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COMPUTER MODELING OF HEAT-DEFORMATION PROCESS MICROPARTICLE SOLIDIFICATION BY FEM ANSYS-CLASSIC CODE

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ABSTRACT: The article deals with the use of the computer numerical methods for the temperature fields analysis by the fast substratum solidification of the discrete liquid microparticle. Material of microparticle is the nickel alloy. A fully molted spherical particle (the radius of particle is 25 μm) is hitting on the solid substratum with initial velocity w_0 = 100 m.s^{-1}. There is a splashing phenomenon of the particle by the heat conduction to the substrate. Results of the computer modeling by ANSYS give the temperature fields in the chosen times and the form chance of the particle.
KEYWORDS: microparticle, solidification, temperature, modeling, ANSYS

❖ INTRODUCTION

Computer modeling of solidification processes affords the opportunity to describe the physical-metallurgical effects which accrue on the metallurgical and micro-metallurgical processes. Substratum solidification introduces phenomena when the molten particle of alloys impinges on the surface of the rigid material (substratum) with certain speed, deforms him and begins heat transfer into substratum. The heat-deformation process begins with fast cooling of molten micro-volume (particle) on the cold surface. Substratum solidification of the melted discreet microparticles constitutes essence of several technological processes: thermal sprayed additive powdery materials, new material production and plasma and flame spraying [1]. The contribution shows discrete approach for numerical simulation of the deformation behavior and heat transfer of melted spherically micro-particle after impact on to steel substratum topside.

❖ MATEMATICAL MODEL

Temperature field introduces distribution of immediate temperatures in searched region is a function T = f(x,y,z,t) generally. Temperature field is described by Fourier-Kirchhoff differential equation of parabolic type in the modification pro cylindrical coordinate system r,φ,z for isotropic material, initial and boundary conditions definition and without heat volume generation [2]

$$\frac{\partial T}{\partial t} = \frac{\lambda}{c_p \rho}\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right), \qquad [\mathrm{K.s^{-1}}] \quad (1)$$

where $\frac{\partial^2 T}{\partial \varphi^2} = 0$, λ is thermal conductivity coefficient [W.m^{-1}.K^{-1}], c_p specific heat at p = const. [J.kg^{-1}.K^{-1}], ρ density [kg.m^{-3}].

Heat transfer on particle-substrate contact zone is expected like perfectly, Fig. 2. For region Γ_2 and for heat flux we have on the particle-substrate contact zone the boundary condition with the form of Fourier law of heat conduction

$$-\lambda_s\, gradT = -\lambda_{sb}\, gradT\,, \qquad [\mathrm{W.m^{-2}}] \ (2)$$

where λ_s is thermal conductivity coefficient of the particle solid phase and λ_{sb} is thermal conductivity coefficient of substratum.

The drop solidification process is modeled as quasi-equilibrium task. In the solidification region Γ_1 in Fig. 2 is for heat flux in direction y wrote:

$$\rho \Delta h_t \frac{d\xi}{dt} = \lambda_L \left(\frac{dT_L}{dy}\right)_{y=\xi} - \lambda_S \left(\frac{dT_{sol}}{dy}\right)_{y=\xi}, \qquad [W.m^{-2}] \quad (3)$$

where Δh_L is latent heat [J.kg^{-1}], λ_L is thermal conductivity coefficient of melted particle material, $d\xi/dt$ is speed of solidification front [m.s^{-1}], T_L temperature of melted material [K], T_{sol} solidification temperature of alloy [K].

Heat transfer from the particle surface into surroundings is solved by Newton's law with combined convection heat transfer (convection + radiation). For the combined heat transfer coefficient is given by the relation:

$$h_{comb} = h_{conv} + h_R = \varepsilon_{1,2}\sigma_0\left(T_s^2 + T_r^2\right)\left(T_s + T_r\right), \qquad [W.m^{-2}.K^{-1}] \quad (4)$$

where h_{conv} is convection heat transfer coefficient [W.m^{-2}.K^{-1}] [2], $\varepsilon_{1,2}$ mutual particle surface emissivity and ambient [-], σ_0 the Stefan-Boltzmann constant, $\sigma_0 = (5{,}67032 \pm 0{,}00071).10^{-8}$ [W.m^{-2}.K^{-4}], T_s particle surface temperature [K] (area A_1, Figure 2) and T_r is ambient temperature [K].

The dimensionless diameter change of the drop in an impact on the substrate depend on the time t [μs] specified in interval 0÷1.2 μs according [3] as follows, Figure. 1:

$$d/d_{part} = 0{,}043 + 5{,}9915t - 4{,}456t^2 + 1{,}624t^3. \qquad [-] \quad (5)$$

The dimensionless height of the deformed drops to the initial diameter is described by equation:

$$h/d_{part} = 1 - 0{,}953t - 0{,}112t^2 + 0{,}291t^3. \qquad [-] \quad (6)$$

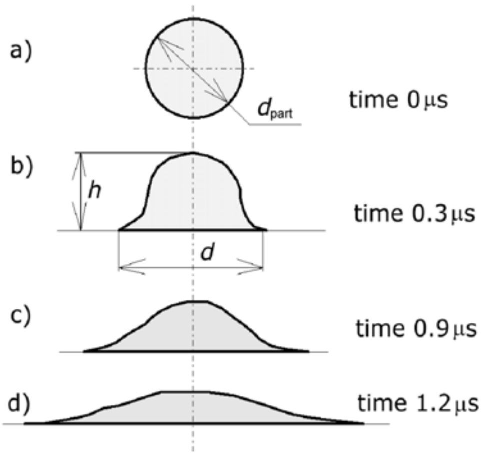

Figure 1. Droplet deformation at impact on substrate plane

❖ SIMULATION MODEL

Simulation model is based on nickel alloy VUZ SDK-52 [4]. The chemical composition (weight %) is in Table 2. The task is solved by finite element method and the thermal task is designed as axisymmetric, transient and non-linear. Geometrical conditions were obtained from equations (5) and (6). In Table 1 are shown thermophysical properties for droplet and the substrate materials [6]. Thermal boundary conditions are represented by equations (2) and (4). Ambient temperature at the place of impact of droplet is constant and chosen T_r = 293.15 K (equation 4). Initial conditions: pro time t=0 is particle initial temperature alloys T_L = 1473 K and substratum temperature T_{sb} = 303.15 K.

Model expects that the diameter off droplet is 50 □m and its speed before the impact on to totally smooth substratum is 100 m.s^{-1}. The droplet trajectory is coincident with normal line to substratum surface. The deformation of the drop begins after the contact with substratum in time 0 s and discrete chosen shapes are showed in Figure. 1. The volume of the particle is during the heat-deformation process invariable.

Specific latent enthalpy, Δh_t = 420 kJ.kg^{-1} is respected in the simulation model. The method of modified specific heat capacity in the temperature range T_L and T_{sol} is used, see Table 1. The quasi-equilibrium liquids temperature of alloys SDK 52 is T_L = 1393 K and solidus temperature T_{sol} = 1223 K [6]

Table 1. Thermal properties of alloy SDK-52 and steel DIN 1.0570

Temperature [K]		293	473	673	873	1073	1218	1223	1393	1398	1473
droplet SDK 52 (nickel)	λ [W.m^{-1}.K^{-1}]	57	54.7	48.8	53.5	58.2	58	58	58	58	58
	c [J.kg^{-1}.K^{-1}]	467	515	544	544	544	544	2644	2644	544	544
	ρ [kg.m^{-3}]	8900	8893	8885	8877	8870	8864	8864	8857	8857	8854
substrate steel DIN 1.570	λ [W.m^{-1}.K^{-1}	43.9	43.9	43.2	39.2	34.7	30.4	29.9	29.9	33.1	33.1
	c [J.kg^{-1}.K^{-1}]	463	477	515	567	634	705	705	710	710	710
	ρ [kg.m^{-3}]	7775	7746	7691	7637	7583	7530	7530	7527	7527	7524

Table 2. Chemical composition (weight %) of alloy SDK-52

Cr	Si	B	C	Fe	Ni
10 %	3.5 %	2.5 %	max. 0.3 %	max. 0.3 %	residue

The simulation of substrate solidification is divided into two stages. In first stage reduces droplet (ball shaped) after contact with the substrate surface its speed of 100 m.s^{-1} at the speed 0 m.s^{-1} and starts the heat transfer on the area Γ_2 from droplet into the substrate, Figure 2. Time of first stage 1.2 μs is taken account. For interval time up 1.2 to 15 μs (Stage 2) will not change shape and micro-volume of the droplet, Figure 1d and heat transfer runs into substrate.

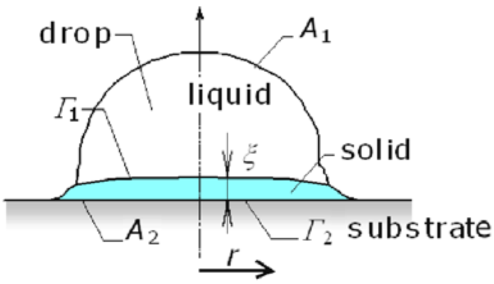

Figure 2. Scheme of created simulation model for time 0.3 μs

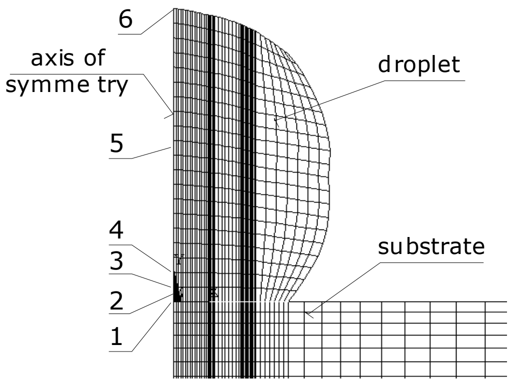

Figure 3. Generated mesh for impact time 0.05 μs

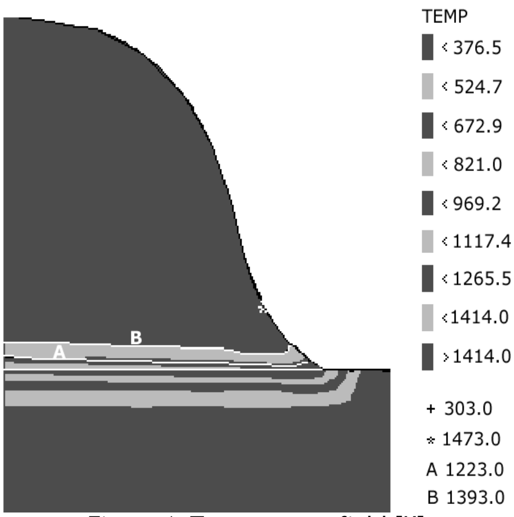

Figure 4. Temperature field [K] in time 0.3 μs

It was created jointly 9 meshes for chosen times in interval from 0 to 1.2 μs. Every mesh had the same volume and the geometry corresponded with equations (5, 6). The main idea for mesh generation was the compatibility for nodes of all meshes, i.e. one node position is moved with the shape changes for all discrete geometrical models. This meshing philosophy enable use the restart procedure of temperature field, which was solved for previous time. For solved thermal task was used axis-symmetric solid element Plane77 with parabolic base function. Generated mesh for impact time 0.05 μs is shown for example in Figure 3.

Computer modeling of substrate solidification process takes into account a thermal perfect contact for each shape deformation phase.

❖ OBTAINED RESULTS AND DISCUSSION

The obtained results are showed in the form of temperature fields contours for chosen times in Figures 4-6. Time dependences of temperature for chosen points of the particles model, Figure 3, are on the graph on Figure 7. In Figure 4 is showed the solidificated area of particle with ξ = 0.52 μm (ξ is the distance from the substrate surface in symmetry axis direction y up to solidification interface). The temperature difference for distance ξ = 0.52 μm is ΔT= 86 K. From the left side of equation (2) is calculated instantaneous density heat flux of particles into the substrate, q = 9.6E9 Wm^{-2}. The adequate value of total heat flow for area Γ_2, according to the geometry in Figure 2, is ϕ = 9.7 W. The figures show high levels of heat flow densities on the border of Γ_2, which results in hypothermia, melt under Figure 7 (curve 1) and under quasi-steady-state solidus temperature. Figure 5 shows the temperature field in the deformed particle at 1.2 μs. Shape deformation of the particles has finished with increasing time. The solidified alloy volume prevents melted phase change the rest of the particles shape. For the impact time greater as 1.2 μs is the shape of impacted droplets constant. In Figure 6 is temperature field in the particle at time t = 8.7 μs, when the solidus temperature reaches the upper part of droplets. This means that time 8.7 μs is the time required for solidification of the entire volume of droplets of molten alloy 52 SDK with diameter 50 μm which hits the substrate with initial speed of 100 m.s^{-1}.

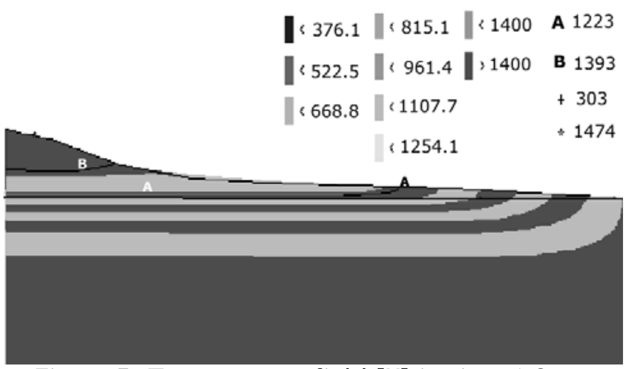

Figure 5. Temperature field [K] in time 1.2 μs

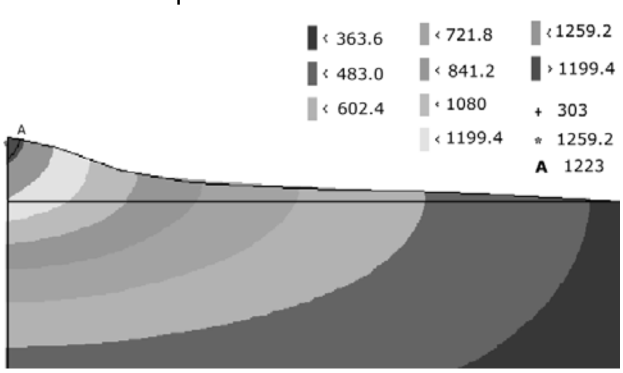

Figure 6. Temperature field [K] in time 8.7 μs

From Fig. 7 it is clear that the impact of particles on the substrate surface occurs very quickly supercooling of the melt in the contact zone to approximately 1143 K. The simulation model shows that the effect of recallescention not increases the temperature on the liquids value.

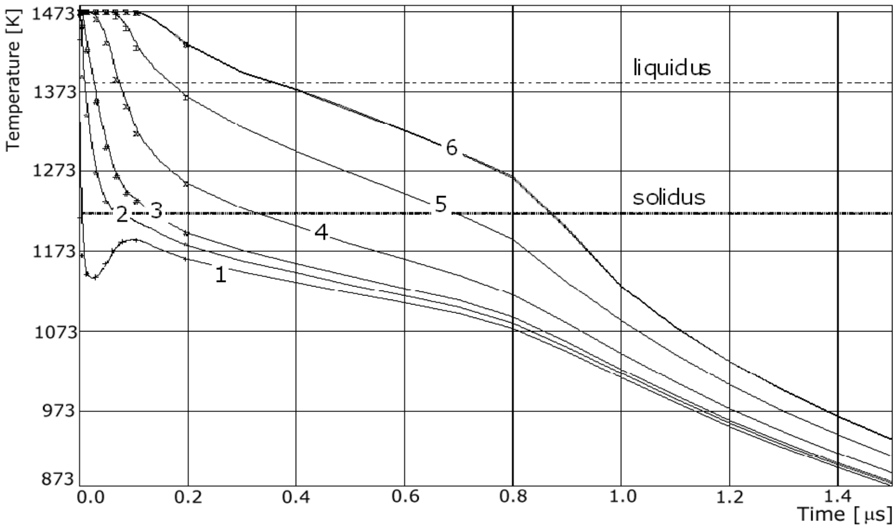

Figure 7. Temperature fields [K] in time

❖ CONCLUSION

The method of numerical simulation enables us to define semi-quantitative thermal effects in the process of rapid solidification of microparticles, albeit at the cost of some simplification which does not suppress the nature process.

Heat transfer from the particles surface into the surrounding (area A1, Figure 2) has no observable effect on the temperature fields in solidificated alloy. The process can be chosen in conditions considered to be adiabatic.

On the basis of solved temperature fields and of metallographic analysis can be created assumptions for more realistic analysis of rapid solidification for melted microparticles at substrate impact process.

The method of computer modeling using the mesh discretisation of chosen phases deforming particles is suitable for application in the classic FEM software. Higher level modeling requires the use of CFD and CFX software.

❖ ACKNOWLEDGMENT

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