Computer simulation of spray deposition process for $Al_{1.0}Si_{0.6}Mg_{0.6}Mn$ alloy

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1. Introduction

The spray deposition process is the combination of a rapid solidification of the disintegrated droplets after atomization and a subsequent slower cooling of the bulk material after deposition. The resulting material properties are critically controlled by a number of process parameters, such as the superheat of the melt, the gas pressure, the ratio of the flow rate of the molten material and the atomization gas or the flight distance of the disintegrated droplets. By optimization of the relevant process parameters, the spray deposition process becomes suitable to produce homogenous, segregation-free materials with fine grain structures, increased solubility of alloying elements and small sized precipitates [1]. The details of the spray deposition process and properties of aluminum alloy can be found in ref. [1-9].

Some authors pointed out an undesirable increase of porosity in characteristic regions of the deposit [2, 3], which can be explained by the disturbance of the ratio between the deposition rate and deposit surface cooling rate, during the deposition process.

To reduce the experiment costs and the research period, numerical simulation is widely used and has been proven to be an effective way to optimize the process parameters and give guidance for design of atomizer, during the development of spray process equipment [4].

The aim of this investigation is modeling of the spray-deposition process for different aluminum alloys. Numerical simulation software has also been developed which has possibilities of adjusting both different materials and variation of the corresponding process parameters. Using of this numerical simulation, selection of optimal parameters for spray deposition process is much easier and, thus, impact on reducing of the porosity of the obtained deposits.

2. Model formulation

The basic stages of the process are: gas atomization of molten alloy and deposition of spray particles onto the substrate [2] (Figure 1).

The computer program is based on three physico-mathematical algorithms: (a) temperature-velocity profile of particles after gas atomization of molten alloy, (b) deposition rate in the spray cross-section area, and (c) spray deposit cooling conditions. On the basis of initial physical assumptions, algorithms are developed in a sufficiently dense numerical solving pattern, to provide enough accuracy of the calculation.

3. Atomization and the temperature-velocity profile of spray particles

The velocity profile of the particles is defined by dependence of gas velocity at particular distance from the atomizing nozzle and it can be described by an empirical relation for the particular nozzle [7]:

$$V_g = V_{go}(1 - D/D_0)^2 \tag{1}$$

Where are: V_g (m/s) – gas velocity; V_{g0} (m/s) – initial gas velocity; D_0 (m) – characteristic distance for gas velocity decrease; D (m) – distance from nozzle. These quantities are functions of atomization and nozzle parameters.

The velocity profile of particles in the gas stream, defined by (1), is obtained from the next differential equation, which is involved numerically [3]:

$$m\frac{dV_d}{dt} = C_{drag} \cdot \rho_g \cdot V_r^2 \cdot \frac{A}{2} + mg \tag{2}$$

where are: m (kg) – mass of the particle; Vd (m/s) – velocity of particle; $V_r = V_g - V_d$ – velocity of the particle relative to the velocity of the gas, ρ_g (kg/m³) gas density; A (m²) – cross-section area of the particle and C_{drag} – drag coefficient.

Temperature profile of particle is obtained by numerical solving of Eqs. (3)-(5):

$$mC_d\Delta T = h \cdot A \cdot \left(T_d - T_g\right) + \sigma \cdot \varepsilon \cdot A \cdot \left(T_d^4 - T_g^4\right) \tag{3}$$

where are: T_d (K) – temperature of the particle; T_g (K) – temperature of the gas stream, ΔT (K) – temperature change of the particle; C_d (Jkg⁻¹K⁻¹) – specific heat of the particle; h (Wm⁻²K⁻¹) – heat transfer coefficient; σ – Stefan-Boltzmann constant and ε – emissivity.
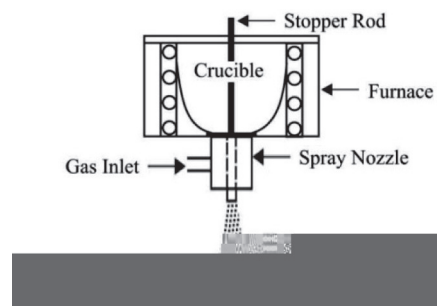

Figure 1. Schematic presentation of the spray deposition process.

The first term at the right side in Eq. (3) refers to convection described by the heat transfer coefficient, h, and the second term refers to radiation. Temperature-velocity profiles are calculated for particles of diameters d = 10, 20, ...,250μm, the range of distances D = 0 - 2000 mm. The time step in all calculations is 1.3 μs.

Sudarea şi Încercarea Materialelor

3.1. Deposition rate

The deposition rate is determined by the normal Gaussian distribution:

$$V_y = V_0 \cdot e^{-\beta R^2} \tag{4}$$

where are: V_y (m/s) – deposition rate; V_0 (m/s) – deposition rate at spray axis; β – radial distribution coefficient and R – distance from the spray axis.

Deposition rate at spray axis, V_0, is the function of a melt flow, distance and spray cone angle. The radial distribution coefficient depends on distance and cone angle. Deposit growth on the rotating substrate is numerically calculated with time step of 50ms. Rotation period of substrate is 1 second. To accomplish the necessary deposition rate, the substrate axis of rotation is placed at the certain distance from the spray axis, DC.

3.2. Deposit cooling conditions

The solid phase content, g, in the spray before compacting must be in the range g = 0.7 to 0.9 [2, 7]. It can be considered that a thin layer of semi-solid/semi-liquid material exists on the spray-deposit surface. It is also assumed that below this layer the material is at a solidification range temperature in such way that only the solidification rate of this thin surface layer should be discussed. This assumption is based on the fact that cooling of the deposit surface throughout the substrate becomes negligible already after approximately 80mm of deposit height, because of the high porosity at the substrate deposit boundary [2, 3], as well as removing the substrate from the compact surface. This condition is realized by preheating the substrate in initial stage of spray deposition. This allows considering the cooling of the deposit, only in the stream of atomizing media.

Spray deposit surface cooling is characterized by the solidification rate [8] which is given by:

$$V_{fs} = \frac{h \cdot \Delta T_c}{(1-g)H_{fs}\rho_m} \tag{5}$$

where are: V_{fs}(m/s) – solidification rate; ΔT – temperature difference between spray and gas; $\Delta T_c = T_{sp} - T_g$, T_g – gas temperature, T_{sp} – average spray temperature; ρ_m – density of solid phase and H_{fs} – latent fusion heat of the material.

3.3. Incoming data

The necessary process parameters and material constants, for solving previously defined problem, are specified in Tables 1and 2. The applied gas in numerical simulation is nitrogen. The adopted parameters of the apparatus in the calculation are:

- spray cone angle is 15º ,
- characteristic distance for gas velocity decrease D_0 = 5m.

Granulometric distribution of alloy particles represents the input data for numerical simulation and is determined on the basis of the atomization parameters and experimental work given by Tomic [9].

4. Results and discussion

Mathematical model of the spray deposition process constitutes a system of equations (1)-(5), which is solved numerically by Runge – Kutta method. The numerical computer simulation is developed in order to define process parameters and to obtain deposits with exactly determined geometry and controlled level of porosity. Some relevant process parameters for the spray deposition process and controlling of the grain size, as the type of gas, and nozzle parameters, are constant parameters in this work, while some are variable, like the type of used metal powder, distance between nozzle, and substrate surface and its type.

After the selection of material and corresponding process parameters, this software enables graphic presentation of deposit growth onto the rotating substrate and deposition conditions.

Substrate distance for spray compacting is chosen in such a manner that the content of solid phase of the spray is provided to be g = 0.8 [2, 3].

Table 1. Parameters of used gas in the simulation of spray deposition process

Gas parameters		
pressure	p	1,2 MPa
initial velocity	V_{g0}	600 m/s
dynamic viscosity	μ_g	$1.7 \cdot 10^{-5}$ kg/ms
specific heat	c_g	1040 J/kgK
density	ρ_g	1.25 kg/m³
thermal conductivity	k_g	0,024 W/mK

Table 2. Parameters of used alloys in the simulation of spray deposition process

Alloys parameters		
Melt stream diameter	D_1	0.005 m
Melt flow rate	I_m	0.03 kg/s
Melt superheat	TSH	715 ºC
Melt density	ρ_m	2550 kg/m³
Solidus temperature	T_s	555 ºC
Liquidus temperature	T_1	650 ºC
Fusion heat	Q_m	396 kJ/kg
dynamic viscosity	μ_d	0.0042 kg/ms
thermal conductivity	k_d	213 W/mK
specific heat of alloy	c_d	886 J/kgK

A presentation of deposit growth for t = 1200s and substrate diameter D_{sb} =150mm is given in Figure 2. The thickness of deposits is greatest near the centre of rotation and decreases towards the periphery. Larger is the thickness of the deposite non-uniformity is more pronounced. Thinner deposits had almost uniform thickness.

Figure 3 represent distribution of V_y/V_{fs} ratio across the deposit. The numbers in oblique brackets on Figure 3, represent V_y/V_{fs} ratio. In the central area of deposit this parameter has a maximum, $(V_y/V_{fs} = 1)$. Deposit height has a maximum in the same area to, and we can expect minimum of porosity in this case.
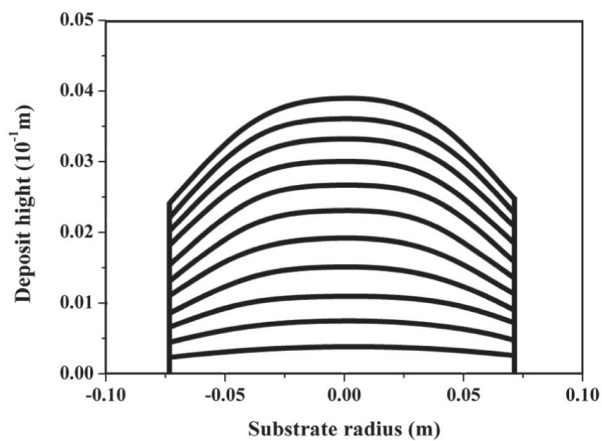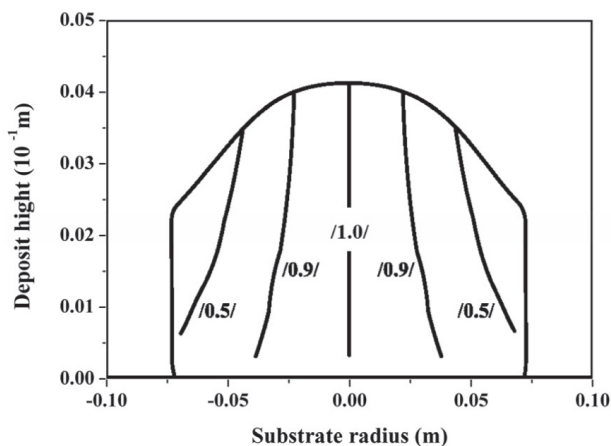
Figure 2. Deposit growth for D = 400mm.

Figure 3. Predicted variation of V_y/V_{fs} ratio across the deposit.

The very important condition for growth of good quality spray deposit is that the solidification rate of the semi-solid/semi liquid surface layer is equal to the spray deposition rate. Disruptions of this condition produce undesirable porosity and microstructure of the final deposit.

5. Conclusion

In this work was performed modeling of spray deposition process of materials with complex chemical composition onto rotating substrate. Solving the mathematical model is done numerically and own software was developed. The results of numerical simulations show that:

If solidification rate of the semi-solid/semi liquid surface layer is equal to the spray deposition rate, then the good quality spray deposit can be expected, especially in the central deposition area (between substrate rotation axis to $R_{sb}/2$).

With increasing distance from the deposit axis, the ratio V_y/V_{fs} decreases, causing increase in porosity.

Results of the numerical simulation can be useful for selection of the optimal spray deposition process parameters.

Acknowledgements

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