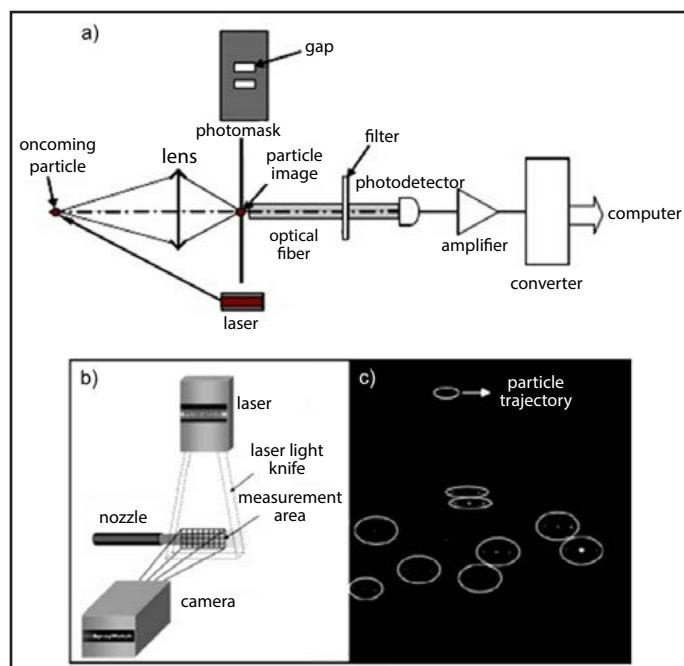


Fig. 4. Stand for measuring gas/particle velocity: scheme of DPV-2000 stand (a), additional laser backlight support (b) and diode laser backlit particles (c) [18,20]

An alternative method used for velocity measurement during spraying is the laser-based velocity measurement with the Doppler method, yet this method is time-consuming and, in consequence, costly. In addition, this method is also troubled by problems accompanying the implementation of the stand due to significant temperature changes during the process. The LDV method was used, among others, by S.V. Klinkov [21,22] or A.N. Papyrin [23].

Modelling of Powder Particle Deformation

The use of numerical methods enables the analysis of deformation courses, powder particle and substrate temperature as well as the determination of the critical gas/powder velocity [1]. The critical velocity criterion adopted is the presence of adiabatic shear bands in the material. In the numerical model the rapid temperature increase with the simultaneous stress decrease is regarded as the moment of adiabatic shear band appearance [24]. The joint requires a temperature equal to 60% of the material melting point, and such a temperature is adopted for the determination of critical velocity [25] (Fig. 5).

Modelling the particle impact against the substrate is performed using software packages, e.g. Autodyn [26], LS Dyna [27] or Abaqus [28]. The model tends to include one particle and the

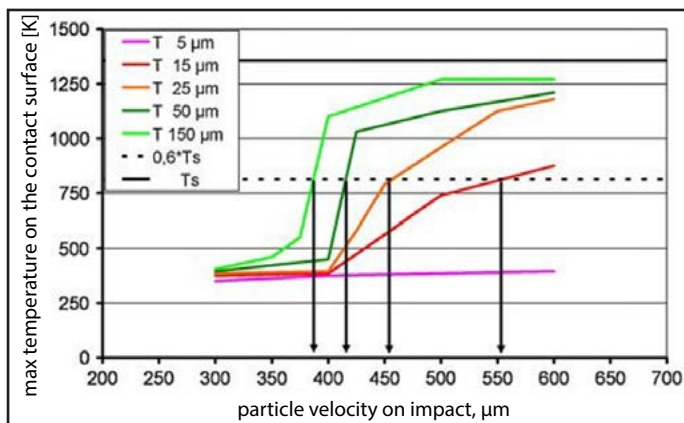


Fig. 5. Temperature on the powder-substrate contact surface during spraying in the function of velocity for various copper particle sizes [25]

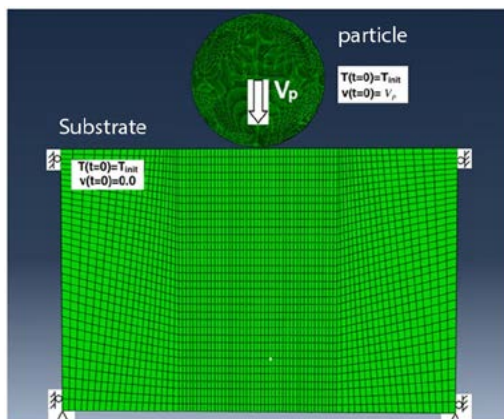


Fig. 6. Computational model scheme for the particle hitting the substrate

substrate. Particle agglomerates are modelled rather rarely [29]. The substrate is usually modelled as the cylindrical surface, whereas the particle is usually spherical. Figure 6 presents the exemplary computational model scheme along with boundary conditions.

In spite of the commonly known correlation between the application efficiency and the impact angle, most simulations are performed for the impact taking place at the right angle [1]. This results from the fact that in most of the tests, emphasis was given to the binding mechanism of the particle and the substrate depending on the types of interacting materials, velocity, temperature, particle oxidation degree and temperature as well as substrate preparation. It is possible to use the symmetrical model and, as a result, limit the simulation time [1,30-32]. Few simulations for impacts at an angle revealed the reinforcement of the energy dissipation effect by friction and, in consequence, the presence of local shear instabilities. The moment tangent component appearing in such a case can be responsible for particle tearing off [25].

The material model used is the Johnson-Cook model. It is commonly used for modelling the behaviour of metal alloys in conditions of high deformation velocity, e.g. for impacts at a significant velocity. In addition, the model takes into consideration the thermal plasticisation and, due to this fact, can be used within a wide temperature range.

Due to significant deformations of mesh elements causing the unrealistic appearance of the particle-substrate contact line, it is often necessary to additionally use the Johnson-Cook model or the Lagrange-Euler adaptive mesh [27,28,34,35]. The analyses revealed that numerical simulations show significant convergence with experimental results [36]. The exemplary comparison of the copper particle deformation due to the impact against the substrate while spraying (numerically calculated and experimentally tested) is presented in Figure 7.

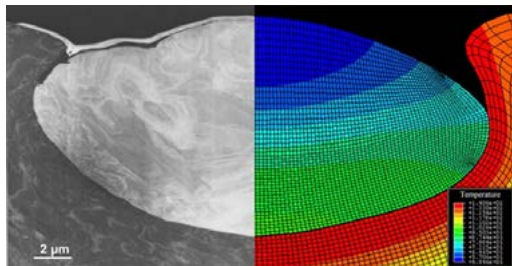


Fig. 7. Deformation of the copper particle sprayed using the Cold Spray method: the TEM photograph (a) and numerical calculations (b) [36]

As regards the combination of particle velocity and temperature during spraying for specific parameters and the particle impact simulation, it is possible to optimise the process both in terms of efficiency and properties of coatings. Using the coefficient η equal to the impact velocity-critical velocity ratio, it is possible to roughly assess coating parameters (see Figure 8a) [37,38]. The market already offers commercial software applications based on this ratio, enabling the drawing of charts related to coating properties and efficiency in the function of process parameters (Fig. 8b). The dependence between the coefficient η and the

coating adhesion results from the fact that the higher the impact velocity in relation to the critical velocity, the greater the area of particle joint with the substrate and, as a result, the greater the adhesion [39]. The example of such a joint area is presented in Figure 9 [39]. If the area reaches 100% of the contact area, the maximum adhesion (close, even to the sprayed material strength value) is obtained [37-39]. However, it should be noted that increasing the velocity is possible only to a certain value, which if exceeded does not lead to the increase in efficiency and improvement of coating properties but leads to degradation caused by the excessive particle deformation [25].

Cold Spray Method Application Potential

The wide Cold Spray method application range justifies the usability of numerical analyses. Taking into consideration the anticipated development of this technique it is necessary to expect its application potential. Thermally sprayed

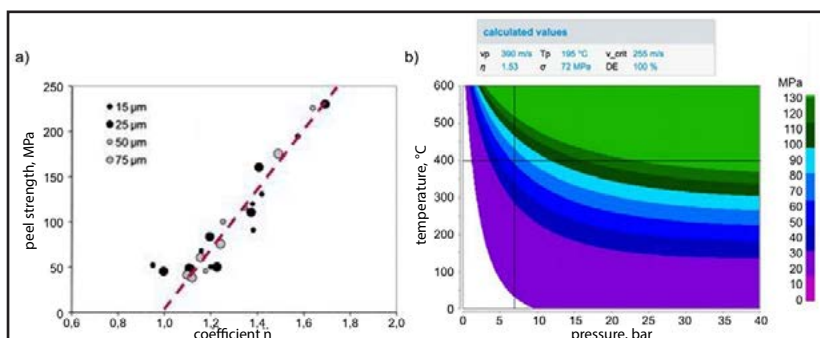


Fig. 8. Adhesion of copper coatings sprayed using the Cold Spray method in the function of coefficient η for various sizes of particles (a), chart of parameter selection for zinc in the function of temperature and gas pressure (b) [37,38]

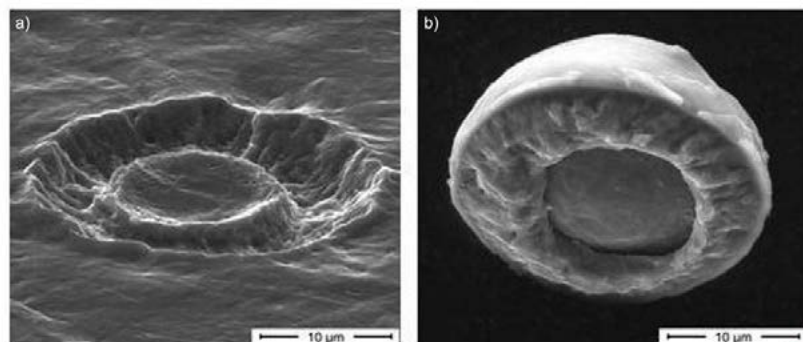


Fig. 9. Trace after the removed Ti-6Al-4V particle for Ti (parameters $T = 780^{\circ}\text{C}$, $p = 3.8 \text{ MPa}$, nitrogen) (a) and the particle itself (b)

coatings are usually evaluated taking three aspects into consideration, i.e. adhesion to the substrate, porosity and oxide contents in the layer. Presently, Cold Spray enables the obtaining of coatings characterised by very low porosity and oxide content and, at the same time, high adhesion. Until today it has been possible to obtain layers of powders of many materials and even composites and cermets. In addition, the lack of thermal stresses in the layer and substrate increases the Cold Spray method application spectrum in comparison with other spraying methods. Cold Spray can be used for applying coatings on all engineering materials, i.e. metal alloys, plastics, ceramics, glass and composites. Already today the Cold Spray sphere of applications is vast and includes, primarily, the following areas [33]:

- anticorrosive protections,
- thermo and electroconductive tracks,
- prototyping (making spatial structures),
- regeneration of tools and machinery parts,
- filling losses in casts and machined elements,
- heat resistant coatings,
- coatings of increased abrasive wear resistance,
- layers resistant to cavitation damage,
- coating with reduced friction coefficient,
- applying metallic filler metals,
- plastic spraying,
- intermediate layers in welding,
- protective and sealing layers,
- nanolayers,
- porous layers,
- decorative layers,
- special applications.

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