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# Numerical simulation EF/VOF to study the influence of the surface condition of the formation of the slats of a nickel deposit produced by plasma spraying

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*ABSTRACT.* The goal of the present work is within the framework of a better comprehension of the production of a coating by plasma projection. It concerns the numerical study of the formation of splats whose stack on the substrate leading to the coating of the substrate. The application of the model, two-dimensional, uses the finite element method and the fluid volume method (VOF) to solve the governing equations, and to enable to study the impact, the spreading out and the solidification of a ceramic drop on a metal substrate and the change of the temperature of the substrate. It predicts the morphology of the slate and eventual splashes during spreading. The results were compared with the results of other authors simulations, obtained under the same conditions. Through this study, it was found that the condition and the preheating of surface play a very important role in the morphology and formation of splats.

*RÉSUMÉ.* Le but du travail actuel est dans le cadre d'une meilleure compréhension de la production d'un enduit par la projection de plasma. Il concerne l'étude numérique de la formation des splats dont la pile sur le substrat menant à l'enduit du substrat. L'application du modèle, bidimensionnel, des utilisations la méthode d'élément fini et la méthode liquide de volume (VOF) de résoudre les équations de gouvernement, et de les permettre d'étudier l'impact, étendre et la solidification d'une baisse en céramique sur un substrat en métal et la variation température du substrat. Il prévoit que la morphologie de l'ardoise et le certain éclabousse pendant la propagation. Les résultats ont été comparés aux résultats d'autres simulations d'auteurs, obtenus dans les mêmes conditions. Grâce à cette étude, il a été constaté que l'état de surface et le préchauffage jouent un rôle très important pour la morphologie et la formation des lamelles.

*KEYWORDS:* finite element, formation of splats, numerical simulation, plasma spraying, volume of fluid (VOF).

*MOTS-CLÉS: élément fini, formation de lamelles, simulation numérique, projection plasma, volume of fluid (VOF).*

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## 1. Introduction

Among all phenomena which utilize the impact of drops on a surface, the production of coatings per pulverization or plasma, are industrial processes used very much. This type of process is also used in many areas, such as inkjet printers, standard cleaning product, and car paints. All uses have as a common objective to cover a surface by a material with minimum matter and low regular thickness, in order to ensure the insulation, better properties or simply the esthetics of the finished product (Fauchais *et al.*, 2001).

The realization of coatings per pulverization of fine droplets on a surface to be covered is a subject with increasing research. In order to include/understand the morphology of the coating (Sayed, 2004), it is interesting to examine the dynamic and thermal phenomena on drops which will create the fine layer (Pasandideh-fard *et al.*, 1998), at the droplets scale. These initially liquid particles are crushed on the substrate, are spread out or burst, cooled during their contact and more or less solidified during a time period more or less long depending on the frequency and conditions of impact (Escure *et al.*, 2001; Goutier *et al.*, 2012).

Physics phenomena around the crash behaviour of a drop still today poorly controlled, although many studies, experimental and numerical, have improved the understanding of the flow of the liquid particles (Ahmed *et al.*, 2001) have studied numerically impact and solidification of an aluminium droplet on rough substrates, using a two-dimensional axisymmetric model. Their results show that the droplet impact on a rough substrate is almost always accompanied by splashing. However, the degree of splash decreases with increasing roughness (Cedelle *et al.*, 2006), also studied the influence of stainless steel substrate preheating on the surface topography and on millimeter- and micrometer-sized splat formation. Their results show that the resulting splats are in the shape of disc when the substrate is preheated at the top of the temperature of transition. And that the presence of the nonpeak increases the contact angle of the liquid on the tierce substrates reducing the thermal resistance of contact at the interface. Other work has provided a theoretical model, based on the volume of fluid (VOF), to study the droplet spreading and solidification Whereas the surface tension, solidification and thermal contact resistance (Zhang *et al.*, 2001; Zirari, 2011) and they noticed that the size, speed, and temperature of a droplet of both the substrate and the temperature of the material play significant roles in the morphology of the impact and the solidification rate.

Fataoui *et al.* (2010) has shown, in the two-dimensional axisymmetric model coupling, the impact speed and the solidification, that solidification starts when the drop reaches a temperature below the melting temperature, which contributes to faster freezing the material and decreases the kinetic energy of the system which reduces the spread rate.

Zhang *et al.*, (2017) have studied the extension of the lifespan of pulling-straightening rollers, for this purpose they have prepared a conventional zirconia thermal barrier (TBC) coating and nanoscale zirconia on the roll surface of H13 steel and observed using a confocal laser remelting microscope and a thermomechanical simulator. The properties of TBCs prepared by plasma spraying and laser remelting were examined separately. Calculations of the surface temperature distribution of the roll are made with ABAQUS. They have proven that TBCs can extend the life of the roll. Unlike conventional plasma spray coating, laser remelting and nano-scale zirconia particles can reduce the number of pores and microcracks in coatings and thus improve the quality of TBCs. Both methods also contribute to the thermal shock resistance of TBCs. This research on the properties of TBC provides a solid foundation for the application of TBC on pulling-straightening roller.

In this study we are interested in modeling and digital simulation of impacts dynamic coupled with cooling and solidification of the droplets. Our numerical study aims to integrate the key parameters as well as possible to act on the solidification of a plate under conditions of plasma projection: temperature of the substrate, and of the jet. In order to be able to compare our calculations resulting from a numerical strategy, considering dynamic coupling, and heat transfer, with experimental data, we chose nickel as the projected material, which is molten on a substrate of rough surface of stainless steel.

The work done is organized as follows: section 2 presents the mathematical model, section 3 describes the results obtained and interpretations, section 4 gives a comparison between the cases studied and finally a conclusion.

## 2. Mathematical formulation

Numerical simulation of drop impact on a substrate calls upon the solution of several equations which couple the thermal and dynamics aspects. This part is dedicated to the presentation of the equations and the numerical method used which enable to solve them. The thermo-physical properties of the materials are given in Table 1 (Xue *et al.*, 2006) The physical domain with boundary conditions is illustrated in Figure 1.

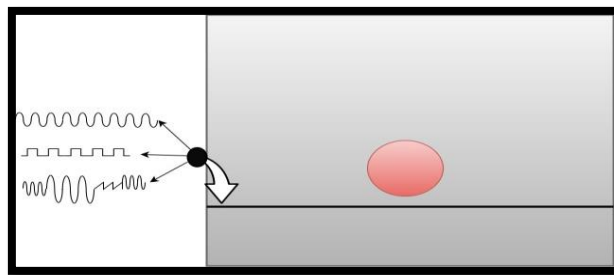


Figure 1. Physical domain of a nickel droplet impacting a substrate

*Table 1. Thermo-physical properties of nickel and stainless steel*

| properties                              | Nickel    | Stainless steel |
|---|-----------|-----------------|
| Density [kg/m <sup>3</sup> ]            | 7900      | 7900            |
| Melting point [°C]                      | 1453      | -               |
| Heat of fusion [J/kg]                   | 310,000   | -               |
| Kinematic viscosity [m <sup>2</sup> /s] | 6.E-7     | -               |
| Liquid thermal conductivity [W/(mK)]    | 90.7      | -               |
| Liquid specific heat [J/(kgK)]          | 609       | -               |
| Surface tension [N/m]                   | 1.778     | -               |
| Solid thermal conductivity [W/(mK)]     | °C        | °C              |
|   | 527 67.6  | 127 16.6        |
|   | 727 71.8  | 327 19.8        |
|   | 927 76.2  | 527 22.6        |
|   | 1227 82.6 | 727 25.4        |
|   |           | 927 28.0        |
|   |           | 1227 31.7       |
| Solid specific heat [J/(kgK)]           | °C        | °C              |
|   | 527 530   | 127 515         |
|   | 727 562   | 327 557         |
|   | 927 594   | 527 582         |
|   | 1227 661  | 727 611         |
|   |           | 927 640         |
|   |           | 1227 682        |

**2.1. Dynamic model**

In the VOF method, the cell containing a fluid is governed by the following equations (Abdellah El-Hadj *et al.*, 2010).

$$\vec{\nabla}(\alpha \cdot \vec{\nabla})=0 \tag{1}$$

$$\frac{\partial(\alpha \cdot \vec{\nabla})}{\partial t} + (\alpha \cdot \vec{\nabla} \cdot \vec{\nabla}) \vec{\nabla} = -\frac{\alpha}{\rho} \vec{\nabla} p + \nabla^2 \vec{\nabla} + \frac{\alpha}{\rho} \vec{F}_b \tag{2}$$

Where  $V$  is the velocity vector,  $\rho$  is the density,  $p$  is the pressure,  $\alpha$  is the fraction of fluid volume (kinematic viscosity) and  $(t)$  the time. The body force applied to the fluid. The surface tension is an important parameter that contributes in to the deformation of the droplet. It is considered as a volume force applied to the free surface of the liquid. The electrostatic forces between the molecules of the surrounding gas are very small compared to those of the liquid due to their molecular distances. The resultant of the forces is directed toward the inside of the particle. This force characterizes the liquid surface tension (N/m). The liquid evolves spontaneously to minimize its surface tension (its free surface energy). According to the VOF methodology, the fraction volume of fluid  $\alpha$  is used for the whole domain where its value indicates the presence or the absence of the fluid. We attribute the value of 1 for a point occupied by the metal and 0 in the other domain part. The mean value in the element presents the function of the fluid volume occupied by the metal.

$$\alpha = \begin{cases} 1. \text{inside the fluid} \\ 0 < \alpha < 1. \text{contain a free surface} \\ 0. \text{empty cell} \end{cases} \quad (3)$$

The element with  $\alpha$  value of  $\alpha$  between 0 and 1 contains the free surface or the interface. To find  $(x,t)$  for all points of the domain of the interface it necessary to solve the transport equation.

$$\frac{\partial \alpha}{\partial t} + V \cdot \nabla \alpha = \frac{d\alpha}{dt} \quad (4)$$

With  $\alpha(x, 0) = \alpha_0(x)$

## 2.2. Heat transfert model

The SH Method is used in order to take into account the phase change in the metal particle. This formulation uses the equivalent specific heat which takes in account the latent heat in the energy equation as (Manual of Ansys ver 11):

$$\frac{\partial(\rho h)}{\partial t} = \rho C_p \frac{\partial T}{\partial t} - \rho L_f \frac{\partial f_s}{\partial t} = \rho C_p^{eq} \frac{\partial T}{\partial t} \quad (5)$$

Where  $h$  is the enthalpy,  $T$  is the temperature,  $C_p$  is the metal specific heat,  $C_p^{eq}$  is the equivalent specific heat,  $L_f$  is the latent heat of fusion and  $f_s$  is the solid fraction.


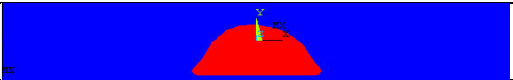

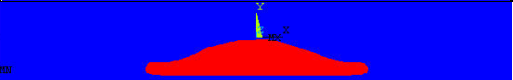

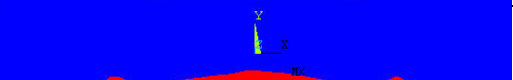

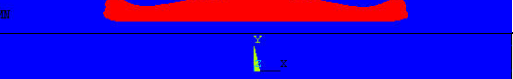

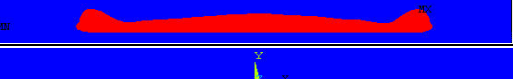

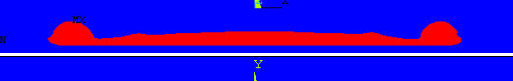

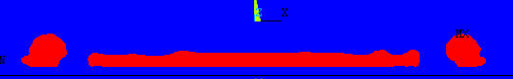

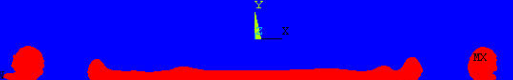
## 3. Results and discussion

### 3.1. Validation of the model

Table 2 represent the results of simulation of the other authors and them ours respectively, for the impact of a Nickel droplet on a rough stainless steel substrate for the same conditions of (Xue *et al.*, 2006). One can note that the dynamic behavior of the droplet as a whole gives an good agreement with that of the experimental images,

the droplet is propagated symmetrically with respect to the point of impact, however, the convex form lowers the slope in time while sliding slowly on the substrate until spreading out completely, it should be noted that the liquid follows the topography of surface, and on rough surface, the flow is vertically disturbed. I.e., when the liquid runs out on surface it tends to follow the form of the surface.

Table 2. Impact of a nickel drop under the same conditions simulated by

| a. simulation   | b. Simulation  |
|---|--|
| <p>0.25 <math>\mu</math>s</p>    |    |
| <p>0.5 <math>\mu</math>s</p>     |    |
| <p>0.75 <math>\mu</math>s</p>    |    |
| <p>1.0 <math>\mu</math>s</p>    |   |
| <p>1.25 <math>\mu</math>s</p>  |  |
| <p>1.5 <math>\mu</math>s</p>   |  |
| <p>2.0 <math>\mu</math>s</p>   |  |
| <p>3.0 <math>\mu</math>s</p>   |  |

### 3.2. Cold substrat

Table 3 represents the temperature distribution during the impact of a droplet in a substrate with rough surface (round-off, square and random). The splats are presented in the form of disc surrounded by a splashed zone. The side matter flows coming from the central part and separates at high speed of the principal edge at the periphery, of the plates in the shape of “finger”, stuck to the central part before “exploding” in fine plates and small droplets to form a crown, is different depending on the surface quality from substrate. The finest central zone corresponds to the zone of impact. Houben *et al.* (1988) and Zhao *et al.* (2015) proposed a model based on the creation of a shock wave. The origin would be then energy coming from the initial impact which would

cause the expulsion of “film” in contact with the substrate and the formation of a crown of the type “splash”. Mostaghimi and its collaborators (Bussmann *et al.*, 1999; Aziz *et al.*, 2000) suggested that the beginning of solidification of the particle intervened at the end of spreading out and consequently could cause a phenomenon of ejection on the peripheral zones with formation of the matter fingers. These results are in contradiction with Gougeon and Moreau (Gougeon & Moreau 2001) which showed that particles are spread out over larger surface because of their initial kinetic energy. When this kinetic energy is completely dissipated, the surface tension causes a surface contraction and the ejection of the liquid of the upper part. The numerical results also indicated that the time of spreading out of the splats, differs depending on the surface quality, for most complicated (random)  $t=4.6\text{ms}$  and that we did not obtain a good spreading out which is due to the large forces of frictions; on the other hand it is noted that in rough surface (square), and because with the sharp angles,  $t=5\text{ms}$  which delays a little the spreading out, but in (round-off) a very good spreading out is obtained a runs time  $t=4.1\text{ms}$ .

Table 3. Distribution of the temperature at the time of the impact of a nickel drop of 2.5mm of diameter on a rough substrate cold of 25°C with impact speed of 2.5m/s

| Time (ms) | Round form | Square form | Random form |
|-----------|------------|-------------|-------------|
| 0         |            |             |             |
| 0.45      |            |             |             |
| 1.35      |            |             |             |
| 2.45      |            |             |             |
| 3.2       |            |             |             |
| 3.95      |            |             |             |
| 4.6       |            |             |             |
| 5         |            |             |             |

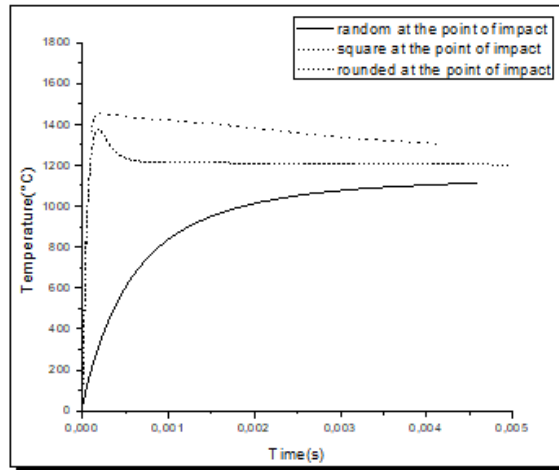
Figure 2a, b, and c shows clearly appearance of zones of good and of bad contacts with the interface particle/substrate suggesting a bad transfer of heat transfer from the particle towards the substrate, which involves a low speed of cooling. The effect of “splashing” of the nickel splats is marked here, probably because of a lower viscosity.

One can also note that, at the very first moments following the first contact of the drop with the target, the temperature of substrate at the point of impact increases quickly (Figure 3.a) and thermal resistance decreases. After a partial spreading out, the surface of contact between the substrate and the drop increases, whereas the temperature of the substrate remains quasi-constant. The temperature of substrate increases much more slowly whereas the temperature of surface of the drop drops;

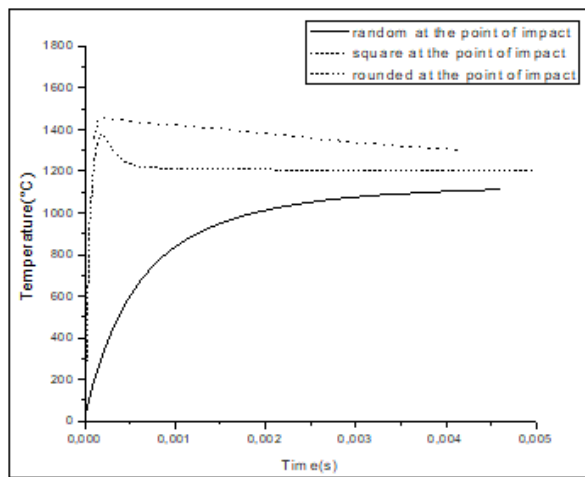
thus the associated resistance of contact increases, which supports the radial thermal diffusion process in the plate.

Figure 3 compares the factor of spreading out of the nickel drop in the suggested model (between the three forms of roughness).

The spreading out and the shape of the drop are similar during the impact for the three forms. For example, in the round form, at the moment  $t=4.1\text{ms}$ , the drop stabilizes and takes the form of the final spreading out. The results of the model presented are very close for the three forms. In our model, we take into account the effect of solidification on the viscosity forces before spreading out, which are corrected after each time step under the transfer effect of heat in the particle.

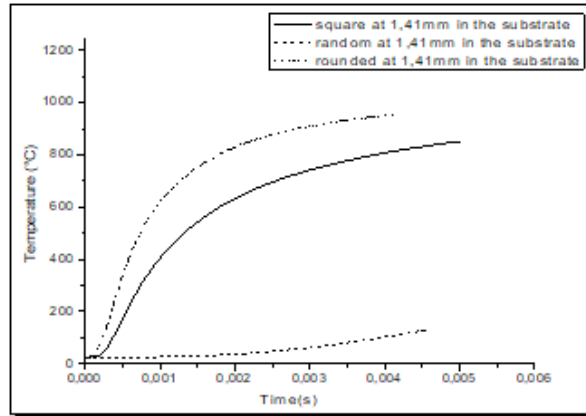


a



b





C

Figure 2. Results of simulation for temperature profile in time for three positions in the rough stainless steel substrate

Moreover, Figure 4 illustrates the distributions of the pressure at the point of impact during spreading out of the drop; initially the pressure is higher at the point of impact (under the plate) which produces a low resistance of contact, hence a good drips/substrate interaction. The pressure disintegrates towards zero very quickly. It should be noted here that, the increase in pressure at the impact in the round form is larger than in random and square one which supports better promotes the collision of lamellae on the substrate in this case better than in both the two other cases.

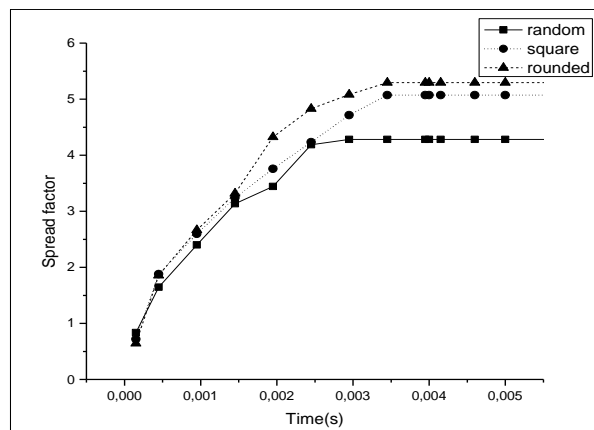


Figure 3. Spread factor of nickel drop 2.5 mms in diameter with impact speed of 2.5m/s on a rough substrate

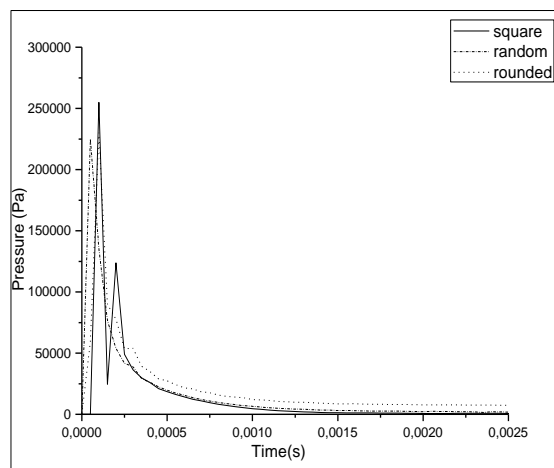


Figure 4. Results of simulation for profile Pressure at the point of impact in the three forms of roughness

### 3.3. Hot substrat

Table 4 represents the distribution of the temperature during the impact of a droplet in a hot rough substrate (random, round and square). This pre-heating led to a transition in morphology from the splats from the “splashes” in the shape of a disc. In a nickel splat, it is possible to observe three quite distinct zones. A first mean zone in the center of the splat, which corresponds to the initial impact, surrounded by a thicker zone in two successive waves.

The pre-heating of substrate delayed the beginning of solidification a little, so that the center of the splats is slightly larger, and the splashes are a little reduced. However, the change was relatively minor. The change in form of the splat (Table 4) cannot be explained by the change of the surface temperature only. It was shown by (Pershin *et al.*, 2003; Yang *et al.*, 2013) that the heating of a steel plate produces an oxide coating on its surface, which can involve an increase in the resistance of contact between the droplets and the substrate.

Figure 5 represents the numerical results of the pressure profile at the contact point. We also notice, initially that the pressure is higher at the point of impact (under the plate) which produces a low resistance of contact (good interaction drips/substrate) for the surface quality (round-off and square), then it disintegrates towards zero very quickly. The pressure of impact is insufficient at the edge of the splat to free itself from the pressure capillaries, roughness and the pressure of gas which involves a bad contact on the external zone. Moreover the surface tension, intervening towards the end of the spreading out of the particle (Madejski 1976; Fukunama & Ohmori 1994;

Pakseresht *et al.*, 2015), causes the withdrawal at the edge of the splat which can explain the formation at the edge.

Table 4. Distribution of the temperature at the time of the impact of a nickel drop of 2.5mm of diameter on a hot rough substrate of 360°C with impact speed of 2.5m/s

| Time (ms) | Round form | Square form | Random form |
|-----------|------------|-------------|-------------|
| 0         |            |             |             |
| 0.45      |            |             |             |
| 1.45      |            |             |             |
| 2.45      |            |             |             |
| 2.95      |            |             |             |
| 3.95      |            |             |             |
| 5.40      |            |             |             |

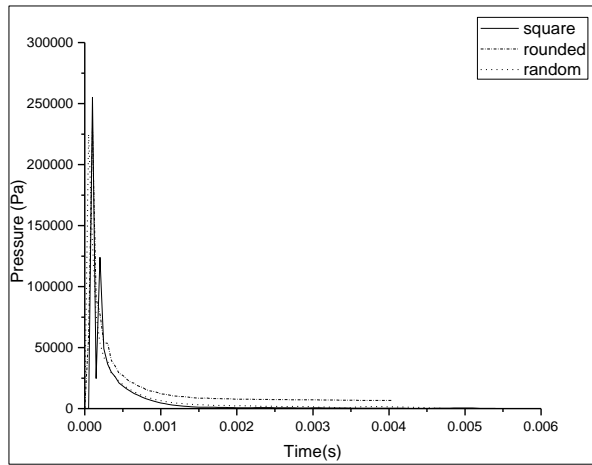


Figure 5. Results of simulation for profile pressure at the point of impact for the three form of roughness

Figure 6 represents the temperature profile at the contact point of a nickel drop during spreading out; one notes that, at the first contact of the drop with the target, the temperature of this point quickly increases, after a partial spreading out the heat-transfer on the surface increases and the temperature of this point remains quasi-constant.

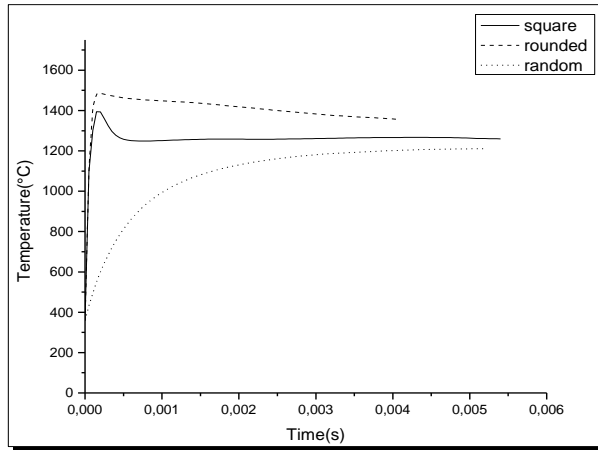


Figure 6. Results of simulation for profile temperature at the point of impact in the three forms of roughness

Figure 7 compares the factor of spreading out of the nickel drop in the suggested model (between the three forms of roughness). The spreading out and the shape of the drop are similar during the impact for the three forms, but the time of spreading out is a little longer for square form.

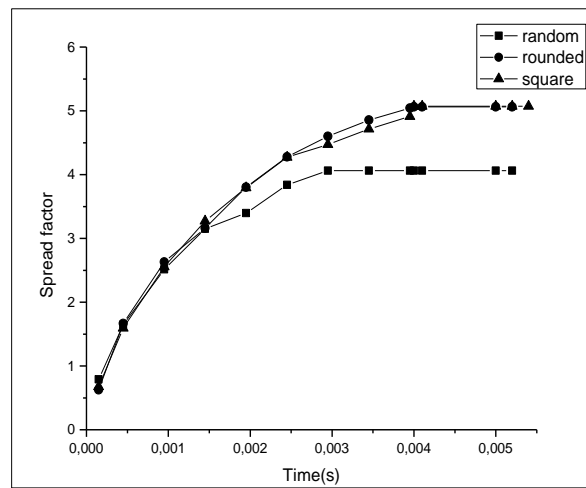
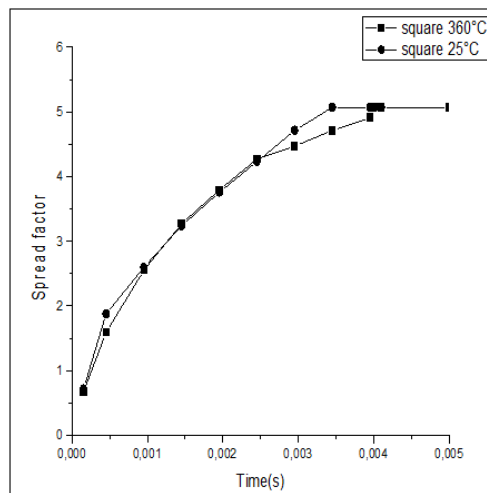
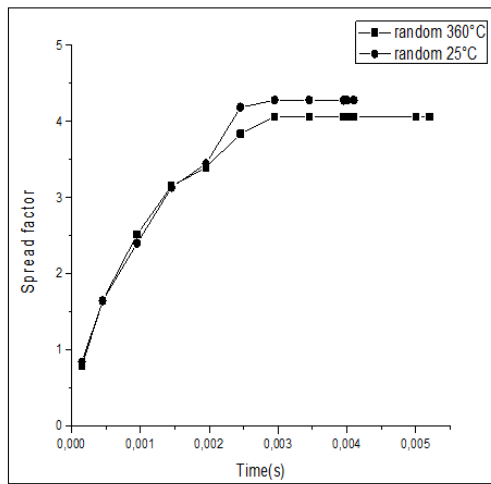


Figure 7. Factor of impact in the three forms of roughness

#### 4. Results comparison

The numerical results showed that the surface quality of substrate plays a big role for the spreading out of a drop, plus surface is rough plus the liquid has difficulty in follow these forms. Thus the liquid which runs out perpendicular to these obstacles is projected vertically because of its inertia. As it is indicated in the figures previously, spreading out is difficult in the random form (form complicated) and in the form square (sharp angle).

The pre-heating of substrate led to a transition from morphology of the splats of form splashes to the shape of disc. Moreover centers of the splats are slightly larger than those of the splats obtained on a cold substrate. It delays a little solidification, and it decreased the splash.



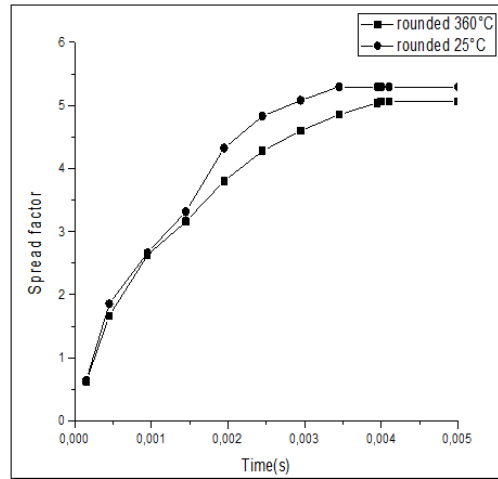


Figure 8. Comparison between the factors of impact in each form for the two cases

## 5. Conclusion

The simulations are performed in 2D Cartesian. The finite element method is used to solve a set of equations governing the impact of nickel particles on a rough surface. The VOF method has to track the free surface deformation. This model is used to study the impact of melted nickel particles on a stainless steel substrate. The model is in good agreement with experiment and the previous digital data. According to the numerical simulations, this model showed that:

- The surface quality exploits a part of the spreading out of the lamella and for which we adopted the best spreading out for the (round) form for the two cases.
- The values of the thermal resistance of impact of the droplets on a substrate are of a crucial importance in simulations of the impact of fused metal of the droplets.
- The substrate preheating retards solidification and reduces splashing.

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