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#### Simulation the solidification process in composites materials with aluminum alloy matrix

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### Abstract

The research objective was to establish a criterion with which to assess whether a particle will be included in the metal matrix without being expelled before the solidification front. To this purpose, a program has been used that simulates the heat transfer by means of finite elements. In the simulation, the Al - 11.8 Si, Al - 4.4 Cu - 0.5 Mg, Al - 4.5 Cu - 1.5 Mg alloys have been considered with  $Al_2O_3$ , graphite, SiC, TiO<sub>2</sub>, ZrO<sub>2</sub> and mica particles as dispersed material. The paper shows the influence of some factors such as the particle conductivity, the matrix conductivity and the particle temperature upon the solidification front geometry and upon the probability that the dispersed material is not expelled before the solidification front.

## **1** Introduction

It is known that one from the most important factors which influences the final quality of the composites materials is solidification process. To obtain a composite material with a high uniformity of dispersed material and high mechanical properties is impossible without a strict control of the solidification process parameters. From all parameters which have influence over the solid front geometry we are focused over the effect of the material properties and particle temperature. For this we realize a computer program which simulates the heat transfer using finite element method and we tried to establish a criteria to appreciate if the matrix structure includes particle from the beginning.

# 2 Mathematical model used to simulate the solidification process

The equation used to describes the heat flow during the solidification process in two coordinates for transient regime is the following:

$$\frac{\partial}{\partial x} \left[ \lambda \left( T \right) \frac{\partial T}{\partial x} + \lambda \left( T \right) \frac{\partial T}{\partial y} \right] = \rho C_{p} \frac{\partial T}{\partial t}$$
(1)

where T represents temperature,  $\lambda$  - conductivity, C - specific heat, t - time and  $\rho$  - density. The initial condition (2) and boundary condition (3) attached to Eqn. (1) to obtain a complete model are:

$$T = T_0, t = 0$$
 (2)

$$\lambda \left(\frac{\partial T}{\partial x}n_{x} + \frac{\partial T}{\partial y}n_{y}\right) + \alpha \left(T - T_{0}\right) = 0, \quad \forall P(x, y) \in S_{\alpha}$$
(3)

where  $T_o$  represents temperature at initial moment and  $\alpha$  is the heat transfer coefficient on the surface  $S_{\alpha}$ .

During the solidification process a significant factor is the latent heat which works like an external source of heat. To obtain a valuable model it is necessary to include this factor in our mathematical model. There are a lot of methods to include this external source in the heat transfer model. We use the following relation:

$$C'_1 = C_1 + \frac{L}{\delta T}$$
(4)

where C'<sub>1</sub> represents the specific heat which include the latent heat, C<sub>1</sub> - specific heat without latent heat, L - latent heat and  $\delta T$  - the differences between liquidus and solidus temperatures.

Because the analytical equations cannot be used to realize the computer program it is necessary to transform it into an integral model. Knowing the differential equation (1), initial (2) and boundary condition (3) the integral equation for mathematical model is:

$$\pi = \int_{\mathbf{V}} \frac{1}{2} [\lambda_{\mathrm{T}} (\frac{\partial \mathrm{T}}{\partial x})^{2} + \lambda_{\mathrm{T}} (\frac{\partial \mathrm{T}}{\partial y})^{2}] d\mathbf{V} + \int_{\mathbf{V}} \rho C_{\mathrm{p}} \frac{\partial \mathrm{T}}{\partial x} d\mathbf{V} + \int_{S_{\alpha}} \frac{\alpha}{2} (\mathrm{T} - \mathrm{T}_{\alpha}) d\mathbf{S}$$
(5)

Having in view that the analyzed domain V can be broken into finite elements with quadrilateral shape, using the linear functions we can describe the temperature with the following equation:

$$\hat{T}(x,y,t) = N_1(x,y)T_1(t) + N_2(x,y)T_2(t) + N_3(x,y)T_3(t) + N_4(x,y)T_4(t)$$
(6)

where  $N_1(x,y)$ ,  $N_2(x,y)$ ,  $N_3(x,y)$  and  $N_4(x,y)$  represents shape functions and  $T_1(t)$ ,  $T_2(t)$ ,  $T_3(t)$  and  $T_4(t)$  the temperatures in finite element nodes. With this last relation and imposing the stationary conditions for Eqn. (5), we have the following equation:

$$\sum_{1}^{n} \left( \int_{V^{e}} B^{T} D B T^{e} dV + \int_{V^{e}} \rho C_{p} \frac{\partial}{\partial t} N dV + \int_{S^{e}_{\alpha}} N_{N^{T}} T^{e} dS + \int_{S^{e}_{\alpha}} \alpha T_{\alpha} N^{T} dS = 0$$
(7)

In matriceal form this equation can now be written as follows:

$$K_1^{e}\dot{T}^{e} + (K_2^{e} + K_3^{e}) \cdot T = K_4^{e}$$
 (8)

After assembling all elements of analyzed domain we obtain the final equations:

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$$K_1T + (K_2 + K_3) \cdot T = K_4$$
 (9)

To obtain the temperatures in transient regime we use finite differences method. The equation which gives the initial temperatures for a new cycle of computing is:

$$\left(\frac{2}{\Delta t}K_{1}+K_{2}+K_{3}\right)\cdot T_{n+1} = \left(\frac{2}{\Delta t}K_{1}-K_{2}-K_{3}\right)\cdot T_{n}+\left(K_{4,n+1}+K_{4,n}\right)$$
(10)

Using this last equation we can compute all temperatures at time t+dt if we know the temperature at time t.

## 3 The computer program

Starting with mathematical model described we realize a computer program to simulate the heat transfer during the solidification process. The computer program, SimCAD v.2.0, written in Pascal language, take in account the internal sources and variation of material properties with temperature. The program use over 10.000 finite elements to obtain an accurate geometrical description of the domain. The necessary time to compose the problem and to solve the equations system is about 60 seconds for a Pentium 166MHz system.

The successive approximation method with a variable suprarelaxation factor is used to solve the equation system. The computer program has routines for automeshing the analyzed geometry and to display the results in graphic mode. The program has been tested for some applications in reheating <sup>1</sup> and castings <sup>2</sup> domains. Results obtained from simulation are close to the results obtained from industrial measurements.

## **4** Numerical experiments

## 4.1 The effect of the particle conductivity / matrix conductivity ratio on the solidification front geometry

A spherical particle situated before the solidification front has been considered in order to study how the material properties of the matrix and the dispersed material affect the solidification front geometry. The numerical experiment is made for a composite material based on aluminum alloys. As dispersed material, particles of various materials are considered, as shown in Table 1.

Matrix	Particle	$K = \lambda_p / \lambda_m$
Al - 4.5 Cu - 1.5 Mg	mica	0.0027
Al - 11.8 Si	ZrO <sub>2</sub>	0.0198
Al - 11.8 Si	Al <sub>2</sub> O <sub>3</sub>	0.0220
Al - 11.8 Si - 1.5 Mg	TiO <sub>2</sub>	0.0523
Al - 11.8 Si - 1.5 Mg	graphite	0.1160
Al - 4.4 Cu - 0.5 Mg	SiC	0.3915

Table 1 Materials used in simulation

The initial temperature for both, matrix material and dispersed material was considered as 720°C. In the simulation of solidification, the transient heat transfer was solved numerically by finite element method and the temperature field was determined. The domain was broken in 8.000 finite elements and the time used by computer to simulate heat transfer for each numerical experiment was about 300 seconds.

The simulation results and the solidification front geometry are shown in Figure 1 a,b,c,d,e and f.



Figure 1: The effect of the  $K = \lambda p / \lambda m$  ratio on the solidification front

As shown in the above figures, the solidification front geometry is strongly affected by the material properties of the dispersed material. In all cases, the occurrence of a prominence in front of the particle is apparent and this prominence tends to continually push the particle in the liquid. The occurrence of this prominence is determined by the presence of the particle that reduces the local heat flow from the liquid phase.

The smaller the prominence increase the probability of inclusion of the particle without being expelled before the solidification front. When using SiC (K=0.3915) as dispersed material, the solidification front is almost plain and better particle inclusion conditions are ensured than when mica is used as dispersed material (K=0.0027).

## 4.2 The effect of the particle temperature upon the solidification front geometry

To quantify how the particle temperature affects the solidification front geometry, a simulation series has been made when the mica particle temperature has been 720°C, 850°C, 1050°C and 1200°C. The configuration of the solidification front is shown in Figure 2 a,b,c,d.



Figure 2: The effect of the particle temperature upon the solidification front geometry

As seen from these simulations, the size of the prominence before the solidification front decreases with the increase of the dispersed material temperature. When the particle is heated at 1200°C, the solidification

front becomes almost plane, ensuring better particle inclusion conditions in the base matrix.

## **4.3** A criterion for the assessment of the inclusion probability of the particle in the metal matrix

A criterion that allows the accumulation of the effect of various parameters that affect the probability that a particle is expelled during solidification is of paramount practical importance. From the analysis of the simulation results, such a criterion could be the size of the prominence appearing before the particle during solidification. By using such a criterion obtained by simulation, one can quantify how various parameters affect the solidification front geometry. Conclusions can be made technologically as to how various parameters affect the dispersion of the particles in the base matrix.

### Conclusions

A series of practical conclusions can be made as a result of the numerical experiments. Some of them are the following:

- the ratio between the particle conductivity and the matrix conductivity strongly affects the inclusion probability of the dispersed material in the metal matrix;
- along with the material properties of the particle and metal matrix, the increase of the particle temperature improves the inclusion conditions of the dispersed material in the metal matrix;
- considering the numerical results shown above, one can conclude that the size of the prominence before the solidification front can be used as a criterion that allows the assessment of the influence of various factors such as particle conductivity, matrix conductivity and particle temperature upon the probability that the particle is not expelled before the solidification front.

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