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Simulation of β – α Transformation In Ti-6Al-4V using Cellular Automata

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***Abstract*— The transformation from β titanium to α titanium is a fast process, andhence simulation of the process is a reliable technique for the understanding of their microstructural evolution and the morphology of the transformed phase. Cellular Automata (CA) is the technique used here for the simulation. In this technique, the considered lattice is divided into a number of cells and based on the property determining parameters of the material, dependent variables are calculated for each cell. Initial Ti-6Al-4V microstructure is mapped to the MATLAB by an image. Based on the assumptions and the thermodynamic properties of Ti-6Al-4V all relevant properties and microstructure is captured by incorporating nucleation and its growth and vanadium diffusion. Vanadium diffusion is solved by Finite Difference Method using appropriate boundary conditions. The simulation is done for three different cooling rates 10, 20 & 30˚C/s.**

***Keywords*—Titanium alloy, Ti-6Al-4V, Phase transformation, Simulation, Cellular Automata**

INTRODUCTION

Titanium has an excellent combination of properties such as strength, ductility, toughness, corrosion resistance, especially in the presence of oxidizing acids. Also, Titanium has a very high strength to weight ratio which makes it an excellent choice for the aerospace industry. The other major application is in chemical industry. As Titanium is very expensive compared to other metals, its applications were limited. But in the recent years, the automotive industry has started using Titanium for the production of high performance cars because of the high strength to weight ratio. Due to its high resistance to corrosion, they have found huge application in the biomedical industry such as for prostheses, implants etc. Even the sports industry started using Titanium for producing several high-performance equipment and sports gears such as bicycles, badminton and tennis rackets etc.

Titanium exists in two stable allotropic forms, one at higher temperature and the other at lower temperature with the β transformation temperature (T_β) being at 882˚C. The allotropic form of Titanium alloy at lower temperature is called α titanium and the form at higher temperature is called β titanium. The α titanium exists as hexagonal close packed (hcp) structure and β titanium exists as body centered cubic (bcc) structure seen in Fig. 1 [1]. Titanium are presently used in industries in the form of different types of alloys.

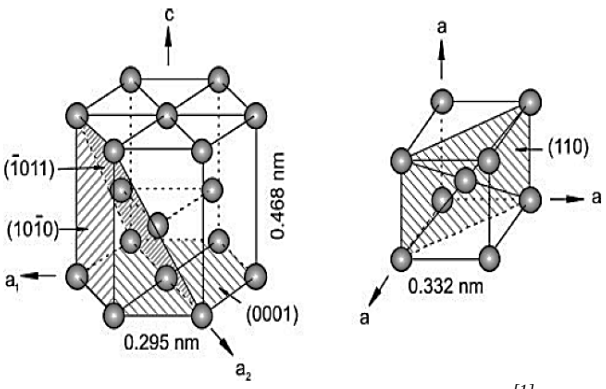

Fig. 1 Crystal Structure of hcp α and bcc β[1]

Several numerical simulation techniques are used for microstructure evolution. Some of the methods used are vertex models, Potts-Mote Carlo models (MC), phase field models and cellular automaton models(CA). The microstructural evolution process and microstructure properties can be accurately produced using these methods. In the vertex model, the calculation for finding the vertex driving force and the vertex equations are very complex. So, its use has been limited in the recent years. Monte Carlo (MC) method is used for simulation of grain growth, recrystallization and phase transformation. The lowest energy principle is used for determining the microstructural evolution. There is no switching rule and the variables are updated subsequently in each time interval. Phase Field method can be used to describe evolution kinetics of microstructural systems. To describe the complex

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evolution, in this method, some necessary variables are introduced. The main disadvantage of this method is that it is very complex and of all the methods it is the most time consuming [8].

The CA method is used for simulating grain growth, recrystallization and phase transformation. This method uses a switching rule for changing or switching the state of each cell and all the variables that influence the state are updated synchronously. The switching rules are created based on physical models that govern the evolution. All these features make the CA method more feasible than the other methods. Fig. 2 shows the schematic illustration of the CA modelling procedure.

The properties and the application of the Titanium alloys are determined by certain factors which include the phases present, grain size, grain shape, morphology and distribution of the fine microstructure.Ti-6Al-4V,which is an α and β alloy, is one of the most widely used Titanium alloy. In the past few decades, several studies have been conducted to study the microstructure and simulate the evolution process of the Titanium alloys.When Ti-6Al-4V is cooled from temperatures above the β-transformation temperature (T_β), for higher cooling rates, the microstructure obtained is entirely martensitic. For slow cooling rates, the α phase grows and coarsens in form of plates or needles [9]. Two morphologies of α phase nucleates during slow cooling rates from temperatures above the T_β: α GB (for α grain boundary) layer which forms at the β / β grain boundaries and α W (for α Widmanstatten) platelets which grow within the β grains. They also mentioned two types of αW structures and related their morphologies to temperature [10].

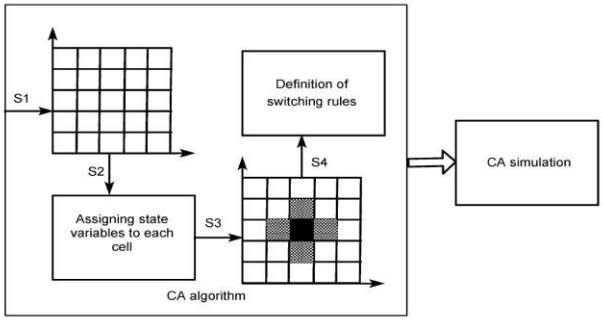

Fig. 2 CA Algorithm[8]

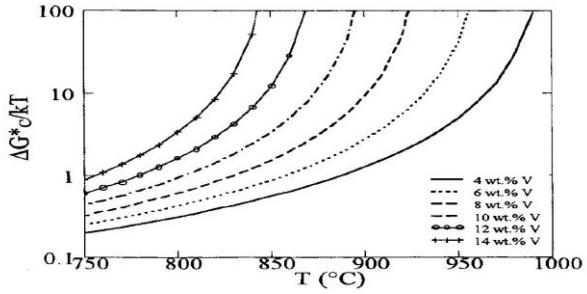

Fig. 3 Nucleation barrier as a function of vanadium Content[16]

The β-α phase transformation kinetics for the Ti-6Al-4V alloy during continuous cooling or under isothermal conditions has been extensively investigated and modeled using the classical Johnson-Mehl-Avrami (JMA) model [11-13]. Malinov et al. [14] studied the isothermal β-α phase transformation kinetics. They obtained two different values for the Avrami index (n). Avrami index n=1.1 for temperatures varying from 900 – 950˚C and n=1.35 for temperatures between 750 – 900˚C. Based on the two different values of n, two different mechanism of alpha formation were suggested: grain boundary nucleation for isothermal holdings above 900˚C, and homogenous nucleation for isothermal holdings below 900˚C. This difference in nucleation mechanism was related to the effect of undercooling. The β-α phase transformation during continuous cooling was also studied using a modified JMA model [15]. A constant value of n = 1.13 is obtained. It was concluded that there was no change in the mechanism of the transformation, and suggested that the α phase nucleates heterogeneously at the β grain boundaries and that the overall transformation rate is controlled by the nucleation rate.

A finite element model (FEM)was proposed to study the kinetics and the morphology of the β-α phase transformation [16]. This transformation was assumed to be controlled by the diffusional redistribution of vanadium between the α and the β phases. The FEM model describes the nucleation and growth process of the α phase. They obtained a numerical solution for the localization and evolution of the α/ β interface using FEM and volume of fluids method. In another study [17], it was found that, martensitic transformation occurred in the α+β Ti-6Al-4V alloy cooled from the β phase range (1020˚C) at 23.1˚C/s. After cooling at 7.3˚ C/s bot dispersed α and α’ martensite where present in the alloy, whereas cooling at 2.5˚C/s or slower only diffusional transformation took place resulting in entirely α structure. The α phase morphology was

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strongly affected by the cooling rate and appeared as Widmannstatten lamellas and equiaxed grains. Lamella or grain size increased if cooling rate is decreased. The β-α transformation kinetics of Ti-6Al-4V was also studied using an approach based on the Johnson-Mehl-Avrami-Kolomogrov (JMAK) model [18]. This approach permits the kinetics parameters to be determined from a single DSC curve of the corresponding cooling rate, by using a simple linear regression. Value of n obtained is n=1.0, which suggests that there is no change in transformation mechanism.

II. OBJECTIVES

1. Simulate the β – α transformation in the titanium alloy Ti-6Al-4V using cellular automata.
2. To study the kinetics of the β – α transformation in the titanium alloy Ti-6Al-4V.
3. To simulate the final microstructure at the end of transformation.
4. To study the effects of cooling rate on the transformation and the final microstructure.

III.GENERAL ASSUMPTIONS

The assumptions made in the modelling of the β-α transformationin Ti-6Al-4V are as follows:

1. The transformation is diffusion controlled.
2. The effect of Aluminium in the transformation is neglected.
3. The nucleation is heterogenous nucleation.
4. The diffusion coefficient D is temperature dependent and is governed by the Arrhenius type equation

$$D = A\exp\left(-\frac{Q}{RT}\right)$$

5. Activation energy for atomic migration is half of the activation energy for diffusion

IV. MODELLING

The α nuclei formation occurs, when the alloy if cooled from the T_β temperature. There is only heterogenous nucleation. So the new nucleus is formed on the β grain boundaries. The nucleation rate is given by the equation [16]

$$N=N_v \frac{k_b T}{h}\exp\left(\frac{-\Delta G_m}{k_b T}\right)\exp\left(\frac{-\Delta G_c^*}{k_b T}\right) \quad ..(1)$$

Where, N_v = number of nucleation sites/unit volume, ΔG_m = activation energy for atomic migration across the interface, ΔG_c^* = the activation energy for nucleation, k_b = Boltzmann constant and h = planck constant. The value for these constants are obtained from published literature [16]. The value for ΔG_c^* is obtained from Fig. 3

The number of nuclei at each time step is calculated using the equation [16]

$$J_0 = \int_{t_0}^{t_n}\int_{S_\beta} N_V \frac{k_b T}{h}\exp\left(\frac{-\Delta G_m}{k_b T}\right)\exp\left(\frac{-\Delta G_c^*}{k_b T}\right) dsdt \quad (2)$$

Fig. 3 shows Nucleation barrier as a function of vanadium content. The moment the number of nuclei increases by one, a new nucleus is created at the β grain boundary. The probability for the nucleus to appear is given by the equation [16]

$$P(x) = P_0 \exp\left(\frac{-\Delta G_c^*(T, C(x))}{k_b T}\right) \quad ..(3)$$

Where C(x) is the vanadium concentration. For a new nucleus occurring on the grain boundary area S_β at the moment t_n is equal to 1.

$$I = P_0 \int_{s_\beta} \exp\left(\frac{-\Delta G_c^*(T, C(x))}{k_b T}\right) dx \quad ..(4)$$

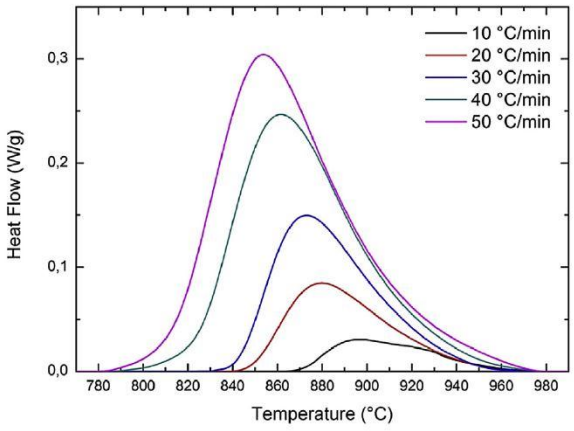

Fig. 4 DSC calorimetry data for Ti-6Al-4V for different cooling rates[18]

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For modelling the growth of the α phase, JMAK equation [18] is usedand is given by,

$$f = 1 - \exp(-kt^n) \quad ..(5)$$

where, f is the phase fraction, k is the reaction rate constant and n is the Avrami index. The Avrami index n is taken from published literatures [18,19] and the rate constant k is found out using the method used by Kherrouba et al. [18].The instantaneous phase fraction can be calculated using the DCS calorimetry data shown in Fig. 4 for different cooling rates using the equation [18]

$$f_i = \frac{\int_{t_s}^{t_i} \frac{dh}{dt} dt}{\int_{t_s}^{t_f} \frac{dh}{dt} dt} \quad ..(6)$$

The growth of the precipitate requires a flux of vanadium atoms from α to β phase, there must be a positive driving force across the interface, which can be calculated by solving the diffusion equation

$$\frac{\partial C}{\partial t} = \nabla.(D\nabla C) \quad ..(7)$$

The diffusion equation is solved using Finite difference method. The diffusion coefficient D is calculated using the equation [16]

$$D = A\exp\left(-\frac{Q}{RT}\right) \quad ..(8)$$

Where A is rate of diffusion, Q is the activation energy for diffusion, R is the gas constant and T the temperature. The value for the constants are taken from published literature [16].

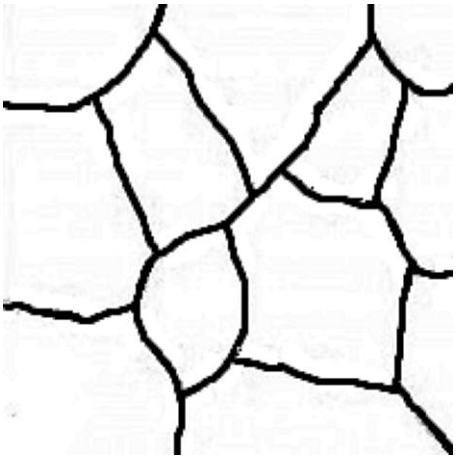


Fig. 5 Initial microstructure of Ti-6Al-4V at 1050° C[19]

Simulation Procedure

1. Size of the specimen is taken as 2000μm X 2000μm. So, a cellular structure containing 200X200 cells are taken, with the area of each cell being 100μm^2.

2. Slow cooling rate are used for the simulation. The cooling rates are 10, 20, 30° C/min. The values for each of the parameters required for the simulation are calculated.

3. The phase state variables and the concentration variables are defined.

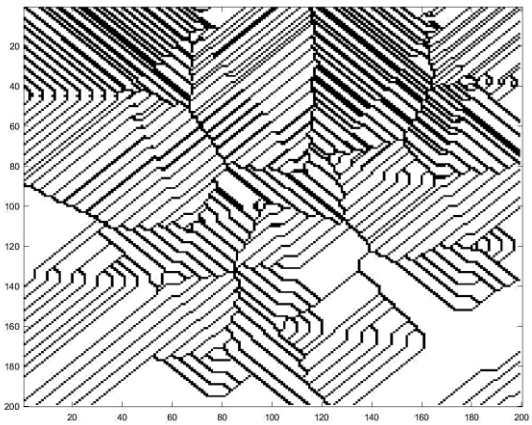
4. The transition rules which govern the switching of cells are defined.

5. The initial β microstructure to be used in simulation is obtained from a published material. A 2000μm X 2000μm size of the grain image is selected and is mapped into the Cellular automata using MATLAB.

6. With the help of MATALAB image processing, the grain boundary cells are identified.

7. When the desired undercooling is achieved, the transformation from β to α starts.

8. The nucleation of α starts at β grain boundaries and is followed by its growth. Random number generation is used for selecting the first site in the grain boundary where the first nucleus occurs.



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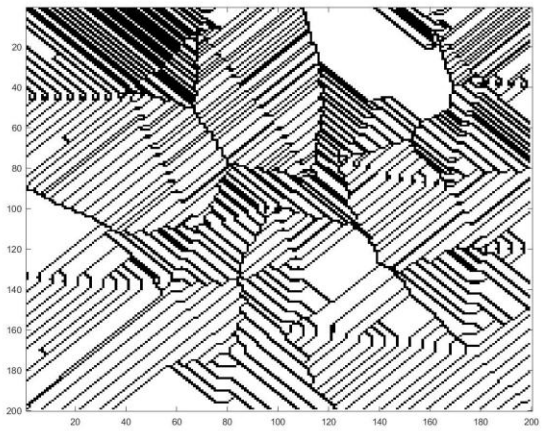

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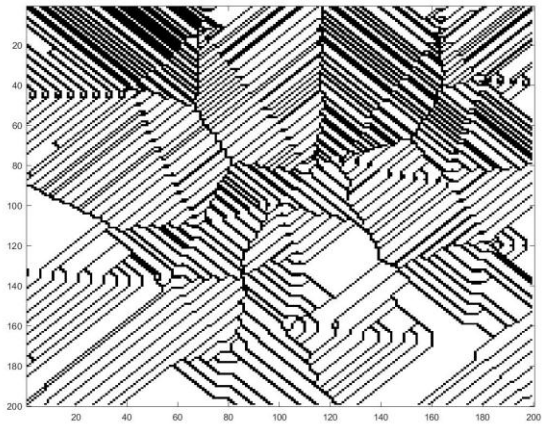

(c)

Fig. 6 Final simulated microstructure for different cooling rates (a) 10˚C/min(b) 20˚C/min (c) 30˚C/min

9. Now, after the first nucleus is created the predefined transition rules are applied to the selected cell and cell is converted to α/β.

10. When the number of nuclei value increases by 1, new nuclei is created at β grain boundaries and the cell is converted to α/β.

11. The phase state variables and concentration variables are updated accordingly.

12. The α/β cells grow.

13. When a cell is completely converted to α, its neighbours become α/β.

14. Determine α phase fraction at the new time.

15. Now update the β phase domain using the updated α phase volume fraction.

16. The vanadium concentration of all the cells are updated

17. Steps 10 through 16 are repeated until all the β phase is converted to α phase or the α phase fraction is equal to 1.

RESULT AND DISCUSSION

The simulation of the β – α transformation in Ti-6Al-4V is a 2D simulation. Simulation was done for three cooling rates 10, 20 & 30˚ C/min. The start temperature for the β – α transformation, for different cooling rates are obtained from the DSC calorimetry data. The final simulated microstructure of Ti-6Al-4V at the end of transformation for the three cooling rates are shown in Fig. 6. From the figure, it is clear that the microstructure for lower cooling rates are much more developed and the grains are thicker than that for higher cooling rates. This is because, at slow cooling rates, there is enough time for the vanadium diffusion to happen and there is enough time for the grains to grow.

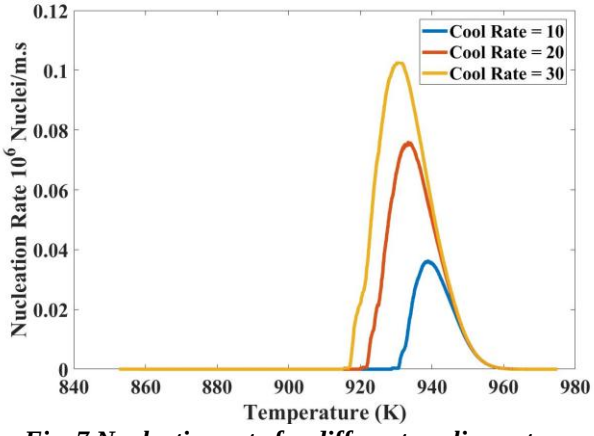

Fig. 7 Nucleation rate for different cooling rates

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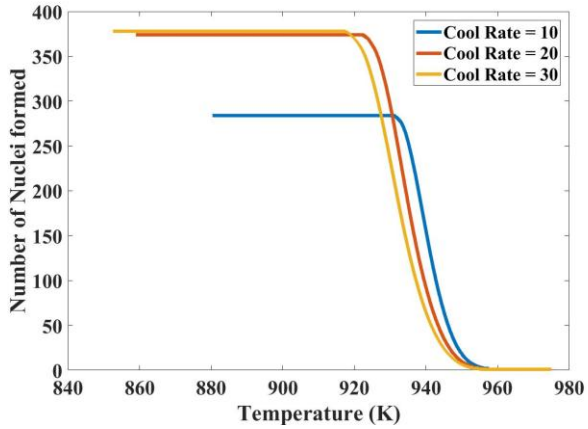

Fig. 8 Number of nuclei formed for different cooling rates

Fig. 7 shows the nucleation rate for different cooling rates. As temperature decreases, the exponential term for atomic migration in the nucleation rate equation decreases, but the exponential term for nucleation barrier increases, which causes a maximum value for the nucleation rate, after which it decreases. Also as the temperature decreases, the number of nucleation sites (i.e. β grain boundary) also decreases because of the growth of α phase, which also explains the maximum value for nucleation rate. Fig. 8 shows the total number of nuclei formed for different cooling rates. As the cooling rate increases, the number of nuclei formed also increases. At slow cooling rates, the nucleation rate is also less (Fig. 7). Also at lower cooling rates the transformation occurs at a slow pace, so that, there is enough time for vanadium diffusion and the growth of the alpha phase, which in turn reduces the number of nucleation sites present. This explains the increase in number nuclei at higher cooling rates.Fig. 9 and 10 shows the α phase fraction amount against temperature and time respectively for different cooling rates. The graphs obtained from the simulation are in close agreement with the results published by katzarov et al. and W. sha et al. [18,19]. This validates the transformation model created.

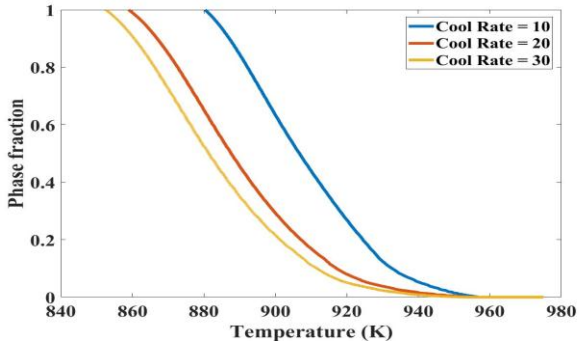

Fig. 9 α Phase fraction vs. temperature for different cooling rates

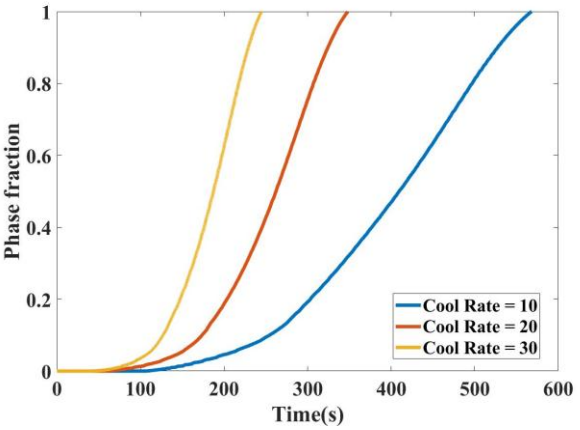

Fig. 10 α Phase fraction vs. time for different cooling rates

VII. CONCLUSION

The β – α transformation is successfully simulated using the proposed model and the results obtained are in close agreement with published results which validates the current model. The following conclusions can be drawn from the results obtained

1. The final microstructure at the end of the transformation is successfully simulated.
2. The microstructure at lower cooling rates are more developed compared to that at higher cooling rates.
3. The grains are thicker at lower cooling rates compared to that at higher cooling rates.
4. As the cooling rate increases, the nucleation rate also increases.

VIII. FUTURE SCOPE

Simulation of microstructure of titanium alloys during various thermomechanical and thermochemical processing is of great interest for several industries. Several research works are being done on this area. The current model is only applicable for continuous cooling at slow cooling rates (<40˚C/min). At higher cooling rates, the transformation is martensitic transformation. Also at higher cooling rates, there is formation of α_{GB} and α_{W} grains. The current model is not capable of simulating the formation of these grains. Only heterogenous nucleation is incorporated in the current model.The effects of the alloying element Aluminium, even though negligible, is not included in the current model.

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