A R C H I V E S O F M E T A L L U R G Y A N D M A T E R I A L S
Volume 54 2009 Issue 2

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THE GRAIN NUCLEATION RATE OF THE AZ91/SiC COMPOSITE BASED ON MAXWELL-HELLAWELL MODEL

SZYBKOŚĆ ZARODKOWANIA ZIAREN DLA KOMPOZYTU AZ91/SIC W OPARCIU O MODEL MAXWELLA-HELLAWELLA

The aim of this work was selection of parameters for the model describing the relationship between the grain density and undercooling. The numerical calculations were performed for the composite material based on AZ91 alloy reinforced by silicon carbides particles. The nucleation rates function of grains based on Maxwell-Hellawell model.

Keywords: numerical simulation, grain nucleation rate, Maxwell-Hellawell model

Celem niniejszej pracy jest dobranie parametrów modelu opisującego zależność gęstości ziaren od przechłodzenia dla krystalizacji kompozytu na bazie stopu AZ91 zbrojonego cząstkami węglika krzemu. Opisana funkcja szybkości zarodkowania ziaren bazuje na modelu Maxwella - Hellawella.

1. Introduction

The composites based on Mg-Al alloy reinforced by silicon carbides are widely applied in the aerospace and motor industry, because of their mechanical properties and low density. The SiC particles are wide used to the reinforcing composites based on the magnesium alloys, because they do not form stable carbides with magnesium.

The numerical simulation of the cast structure requires the knowledge of equations describing the relation between the grain density and undercooling. Hence, the problem of nucleation is a subject of theoretical as well experimental investigations [1-9]. The results of these investigations lead to a different nucleation laws. Generally they bind undercooling degree and the material parameters with the nucleation rate or nucleus density. The most often used model for numerical simulation of the crystallization process is Maxwell- Hellawell model (MH) [2]. The Maxwell- Hellawell model describes the relationship between nucleation rate with undercooling degree, the crystallization temperature, the nucleation time and the chemical composition of the alloy. Appearing parameters in these equations are the so-call parameters of the adjustment. Because their value is not estimated, they have to be empirically qualified for each physical-chemical condition of the liquid metal. In order to determine fitting parameters of solidifying AZ91/SiC composites, the results of experimental investigations were found in the literature [1].

2. Results of numerical simulation

In the year 1975 Maxwell and Hellawell [2] published heterogeneous nucleation model adapted to numerical calculations. The grain's nucleation rate was given by equation:

$$\frac{dN}{d\tau} = Q \cdot (N_0 - N) \cdot exp\left(\frac{-F(\theta)}{\Delta T^2 (T_N - \Delta T)}\right), \quad (1)$$

where:

Q – The nucleation frequency, s^{-1};

N_0 – The total density of nucleation sites, m^{-3};

N – The actual density of nucleation sites for heterogeneous nucleation left after the actual time, m^{-3}.

The nucleation frequency (Q) was assumed to 2.5 x 10^{18} s^{-1} [2]. The total density of nucleation sites (N_0) is also a parameter subject to discussion. Logically, its value should be greater than value of grain density formed during the crystallization process. This way of thinking was confirmed by authors in the paper [2]. They showed that when N_0 parameter increases of four orders of magnitude the calculated grain density increases less than a

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twice. This phenomenon is connected with fact that increase of nucleation rate causes decreases significantly time of whole nucleation process.

Because of small amount of experimental data, the results obtained by numerical modelling can be very useful. The main problem is to predict how the grain density N_v vary or the calculations parameters. The integration of equation (1) shows that the number of nucleus is dependent on time.

For $\Delta t_N = t_F - t_0$

$$N_V = N_0 \cdot \left(1 - exp\left(-Q \cdot exp\left(\frac{-F(\theta)}{\Delta T_{max}^2 (T_N - \Delta T_{max})}\right)\Delta\tau_N\right)\right) \cdot \quad (2)$$

The solidification parameter ($F(\theta)$) was calculated with use of experimental data taken from paper [1]. A. Luo in his work performed thermo and micro-structural analyze of AZ91 alloy and two AZ91 metal matrix composites reinforcement by SiC ceramic particles. The analyzed composites were: MMC-1 with 10% of SiC particles, MMC-2 with 0.5% of SiC particles. The structural analyze of those investigation clearly shows that grain size in composites are much smaller than in alloy without any reinforcement. The results were: 126.9 m for AZ91 with 0% SiC, 41.8 μm for MMC-1 and 79 μm for MMC-2. Additional parameter, the nucleation temperature (T_N), is the temperature on the cooling curve where the cooling rate $\left(\frac{dT}{d\tau}\right)$ rapidly changes. This temperature value means nucleation of magnesium primary phase and it is a start point of emitting of latent heat of crystallization. The nucleation temperature (T_N) was higher for composites (605.7°C for MMC-1 and 601.5°C for MMC-2) than for AZ91 alloy (598.2°C). This phenomenon makes possible nucleation of large number of primary crystals of magnesium. This confirms the thesis about heterogeneous nucleation of primary phase (α-Mg) on the silicon carbide (SiC).

The number of grains was calculated by dividing of volume of casted plate reduced of fraction of SiC particles by volume of grain. It was assumed that every grain is an ideal sphere of average grain diameter.

Maximum undercooling (ΔT_{max}) was calculated as a difference between nucleation temperature (T_N) and recalescence (T_R), fig. 1. This figure was based on data taken from [1]. This figure presents differences between cooling curves in the range of crystallization of the primary phase of magnesium for AZ91 alloy (fig. 1a) and for the composite AZ91/SiC (fig. 1b). The temperature (T_R) was read from cooling curve for time when the cooling rate $\left(\frac{dT}{d\tau}\right)$ is the highest. The process of the crystallization of primary phase can be divided into two stages. First stage starts at the moment when temperature of cooling liquid reaches value of $T=T_N$. There appears parallel phenomena nucleation and grains growth. This process ends at moment when the temperature of crystallizing alloy reaches value of recalescence temperature (T_R). This starts second stage of process – grain growth. Proper determination of every characteristic temperature (T_N, T_R) effects precision of solution of grain growth model (MH model).

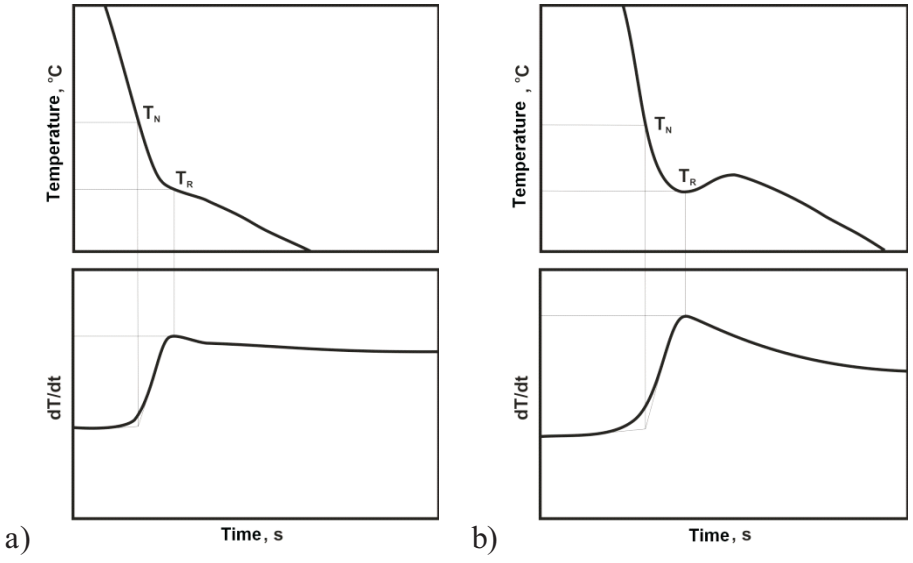

Fig. 1. Run of cooling curve and cooling rate for AZ91 alloy (a) and composite (b) in the range of crystallization of primary magnesium phase base on the literature [1]

To determine lacking parameters of fitting F(θ) equations (2) was transformed into form:

$$F(\theta) = -\frac{1}{(\Delta T)^2(T_N - \Delta T)} ln\left(\frac{1}{Q\Delta\tau_N} ln\left(\frac{N_0}{N_0 - N_V}\right)\right). \quad (3)$$

Using equation (3) and data from table 1 it is possible to calculate values of parameter F(θ) for AZ91/SiC composite of various volume fraction of silicon carbides particles. Results of calculation of parameter F(θ) are also presented in table 1.

Calculated values of parameter F(θ) allow to determine nucleation rate for particular value of undercooling (ΔT). Figures 2 present dependence of nucleation rate on undercooling value for investigated alloy and composites.

Knowledge of effect of undercooling on nucleation rate is not sufficient to determine grain density (N_V). There is requested the conjugation of this equation (1) with differential equation of heat transfer and equation describing grain growth rate. Solution of such set of differential equations allows to predict grain density and run of cooling curve.

TABLE

Parameters of the composite base on the AZ91 alloy reinforced silicone carbides for various volume fraction: 0% SiC, 0.5% SiC and 10% SiC

Parameters	Composite base on the AZ91 alloy		
	0% SiC	0,5% SiC	10% SiC
N_V, m^{-3}	89719685891	370010814499	2259364365630
ΔT_{max}, K	3.8	5.0	9.2
$\Delta\tau_N$, s	7	6	13.4
T_N, K	871.35	874.65	878.85
N_0, m^{-3}	10^{17}	10^{17}	10^{17}
Q, s^{-1}	$2.5 \cdot 10^{18}$	$2.5 \cdot 10^{18}$	$2.5 \cdot 10^{18}$
F(θ), K^3	729505.89	1231896.81	4096674.20

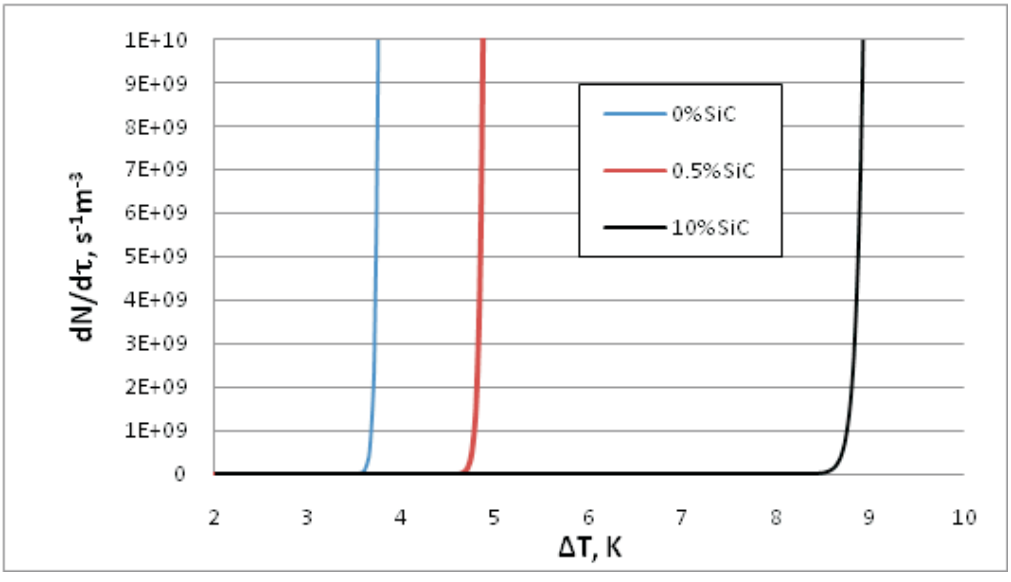

Fig. 2. Graph of the nucleation rate dependent on the actual undercooling

Figure 2 presents kinetic of nucleation of composite AZ91/SiC for various values of volume fraction of SiC: 0%, 0.5% and 10%. Run of nucleation kinetic is similar for every case. The number of forming nuclei increases with undercooling. For each of investigated composites value of nucleation rate increases rapidly starting from particular undercooling value. This undercooling value grows with increase of volume fraction of SiC particles.

3. Summary

Because of lack of sufficient data for fitting parameters calculation in MH model, there is necessary to use statistical method of evaluation of such parameters on the base of experimental results.

Determined fitting parameters can be applied in equation describing nucleation and crystallization of composites. Such obtained model can be used to predict grain density in composites.

Analyzing change of F(θ) parameter depend on volume fraction of SiC particles in AZ91/SiC composite, there can be observed increase of this parameter from F(θ) = 729505.89 K^3 for 0% SiC to F(θ) = 4096674.20 K^3 for 10% SiC. This effect will be the subject of further investigations.

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This paper was supported by AGH University of Science and Technology, no. 10.10.170.300.

Received: 10 May 2009.