Constitutive Model of Particulate-Reinforced Nanocomposites for Thixotropic Plastic Forming

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Abstract: With the consideration of Orowan strengthening effect, a new constitutive model of particulate-reinforced magnesium matrix nanocomposites for thixotropic plastic forming was derived by analyzing relationships among parameters (stress σ , strain ε , strain rate $\dot{\varepsilon}$, liquid phase rate f_L , volume fraction of nano-reinforcement f_p , temperature T). The multiple nonlinear regression method was used to determine the parameters in the constitutive model. A specific constitutive model of SiCp/AZ61 nanocomposites in thixotropic plastic forming was proposed. The calculated values obtained from the constitutive model are in good agreement with the experimental results. Therefore, the constitutive model provides references for the thixotropic forming theory, simulation and fabrication of nanocomposites.

Key words: nanocomposites; thixotropic plastic forming; constitutive relationship; Orowan strengthening effect

Magnesium based alloys have widespread applications, especially in the automotive industries, due to their excellent combination of mechanical properties and die castability. It is particularly worth mentioning that their density is significantly lower than that of aluminum or copper^[1,2]. As it's known to all, micron size ceramic particles which possess low density, stiffness and creep resistance, are added into magnesium based alloys to enhance their mechanical properties. Nevertheless, the ductility of the matrix would be reduced due to the additions of micron size ceramic particles, which limits their applications where good ductility is required^[3].

Particulate-reinforced magnesium matrix nanocomposites (MMNCs), in which the reinforcement particle size is less than 100 nm, are most promising high performance materials with unique mechanical and physical properties. It has been shown that MMNCs balance mechanical properties between nano- and micro-structured materials, i.e., ultimate tensile strength and ductility, 0.2% yield strength, Young's modulus and enhanced hardness^[4,5].

The mechanical properties of nanocomposites depend on many factors, including properties of the matrix, processing method, grain size of the matrix, and reinforcement phase properties such as strength and coefficient of thermal expansion. Recently, semi-solid metal processing techniques have been developed to manufacture wrought magnesium or aluminium alloys, of which thixoforming exhibits both matured technology and obvious economical benefit. Thixoforming is extensively employed to form magnesium or aluminium alloys directly into near-net shape components^[6-8].

Constitutive modeling of MMNCs for thixoforming is a suitable approach to facilitate the development of thixoforming, and it is especially important for designing a composite for sensitive applications with high experimental costs and predicting the mechanical properties of MMNCs as a function of processing conditions, reinforcement and matrix. H. Yan^[9,10] et al. investigated the magnesium matrix composites thixotropic plastic deformation behavior, and the corresponding constitutive model was established. G.

Received date: October 20, 2015

Foundation item: National Natural Science Foundation of China (51364035, 51165032); Loading Program of Science and Technology of College of Jiangxi Province (KJLD14003)

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Bao et al.^[11] carried out a micromechanics study of ceramic particle reinforced metal matrix composites for the high strain rate deformation. In order to predict the rate-dependent plastic flow behavior of the metal matrix composite, a constitutive formula was established. A. Sanaty-Zadeh^[12] has investigated the sole or mixed effects of different active strengthening mechanisms (Orowan, load bearing modeling, Hall–Petch and CTE mismatch) to predict the properties of particulate-reinforced magnesium matrix nanocomposites, by Clyne approach.

However, researches on developing the constitutive model of MMNCs for thixotropic plastic deforming have not been reported yet. In this study, a new constitutive model was developed.

1 Establishment of Constitutive Model

Based on the analyses of the compression behavior of micro sized particulate reinforced composites for thixotropic plastic deformation, it is found that there exists a certain nonlinear relationship among temperature T , strain ε , strain rate $\dot{\varepsilon}$, stress σ , and liquid phase rate f_L . Consequently, the constitutive relationship of micro sized particulate reinforced composites for thixotropic plastic forming was proposed by H. Yan et al.^[10], as shown in following equation:

$$\sigma \propto \exp(a + bf_p + cf_p^2 + d/T) \cdot \varepsilon^n \cdot \dot{\varepsilon}^m \cdot [1 - \beta f_L]^{a_1} \cdot [1 + (\alpha \dot{\varepsilon})^m f_p]^{a_2} \quad (1)$$

where f_L can be calculated as:

$$f_L = \left(\frac{T_M - T_L}{T_M - T} \right)^{\frac{1}{1-K}} \quad (2)$$

Where a , b , c , d , a_1 and a_2 are constants; n is the strain hardening index; m is the strain rate sensitivity index; β is the geometric parameter, α is the correction coefficient; f_p is the volume fraction of micro sized particles in the matrix composite; f_L is the volume fraction of liquid phase; T_M is the melting point of pure metal; T_L is the liquids temperature of base alloy; K is the equilibrium distribution coefficient.

Z. Zhang and D. L. Chen have investigated the effects of Orowan strengthening mechanics in nano particulate reinforced magnesium matrix nanocomposites (particle size ranges from 20 to 100 nm)^[13]. And the results indicate that the Orowan strengthening effect plays a crucial role at strengthening the yield strength in MMNCs and the strengthening effect increases with decreasing the size of nanoparticles. Subsequently, a constitutive relationship of MMNCs for predicting yield strength of intra-granular type is summarized as follows:

$$\sigma_{yc} = \sigma_{ym} (1 + f_1) (1 + f_d) (1 + f_{Orowan}) \quad (3)$$

$$f_{Orowan} = \frac{2G_m b}{\sigma_{ym} (\pi/6 f_b)^{1/3} d_p} \quad (4)$$

Where σ_{yc} is the yield strength of MMNCs; σ_{ym} is the yield strength of the magnesium matrix alloy under the same processing conditions as those of MMNCs; f_1 is the improvement factor in consequence of the load-bearing effect; f_d is the improvement factor related with the enhanced dislocation density in the matrix induced by the thermal mismatch between the reinforcement particles and the matrix; f_{Orowan} is the improvement factor associated with the Orowan strengthening effect; f_p is the volume fraction of reinforcement nanoparticles; G_m is the shear modulus of the magnesium matrix; b is the magnitude of the Burgers vector of dislocations in the magnesium matrix; d_p is the particle size.

With the consideration of Orowan strengthening effect, the constitutive model of composites reinforced with nanoparticles for thixotropic plastic deformation is proposed as follows:

$$\sigma = \exp(a + bf_p + cf_p^2 + d/T) \cdot \varepsilon^n \cdot \dot{\varepsilon}^m \cdot [1 - \beta f_L]^{a_1} \cdot [1 + (\alpha \dot{\varepsilon})^m f_p]^{a_2} [1 + \lambda f_p^{1/3}]^{a_3} \quad (5)$$

$$(\lambda = \frac{2G_m b}{G(\pi/6)^{1/3} d_p})$$

For the intra-granular type of MMNCs in this experiment, the volume fraction of nanoparticles is relatively low, typically about 0.27%~1.12%. Therefore its quadratic form cf_p^2 shall be excluded from consideration. The final form of constitutive model is established as follows:

$$\sigma = \exp(a + bf_p + d/T) \cdot \varepsilon^n \cdot \dot{\varepsilon}^m \cdot [1 - \beta f_L]^{a_1} \cdot [1 + (\alpha \dot{\varepsilon})^m f_p]^{a_2} [1 + \lambda f_p^{1/3}]^{a_3} \quad (6)$$

2 Solution for Parameters in Constitutive Model

In order to determine the parameters in the constitutive model, the multiple nonlinear regression method was used. And Eq.(6) can be transformed into a linear one after taking logarithm.

$$\ln \sigma = a + bf_p + c/T + n \ln \varepsilon + m \ln \dot{\varepsilon} + a_1 \ln(1 - \beta f_L) + a_2 \ln[1 + (\alpha \dot{\varepsilon})^m f_p] + a_3 \ln(1 + \lambda f_p^{1/3}) \quad (7)$$

Where

$$\begin{aligned} y &= \ln \sigma, X_1 = f_p, X_2 = 1/T, X_3 = \ln \varepsilon \\ X_4 &= \ln \dot{\varepsilon}, X_5 = \ln(1 - \beta f_L) \\ X_6 &= \ln[1 + (\alpha \dot{\varepsilon})^m f_p], X_7 = \ln(1 + \lambda f_p^{1/3}) \\ A_0 &= a, A_1 = b, A_2 = c, A_3 = n, A_4 = m \\ A_5 &= a_1, A_6 = a_2, A_7 = a_3 \end{aligned} \quad (8)$$

Therefore, Eq.(7) can be changed into the following form:

$$y = A_0 + A_1X_1 + A_2X_2 + A_3X_3 + A_4X_4 + A_5X_5 + A_6X_6 + A_7X_7 \quad (9)$$

3 Constitutive Relationship of SiCp/AZ61 Nanocomposites for Thixotropic Plastic Forming

The data (σ , $\dot{\varepsilon}$, ε , T , f_L , f_p) in the constitutive relationship were gained based on the thixotropic compression of SiCp/AZ61 nanocomposites. A more detailed description of the experiment was previously reported by us^[14]. The SiC powder with a mean particle size of 100 nm was added into AZ61 matrix uniformly. Statistical package for the social sciences (SPSS) was applied to make the regression calculation and analysis for the above linear Eq. (9). Table 1 lists the common statistical values, including the correlation coefficient R , determination coefficient R^2 , adjusted determination coefficient $\bar{R}^2$ and the standard error of the estimate S . A_4 (the number m) was calculated by repeated selection of α (the correction coefficient) to be in accordance with the number m in X_6 ($\ln[1 + (\alpha\dot{\varepsilon})^m f_p]$). The best fit correction coefficient ($\alpha=58$) was obtained. Since the equation, as shown in Eq.(9) has lots of explained variables, these explained variables should be depended on the adjusted determination coefficient $\bar{R}^2$. As shown in Table 1, $\bar{R}^2$ is close to 1 and it implies that its fit degree is high. Consequently, we can conclude that the proposed constitutive model is reliable and can give accurate and stable results.

Table 2 shows the analysis results of variance. Residual and regression in sum of squares are 2.826 and 22.847, respectively, and the total is 25.673. Meanwhile, residual and regression of mean square are 0.046 and 3.264, respectively.

Standard error of unstandardized coefficients (Std. Error), unstandardized coefficients (B), standardized coefficients, observed value (t) of test statistics in the significance test of regression coefficient and the concomitant probability value (Sig.) are shown in Table 3. And the value of the corresponding variable regression coefficient can be derived from Table 3, as shown in follows: $X_0 = -5.768$, $X_1 = 14.158$,

$X_2 = 3674.674$, $X_3 = -0.535$, $X_4 = 0.245$, $X_5 = 6.076$, $X_6 = -1.663$, $X_7 = 17.834$. The fact that the concomitant probability (Sig.) approximately equals to 0 indicates that it has significant regression. When compared with the regression coefficients, the sensitivity coefficient m ($X_4 = 0.245$) of strain rate which was determined by regressing is in good agreement with the replaced value (m).

Consequently, the following formula is got from Eq. (9).

$$y = -5.768 - 14.158X_1 + 3674.674X_2 - 0.353X_3 + 0.245X_4 + 6.076X_5 - 1.663X_6 + 17.834X_7 \quad (10)$$

By means of the inverse process of converting Eqs.(7) to (9), Eq.(11) was acquired from Eq. (10), as shown in follows:

$$\sigma = \exp(-5.768 + -14.158f_p + 3674.674/T) \cdot \varepsilon^{-0.353} \cdot \varepsilon^{0.245} \cdot [1 - \beta f_L]^{6.076} \cdot [1 + (58\varepsilon)^{0.245} f_p]^{-1.663} \cdot [1 + 0.627f_p^{1/3}]^{17.834} \quad (11)$$

Eq.(11) is the constitutive relationship of SiCp/AZ61 nanocomposites for thixotropic plastic forming.

4 Validation of Constitutive Model of SiCp/AZ61 Nanocomposites for Thixotropic Plastic Forming

Fig.1 shows comparisons between predicted and experimental results in thixotropic plastic compression

Table 1 Constants used for the statistical calculation

Model	R	R^2	$\bar{R}^2$	S
1	0.943 (a)	0.890	0.977	0.22196

a. Predictors: (Constant) X_7 , X_6 , X_5 , X_4 , X_2 , X_1 , X_3 ;

b. Dependent variable: y

Table 2 ANOVA (b)

Model	Sum of squares	df	Mean square	F	Sig.
1 Regression	22.847	7	3.264	66.975	0.000(a)
Residual	2.826	58	0.046	-	-
Total	25.673	65	-	-	-

a. Predictors: (Constant) X_7 , X_6 , X_5 , X_4 , X_2 , X_1 , X_3 ;

b. Dependent variable: y

Table 3 Coefficients (a)

Model		Unstandardized coefficients		Standardized coefficients	t	Sig.
		B	Std. error			
1	X_0 (Constant)	-5.768	4.631	-	-1.246	0.218
	X_1	14.158	56.193	-0.53	-0.252	0.802
	X_2	3674.674	2312.933	0.210	1.59	0.118
	X_3	-0.535	0.031	-5.000	11.277	0.000
	X_4	0.245	0.036	0.708	6.835	0.000
	X_5	6.076	1.661	0.490	3.657	0.001
	X_6	-1.663	0.996	-0.188	-1.670	0.100
	X_7	17.834	6.367	0.472	2.242	0.029

a. Dependent variable: y

Fig.1 Validation of constitutive model: (a) 1 wt% SiC_p/AZ61, 535 °C, 0.1 s⁻¹; (b) 2 wt% SiC_p/AZ61, 550 °C, 1 s⁻¹

processes. The solid lines are the experimental curves, and the dotted lines are the predicted ones. As shown in Fig.1, the results predicted by Eq.(10) agree with the experimental results. It indicates that the proposed constitutive model has fairly high level of forecast precision and practical significance for guiding the thixotropic plastic deformation process of nanocomposites.

5 Conclusions

1) The multiple nonlinear regression method is used to develop the constitutive model of particulate-reinforced

nanocomposites for thixotropic plastic forming. This was done by taking Orowan strengthening effects into account. The calculated values obtained from the constitutive model are in good agreement with the experimental results.

2) The constitutive model has fairly high level of forecast precision and practical significance for guiding the thixotropic plastic deformation process of nanocomposites.

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纳米颗粒增强镁基复合材料触变成形本构模型

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摘 要: 通过分析纳米颗粒增强镁基复合材料半固态触变塑性成形中不同因素(应力 σ 、应变 ε 、应变速率 $\dot{\varepsilon}$ 、温度 T 、液相分数 f_L 、增强颗粒体积分数 f_p)之间的关系, 同时考虑 Orowan 增强机制, 由此提出一种新的本构模型。该本构模型中各参数由多元非线性回归法演算而得。触变塑性成形实验数据与数值模拟数据吻合良好, 证明推导的本构关系可用于触变塑性成形的数值模拟, 并可用来指导复合材料的触变塑性成形工程实践。

关键词: 纳米复合材料; 触变成形; 本构关系; Orowan 增强机制

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