Article ID: 1003-6326(2005)04-0749-05

Microstructure evolution model based on deformation mechanism of titanium alloy in hot forming ①

LI Xiao-li(李晓丽), LI Miao-quan(李淼泉)
(School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China)

Abstract: The microstructure evolution in hot forming will affect the mechanical properties of the formed product. However, the microstructure is sensitive to the process variables in deformation process of metals and alloys. A microstructure evolution model of a titanium alloy in hot forming, which included dislocation density rate and primary α phase grain size, was presented according to the deformation mechanism and driving forces, in which the effect of the dislocation density rate on the grain growth was studied firstly. Applying the model to the high temperature deformation process of a TC6 alloy with deformation temperature of 1 133-1 223 K, strain rate of 0.01-50 s^{-1} and height reduction of 30%, 40% and 50%, the material constants in the present model were calculated by the genetic algorithm(GA) based objective optimization techniques. The calculated results of a TC6 alloy are in good agreement with the experimental ones.

Key words: titanium alloy; grain size; dislocation density; hot forming; microstructure evolution model
CLC number: TG 319 **Document code:** A

1 INTRODUCTION

Titanium alloys have been intensely studied over the last few decades due to their important technological applications. The low density, high specific strength, excellent resistance against corrosion and high temperature strength retention, have prompted the use of titanium alloy in a wide variety of applications ranging from aircraft engine and structural components to bio-applications. It is well known that the microstructure of titanium alloy is very sensitive to the process parameters in deformation process, which also results in a strong sensitivity of the service properties of the workpiece. Therefore, simulation of microstructure evolution in metal forming has been paid more attention to in recent years[1-6].

In order to make an accurate computation for microstructure in hot forming, many researchers have developed diverse microstructure evolution models. Sellars[7] captured an empirical formula for recrystallization behavior by power-law functions of the process parameters, including strain, strain rate and deformation temperature. The application of statistical methods to microstructure prediction of recrystallization after hot forming was carried out by Bailer et al[8]. Ashby[9] applied internal state variables to describe the microstructure evolution. Ding et al[10] coupled fundamental metallurgical principles with the cellular automaton (CA) technique to simulate the dynamic recrystallization process. In recent years, the microstructure evolution of titanium alloy has been paid more attention to. Li et al[11-13] established a model for microstructure evolution during isothermal forming of titanium alloy, by means of the fuzzy set(FS) and artificial neural network(ANN), and applied it to simulate the grain size and the volume fraction of the primary α phase during isothermal compression of a cylinder.

The existing models are accurate enough but lack of adequate capabilities for revealing the internal deformation mechanism. Along with the mechanism and driving forces for the microstructure evolution being fairly well understood inch by inch, a novel model based on the deformation mechanism could be proposed. The internal state variables model not only has the higher reliability in prediction of microstructure, but also can reveal the deformation mechanism, so the internal state variables model gained considerable momentum.

The present work is focused on the identification of mechanism and driving forces for grain growth of titanium alloy. Based on the identified mechanism, a microstructure evolution model including dislocation density rate equation and grain

① **Foundation item:** Project(G2000067206) supported by the National Basic Research Program of China; Project supported by Teaching and Research Award Fund for Outstanding Young Teachers in Higher Education Institutions of Ministry of Education; Project(50475144) supported by the National Natural Science Foundation of China; Project(CX200305) supported by the Doctorate Creation Foundation of Northwestern Polytechnical University **Received date:** 2004-11-08; **Accepted date:** 2005-01-25

Correspondence: LI Xiao-li, PhD; Tel: +86-29-88460465; E-mail: ustblxl@163.com

growth rate equation is proposed. In addition, the genetic algorithm (GA) based objective optimization technique is used to determine the material constants arising in the model from the experimental data of a TC6 alloy at different temperatures, height reductions and strain rates.

2 MICROSTRUCTURE EVOLUTION MODEL

2.1 Dislocation density rate

It is well known that the dislocation structure developed in plastic deformation constitutes a driving force for microstructure evolution, such as recrystallization and grain growth. Dynamic recrystallization (DRX) is commonly associated with high temperature plastic deformation of metallic materials with relatively low-to-medium stacking fault energy. It was pointed out that the stacking fault energy of two-phase titanium alloy is fairly high[14]. Therefore, when the deformation occurs in the two phases region, there is no dynamic (or metadynamic) recrystallization for all the experimental conditions[14].

Dislocation density ρ in hot forming depends on two competing processes: work hardening and dynamic recovery (softening). Kocks and Mecking have pursued a phenomenological approach (the K-M model) to predict the variation of dislocation density with strain for stage III hardening of metals[10]. The model is based on the assumption that the kinetics of plastic flow is determined by a single structural parameter (dislocation density ρ) which represents the entire current structure. In the K-M model, the dislocation storage rate is proportional to $\rho^{1/2}$, and the dislocation annihilation rate is proportional to ρ, so the variation of the mean dislocation density with respect to strain can be expressed as

$$\frac{d\rho}{d\varepsilon_p} = k_1\sqrt{\rho} - k_2\rho \tag{1}$$

where ε_p is the plastic strain, the coefficient k_1 is a constant, k_2 represents a thermally activated process of dynamic recovery by dislocation cross-slip (at low temperature) or dislocation climb (at high temperature), which is a function of temperature and strain rate, and can be described as[15]

$$k_2 = k_{20}\frac{\dot{\varepsilon}_0^*}{\dot{\varepsilon}_p}\left[1 - \exp(-0.7R_c^4\rho^2)\right] \cdot \exp\left[-\frac{Q}{RT}\right] \tag{2}$$

where $\dot{\varepsilon}_0^*$ and $\dot{\varepsilon}_p$ are the reference and applied strain rates, Q is the activation energy for cross slip and recombination, R is the gas constant (8.31 J·mol^{-1} K^{-1}), T is the absolute deformation temperature (K), R_c is a cut-off radius beyond which dislocations cannot cross-slip and recombine, and k_{20} is a proportional constant. The multiplicative factor ($k_{20}\dot{\varepsilon}_0^*$) is used as a fitting constant. In the hot forming of metal, the dislocation density ρ is so large that the $\exp(-0.7R_c^4\rho^2)$ in Eqn.(2) is close to zero. Therefore, Eqn.(2) is simplified as the following equation:

$$k_2 = k_{20}\frac{\dot{\varepsilon}_0^*}{\dot{\varepsilon}_p}\exp\left[-\frac{Q}{RT}\right] \tag{3}$$

Substituting Eqn.(3) into Eqn.(1), the dislocation density rate $\dot{\rho}$ can be written as

$$\dot{\rho} = \alpha_1\sqrt{\rho}\,|\dot{\varepsilon}_p| - \alpha_2\exp\left[-\frac{Q}{RT}\right]\rho \tag{4}$$

where α_1 and α_2 ($= k_{20}\dot{\varepsilon}_0^*$) are the material constants. The right hand side of Eqn.(4) has two terms, the first term characterizes the processes of dislocation storage and the second term characterizes the concurrent dislocation annihilation by recovery. In steady deformation state, the variation of dislocation density is so small as to be ignored, i.e. $\dot{\rho} \approx 0$.

2.2 Grain growth rate

The microstructure of two-phase titanium alloy is composed of two phases: an hcp α phase including the primary α phase and the secondary α (α') phase, and a bcc β phase which are stable at low and high temperatures. For the two-phase titanium alloy, the mechanical performance is affected greatly by the shape and size of primary α phase. So to describe the primary α phase grain growth is the key to the microstructure modeling in hot forming.

In the absence of dynamic recrystallization, grain refinement caused by dynamic recrystallization will not occur. The primary α phase grain growth is composed of the static grain growth, plastic strain induced dynamic grain growth, grain growth and grain refinement due to the variation of dislocation density.

The static grain growth at high temperature can be modeled by

$$\dot{d}_{\text{static}} = \frac{M\sigma_{\text{surf}}}{d} \tag{5}$$

where M is the mobility of grain boundaries and σ_{surf} is the grain boundary energy per unit area[16]. The multiplicative factor ($M\sigma_{\text{surf}}$) is used as a fitting constant, so Eqn.(5) can be expressed as

$$\dot{d}_{\text{static}} = \beta_0 d^{-\gamma_0} \tag{6}$$

where β_0 and γ_0 are the temperature-dependent material constants.

In hot forming, the plastic strain induced dynamic grain growth can be expressed as[17]

$$\dot{d}_{\text{dynamic}} = \beta_1|\dot{\varepsilon}_p|d^{-\gamma_1} \tag{7}$$

where β_1 and γ_1 are the temperature-dependent material constants.

During deformation process, the dislocation density is changing intensely due to the work hardening and dynamic recovery. So the influence of the dislocation density on the grain size is too great to be ignored. Some scholars proposed that the average grain size is inversely proportional to dislocation density in hot forming[18, 19], and can be described by the following equation:

$$d = \frac{K}{\sqrt{\rho}} \tag{8}$$

where K is the material constant.

According to Eqn. (8), the influence of the variation of dislocation density on the grain growth is proposed in this paper:

$$\dot{d}_{dis} = -\beta_2 \dot{\rho}^{\gamma_2} d^{\gamma_3} \tag{9}$$

where β_2, γ_2 and γ_3 are the material constants.

Considering the static grain growth, plastic strain induced dynamic grain growth and the influence of the variation of dislocation density on grain growth, the grain growth rate may take the form as

$$\dot{d} = \dot{d}_{static} + \dot{d}_{dynamic} + \dot{d}_{dis} = \beta_0 d^{-\gamma_0} + \beta_1 |\dot{\varepsilon}_p| d^{-\gamma_1} - \beta_2 \dot{\rho}^{\gamma_2} d^{\gamma_3} \tag{10}$$

By introducing the effect of the dislocation density on the grain growth, the microstructure evolution model is fit for all deformation condition, which overcomes the problems in the material models proposed by some researchers[17, 20] that are only able to model the static grain growth and the dynamic grain growth induced by plastic strain in superplastic deformation.

In summary, the physically based model for microstructure evolution in hot forming of titanium alloy is expressed as

$$\begin{cases} \dot{\rho} = \alpha_1 \sqrt{\rho} |\dot{\varepsilon}_p| - \alpha_2 \exp\left(-\frac{Q}{RT}\right) \rho \\ \dot{d} = \beta_0 d^{-\gamma_0} + \beta_1 |\dot{\varepsilon}_p| d^{-\gamma_1} - \beta_2 \dot{\rho}^{\gamma_2} d^{\gamma_3} \end{cases} \tag{11}$$

where α_1, α_2, β_0, β_1, β_2, γ_0, γ_1, γ_2 and γ_3 are the material constants to be determined from experimental data using GA-based objective optimization technique.

3 APPLICATION OF MODEL TO TC6 ALLOY

3.1 Material

The TC6 alloy was chosen to verify the microstructure evolution model in this study, which is one of the best two-phase titanium alloys with good resistance against heat and corrosion, and has been widely used in the aviation and aerospace industries. The TC6 alloy produced by Baoji Nonferrous Metal Works, China, is of 42 mm in diameter. The chemical composition is shown in Table 1. The heat treatment procedure before isothermal compression tests was as follows: heating to 1 143 K and holding for 1 h, then to 923 K and holding for 2 h, and finally cooling in air to room temperature. The cylindrical specimens with 8mm in diameter and 12 mm in height were machined from the heat-treated bars.

Table 1 Chemical composition of TC6 alloy (mass fraction, %)

Al	Cr	Fe	Mo	Si	Ti
6.29	1.42	0.42	2.71	0.33	Bal.

3.2 Hot compression

The isothermal compression experiments with constant strain rate were conducted at THERMECMASTOR-Z simulator. The specimens and compression rams were heated by high frequency induction heating system under the vacuum condition to avoid oxidation. The specimens were kept for 3 min before the commencement of deformation. After compression, the specimens were immediately quenched by nitrogen gas at the cooling speed of 30 K/s to retain the as-deformed microstructures[21].

3.3 Microstructure tests

The β transus temperature of the TC6 alloy is about 1 233 K. The nominal deformation temperatures were ranged as 1 133, 1 193 and 1 223 K, and the strain rates were 0.01, 1 and 50 s^{-1} for each deformation temperature. The isothermal compression tests were performed with 30%, 40% and 50% reductions in height at each combination of deformation temperature and strain rate. For microstructure measurement of the TC6 alloy, four locations in four directions and a location near the center on equatorial plane of each specimen were chosen. The measurement of microstructure was carried out at Leica LABOR-LUX12MFS/ST microscope for quantitative metallography with QUANTIMET 500 software of image analysis, in which three visual fields at each location of specimens were chosen to measure. The selected experimental results, which are the average values of all the visual fields for each specimen, are shown in Table 2.

Table 2 Primary α phase grain size under different deformation conditions

Deformation temperature/K	Height reduction/%	Grain size/μm		
		0.01 s^{-1}	1 s^{-1}	50 s^{-1}
1 133	30	4.10	4.09	5.78
1 193	40	3.91	3.85	3.85
1 223	50	2.37	3.11	4.16

3.4 Determination of material constants

The optimization techniques for obtaining the material constants arising in the model were based on minimizing the sum of the errors between the experimental and calculated data[22, 23]. For the microstructure evolution model, an objective function was defined in terms of the square of the difference between the experimental and the calculated data of the primary α phase grain size:

$$f(x) = \sum_{j=1}^{n}\sum_{i=1}^{m} w_{ij}[(d_i^c)_j - (d_i^e)_j]^2 \qquad (12)$$

where $f(x)$ is the residual for average grain size, $x(=[x_1, x_2, \cdots, x_s])$ represents the material constants and s is the number of the constants to be determined, $(d_i^c)_j$ and $(d_i^e)_j$ are the calculated and experimental average grain size for the same strain level i and strain rate j, m is the number of the experimental average grain size data for the strain rate j, n is the number of strain rates considered for grain growth, w_{ij} is the weight coefficient. The calculated grain size $(d_i^c)_j$ is not available directly and has to be determined from the grain growth Eqn.(10) by means of a numerical integration method. The determination of material constants within the model is to minimize the above objective function.

By using conventional optimization method, it is very difficult to search the global minimum in the multi-modal distribution space. In order to search the global minimum quickly and effectively, a novel algorithm must be introduced.

Genetic algorithm (GA) is a kind of search algorithm based on the concepts of natural selection and survival of the fittest. GA can model the life evolutional mechanism and search the global minimum quickly in complex system[24]. In this paper, a genetic algorithm based optimization techniques was developed and programmed to determine the material constants in the microstructure evolution model. Sixteen sets of the experimental data of TC6 alloy at deformation temperatures of 1 133 − 1 223 K and strain rates of 0.01 − 50 s^{-1} acted as the sampled data. The determined material constants are listed in Table 3.

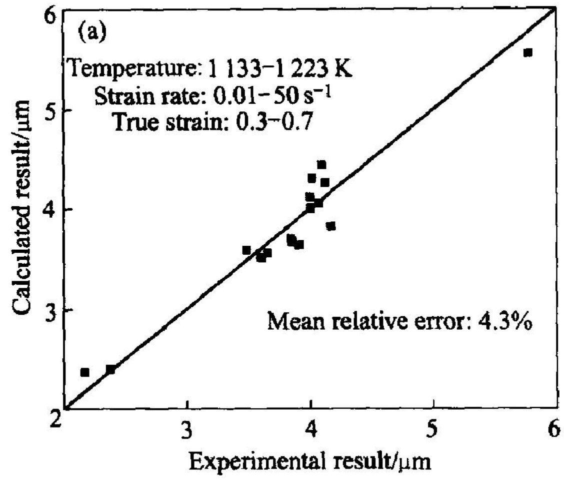
Table 3 Optimized material constants for microstructure evolution of TC6 alloy

α_1	α_2		β_0	β_1
0.737 5	1.0×10^{-9}		0.202 0	0.935 0
β_2	γ_0	γ_1	γ_2	γ_3
2.13×10^{-7}	6.027 8	15.28	0.984 9	3.520 9

3.5 Comparison of calculated results with experimental ones

The model of Eqn.(11) with the material constants listed in Table 3 was used to calculate the grain size of TC6 alloy at high temperature deformation.

The calculated and experimental results of the primary α phase grain size are shown in Fig. 1. The average relative error between the sampled experimental data of the sixteen sets and the calculated is 4.3%. The average relative error between the non-sampled experimental data of the five sets and the calculated, which is not included in the optimizing calculation, is 10.1%. It can be seen that the microstructure evolution model can be used to represent the primary α phase grain size of TC6 alloy at deformation temperatures of 1 133 − 1 223 K and strain rates of 0.01 − 50 s^{-1}.



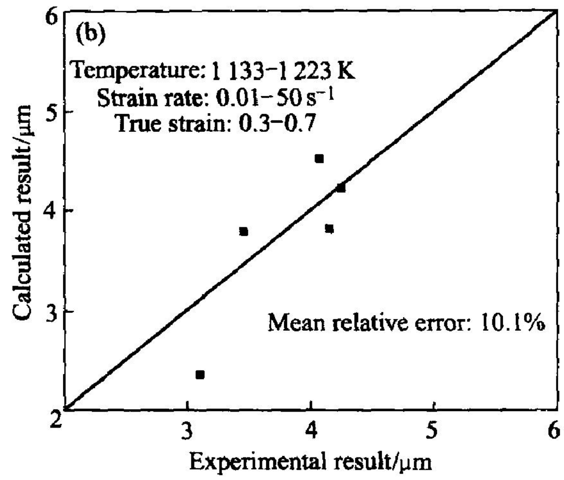


Fig. 1 Comparison of calculated results with experimental ones of primary α phase grain size
(a) —Sampled data; (b) —Non-sampled data

4 CONCLUSIONS

1) Based on the analysis of deformation mechanism and driving forces, a microstructure evolution model including dislocation density rate and grain growth rate was proposed. In the grain growth rate equation, the effect of the dislocation density rate on the grain growth was studied for the first time.

2) The material constants within the model were determined from the experimental data of TC6 alloy in the temperature range 1 133 − 1 223 K and strain rates 0.01 − 50 s^{-1} by the GA-based objective optimization technique. This provides a reasonably accurate fitting over the whole range of temperature and strain rates of current interest.

3) The microstructure evolution model presented in this paper, which are genetic in nature, are applicable over most of two-phase titanium alloy.

REFERENCES

[1] Semiatin S L, Seetharaman V, Weiss I. Hot working of titanium and titanium aluminide alloy —An overview [J]. Materials Science and Engineering, 1998, A1243 (1/2): 1－24.

[2] Kim H Y, Hong S H. High temperature deformation behavior and microstructural evolution of Ti-47Al-2Cr-4Nb intermetallic alloys [J]. Scripta Materiallia, 1998, 38(10): 1517－1523.

[3] Semiatin S L, Bieler T R. The effect of alpha platelet thickness on plastic flow during hot working of Ti-6Al-4V with a transformed microstructure [J]. Acta Materiallia, 2001, 49(17): 3565－3573.

[4] Nemat-Nasser S, Guo W, Nesterenko V F, et al. Dynamic response of conventional and hot isostatically pressed Ti-6Al-4V alloys: experiments and modeling [J]. Mechanics of Materials, 2001, 33: 425－439.

[5] LI M, XIONG A, HUANG W, et al. Microstructural evolution and modelling of the hot compression of a TC6 titanium alloy [J]. Materials Characterization, 2003, 49: 203－209.

[6] LI M, CHEN D, XIONG A, et al. An adaptive prediction model of grain size for the forging of Ti-6Al-4V alloy based on the fuzzy neural networks [J]. Journal of Materials Processing Technology, 2002, 123(3): 377－381.

[7] Sellars C M. Modelling microstructural development during hot rolling [J]. Materials Science and Technology, 1990, 15: 1072－1081.

[8] Bailer C A L, Mackay D J C, Sabin T J, et al. Static and dynamic modelling of materials forging [J]. Australian Journal of Intelligent Information Processing Systems, 1998, 5: 10.

[9] Ashby M F. Physical modelling of materials problems [J]. Materials Science and Technology, 1992, 8: 102－111.

[10] DING R, GUO Z X. Microstructural modelling of dynamic recrystallisation using an extended cellular automation approach [J]. Computational Materials Science, 2002, 23: 209－218.

[11] XIONG A, XUE S, LI M. Microstructure evolution and modeling during isothermal deformation of TC4 titanium alloy [J]. Journal of Plastic Engineering, 2002, 9(1): 14－16. (in Chinese)

[12] LI M, XIONG A. New model of microstructural evolution during isothermal forging of Ti-6Al-4V alloy [J]. Materials Science and Technology, 2002, 18: 212－214.

[13] LI M, LIU X, XIONG A, et al. Microstructure modeling and FE simulation of a titanium alloy during isothermal forging [A]. Mynors D, Ruan X. Proceedings of 4th ICFG Workshop on Process Simulation in the Metal Forming In dustry [C]. Shanghai, China, 2004. 108－120.

[14] Ding R, Guo Z X, Wilson A. Microstructural evolution of a Ti-6Al-4V alloy during thermomechanical processing [J]. Materials Science and Engineering, 2002, A327: 233－245.

[15] Picu R C, Majorell A. Mechanical behavior of Ti-6Al-4V at high and moderate temperatures —Part Ⅱ: Constitutive modeling [J]. Materials Science and Engineering, 2002, A326: 306－316.

[16] Shewmon P G. Transformations in Metals [M]. New York: McGraw-Hill, 1969.

[17] Dunne F P E. Inhomogeneity of microstructure in superplasticity and its effect on ductility [J]. International Journal of Plasticity, 1998, 14(4－5): 413－433.

[18] Estrin Y, Toth L S, Molinari A, et al. A dislocation-based model for all hardening stages in large strain deformation [J]. Acta Materialia, 1998, 46(15): 5509－5522.

[19] Estrin Y. Dislocation theory based constitutive modeling: foundations and applications [J]. Materials Processing Technology, 1998, 80－81: 33－39.

[20] Cheong B H, Lin J, Ball A A. Modelling of hardening due to grain growth for a superplastic alloy [J]. Journal of Materials Processing Technology, 2001, 119: 361－365.

[21] XIONG Ai-ming, HUANG Wei-chao, CHEN Sheng-hui, et al. Effects of heat treatment on microstructure of TC6 titanium alloy [J]. The Chinese Journal of Nonferrous Metals, 2002, 12(1): 206－209. (in Chinese)

[22] LIN J, YANG J. GA-based multiple objective optimisation for determining viscoplastic constitutive equations for superplastic alloys [J]. International Journal of Plasticity, 1999, 15: 1181－1196.

[23] LIN J, LIU Y. A set of unified constitutive equations for modeling microstructure evolution in hot forming [J]. Journal of Materials Processing Technology, 2003, 143－144(20): 281－285.

[24] Castro C F, António C A C, Sousa L C. Optimisation of shape and process parameters in metal forging using genetic algorithms [J]. Journal of Materials Processing Technology, 2004, 146: 356－364.

(Edited by YUAN Sai-qian)