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SIMULATION OF MICROSTRUCTURE EVOLUTION DURING FORGING AND HEAT TREATMENT OF Ti-6Al-3.5Mo-1.5Zr-0.3Si TITANIUM ALLOY

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Abstract

The model of dynamic recrystallization of Ti-6Al-3.5Mo-1.5Zr-0.3Si has been developed based on experimental data and implemented in FEM code QForm. Kinetics of dynamic recrystallization was simulated by Johnson-Mehl-Avrami-Kolmogorov equation. Effect of aging time (1-6 h) and temperature (450-650 °C) on mechanical properties has been experimentally studied. The model of heat treatment of Ti-6Al-3.5Mo-1.5Zr-0.3Si has been developed and implemented in FEM code QForm. The model is capable to predict phase composition and hardness during and after arbitrary heat treatment within studied range. It was found that the highest hardness of Ti-6Al-3.5Mo-1.5Zr-0.3Si can be obtained by aging during 4-6 hours at 550°C after solution treatment at 960°C.

Key words: Simulation, Microstructure evolution, Heat treatment, QForm, Forging

1. INTRODUCTION

Titanium alloys, particularly dual-phase titanium alloys, have been widely used as advanced structural materials in aeronautic applications (Song et al., 2014; Zong et al., 2009). Ti-6Al-3.5Mo-1.5Zr-0.3Si alloy is an α+β heat resistant titanium alloy that is applicable for critical aerospace applications owing to its high strength to weight ratio, good corrosion resistance and a high service temperature up to 500 °C (Li et al., 2002). The alloy is widely used in aircraft engine compressor disks and blades and some airplane components. An understanding of the mechanisms of thermo-mechanical processing of this alloy will be highly beneficial to control its microstructure during manufacturing (Alimov et al., 2018). The objective of this study is to simulate the microstructural evolution during hot forging and to predict the mechanical properties after heat treatment of Ti-6Al-3.5Mo-1.5Zr-0.3Si part.

2. MATERIALS AND PROCEDURES

2.1. Materials

The billet used in the present work was a 55 mm diameter hot-rolled bar stock of Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy. Its measured composition (in wt%) was 5.9 aluminum, 3.27 molybdenum, 1.40 zirconium, 0.2 silicon, balance titanium. The β transus for this material is about 1008 °C. The study of Ti-6Al-3.5Mo-1.5Zr-0.3Si microstructure evolution and heat treatment have been performed in as supplied state. The initial microstructure is shown in figure 1. Microstructure is bimodal with globular α-phase volume fraction of 0.4 and primary α-phase average grain size of 7.4 μm. On the picture you can

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see white grains of α-phase and black intergranular combination of lamellar α-phase and β-phase.

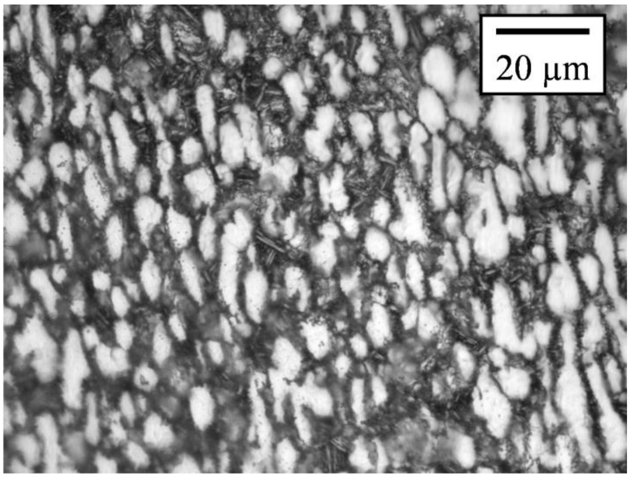

Fig. 1. *Initial microstructure of Ti-6Al-3.5Mo-1.5Zr-0.3Si alloy*

2.2. Microstructure characterization

Microstructure has been characterized using optical microscopy images. The average grain size has been evaluated by Heyn lineal intercept procedure according to ASTM E0112-96. The globular grains have been identified by a ratio between the longitudinal and transversal sizes of no larger than 3:1. The volume fraction of globular α-phase in the bimodal structure has been determined by computing the area occupied by globular grains using an overlain mesh with a cell size of 5 μm.

2.3. Heat treatment

Heat treatments were performed in laboratory oven according to the plan of experiments. Dimensions of specimens were Ø5x9 mm. Solution temperature was 960°C, holding time was 20 min. Quenching was carried out in fresh water with room temperature.

2.4. Hardness measurement

Hardness was measured by HV5 Vickers method by a Durascan 20 tester according to ASTM E92-17 in three points on each specimen.

2.5. Finite element method (FEM) analysis

Simulations have been done by FEM commercial code QForm (www.qform3d.com). FEM analysis has been used to obtain true strain-stress curves by temperature correction for compensation of deformation heating by iterative procedure (Alimov et al., 2018). The inverse analysis technique for determining the flow stress curve has been developed by Cho and Altan (2005) and in presented work we have used this technique for a set of temperature and strain rate conditions. The set of flow curves is given in tabular form. The following objective function was used:

$$\Phi = \frac{1}{K}\sum_{j=1}^{K}\frac{1}{N_j}\sum_{i=1}^{N}\left(\frac{F_{ij}-f_{ij}}{F_{ij}}\right)^2 \qquad (1)$$

where: K – number of flow curves; N – number of points approximating the flow stress curve; F_{ij} – an experimentally determined force at a point, kN, f_{ij} – calculated force at a point, kN.

To minimize the objective function an iterative algorithm and an optimizer have been used.

Also, the friction factor has been determined by means of inverse analysis (Alimov et al., 2018). Input data included the specific sample and dies geometry, kinematics of forming equipment, heating history used in the experiments, Ti-6Al-3.5Mo-1.5Zr-0.3Si flow stress data corrected to exclude influence of deformation heating, thermophysical properties of Ti-6Al-3.5Mo-1.5Zr-0.3Si alloy, the die material, and the value of the friction factor. All data except flow curves and friction conditions have been taken from QForm deformed materials database.

3. RESULTS AND DISCUSSION

3.1. Process characterization

Microstructure evolution of Ti-6Al-3.5Mo-1.5Zr-0.3Si Titanium alloy has been investigated during hot forging of part «Lever» (figure 2).

The technological process consists of following stages: heating to forging temperature 970°C, upsetting, preforming, flash trimming, reheating, final forming, second flash trimming and heat treatment (figure 3). Forging temperature was chosen as equal as β-transus minus 40°C. This temperature provides the greatest plasticity and the lowest flow stress along with ensuring a favourable microstructure

Microstructure characterization and further FEM analysis have been carried out in certain crosscut sections that are shown in figure 4.

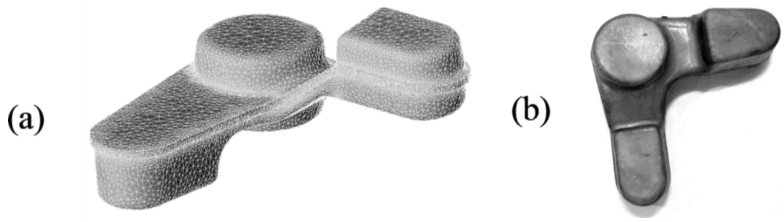

Fig. 2. *Finite element model (a) and the photo of forged part «Lever» (b).*

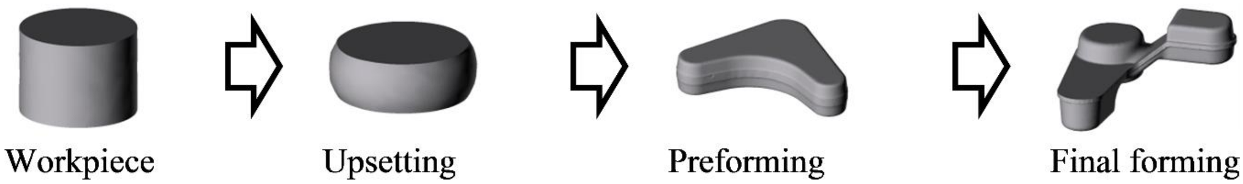

Fig. 3. *Processing route of forging of the part «Lever».*

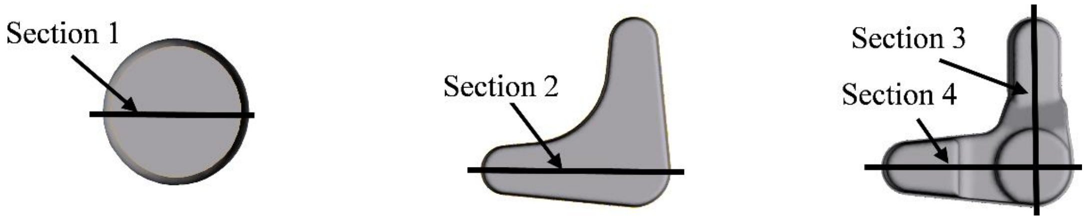

Fig. 4. *The scheme of crosscut sections in the part «Lever».*

3.2. Microstructure evolution model

The main process of microstructure evolution of dual-phase titanium alloys which takes place during deformation is dynamic recrystallization. Recrystallization is a process by which deformed grains are replaced by a new set of nondeformed grains that nucleate and grow until the original grains have been entirely consumed. Due to presence of β-phase grain growth is supressed and its effect could be neglected. The kinetics of recrystallization was simulated by the JMAK (Johnson-Mehl-Avrami-Kolmogorov) equation. In our model the fraction of the volume that has passed through dynamic recrystallization is calculated as follows:

$$X_d = 1 - \exp\left[-\beta_d\left(\frac{\varepsilon-\varepsilon_c}{A_d d_0^{M_d}\dot{\varepsilon}^{L_d}\exp\left(\frac{Q_d}{RT}\right)+C_d}\right)^{k_d}\right] \quad (2)$$

where: β_d, A_d, M_d, L_d, Q_d, C_d, k_d,– constants.

Constants were determined using mean square root method on the basis of experimental measurements of dynamic recrystallized volume fraction.

3.3. Experimental study of microstructure

Typical microstructure after upsetting can be characterized as bimodal with volume fraction of recrystallized α-phase of 0.16 (figure 5a). Macrograph and typical microstructure after preforming are shown in figures 5b, 5c. Microstructure is almost homogeneous with volume fraction of recrystallized α-phase of 0.26.

Macrograph and typical microstructures after final forming are shown in figures 6-7. As we can see there is almost homogeneous microstructure in bosses with volume fraction of recrystallized α-phase of 0.40 and localized flow bands in adapters with volume fraction of recrystallized α-phase of 0.68.

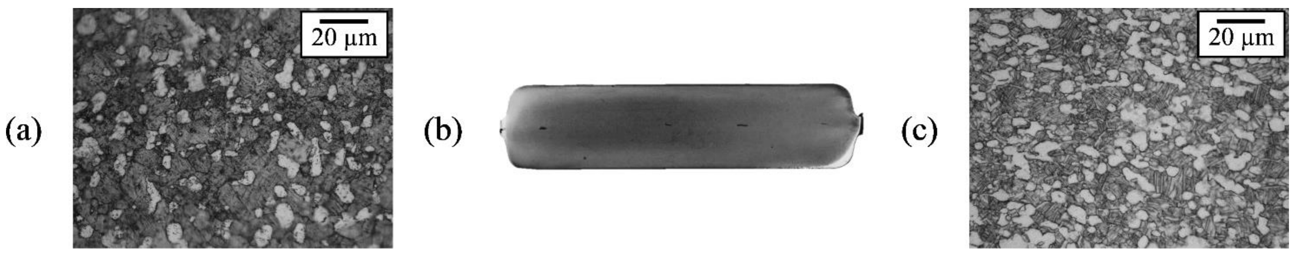

Fig. 5. *Typical microstructure (a) after upsetting (section 1), macrograph (b) and typical microstructure (c) after preforming (section 2).*

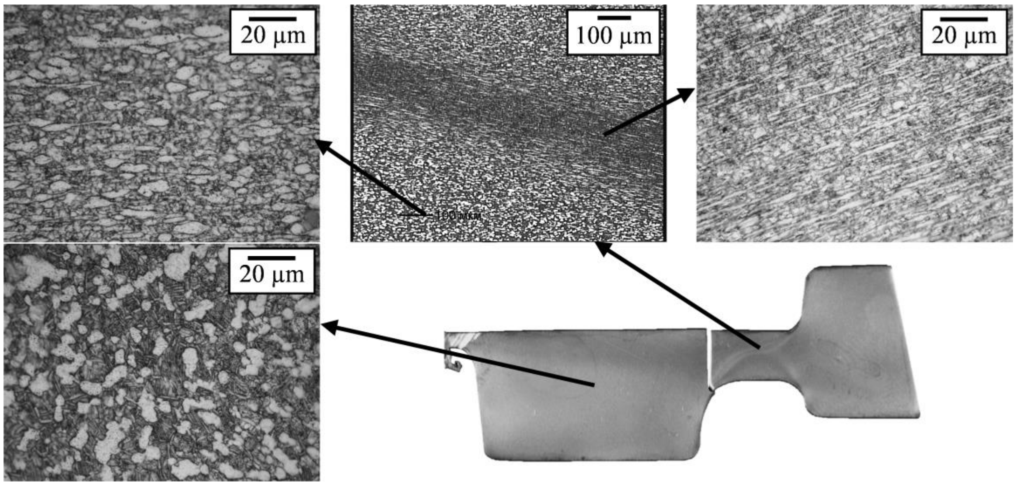

Fig. 6. Macrograph and typical microstructure after final forming (section 3).

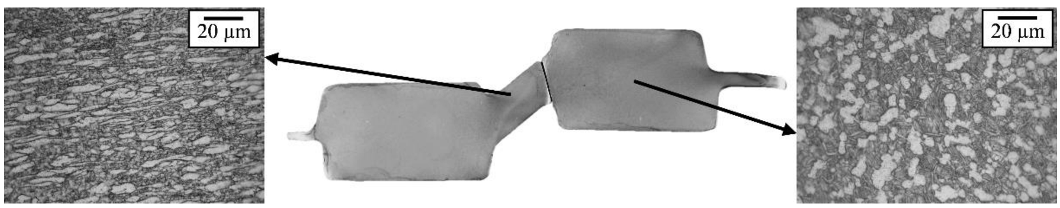

Fig. 7. Macrograph and typical microstructure after final forming (section 4).

3.4. Microstructure evolution simulation

Special microstructure evolution module of FEM commercial code QForm was used for simulation of microstructure evolution of Ti-6Al-3.5Mo-1.5Zr-0.3Si during forging of part «Lever». Measurement points were the same as used in experiments. Predicted distributions of recrystallized volume fraction of α-phase obtained by means of simulation of the technological process in FEM commercial code QForm are shown in figure 8. As we can see predicted recrystallized α-phase volume fraction well corresponds to experimental data (figure 9).

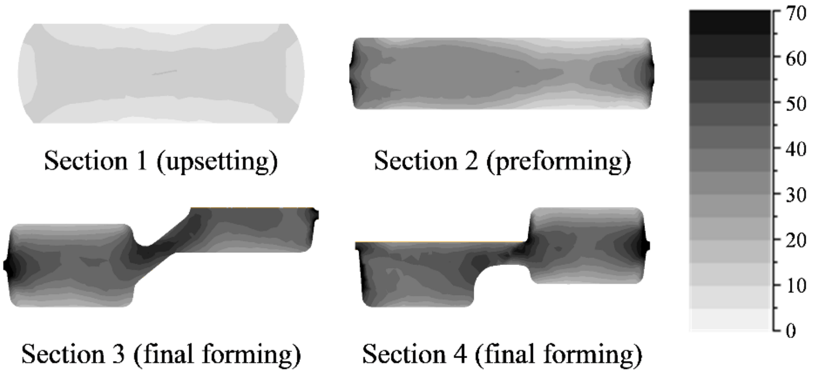

Fig. 8. Recrystallized volume fraction of α-phase (in percents).

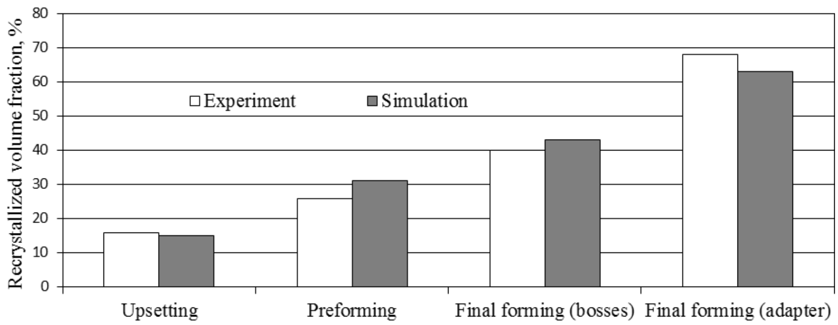

Fig. 9. Comparison of experimental and simulated recrystallized volume fraction.

3.5. Heat treatment model

After forging the part is subjected to heat treatment, which provides final mechanical properties (hardness, yield strength, ultimate tensile strength, toughness, etc.). Typical hardening heat treatment of titanium alloys includes solution heat treatment, quenching and aging. Solution treatment temperature of 960 °C (β-transus minus 40 °C), aging time of 2-8 h and temperature range of 535-675 °C are recommended for Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy (Copley & Langer, 1991). A change in the aging temperature alters the amount of β phase to decompose and affects mechanical properties. Selection of an aging temperature and time is based on the combination of mechanical properties desired after aging.

Data for polymorphic and martensitic transformation required for simulation were taken for titanium alloy Ti-6Al-4V, which is very close to Ti-6Al-3.5Mo-1.5Zr-0.3Si in Al and Mo equivalents.

Polymorphic transformation during heating to solution temperature was simulated using Leblonde-Devaux (Leblond, Devaux, 1984) model taking into account α-β phases equilibrium curve (figure 10).

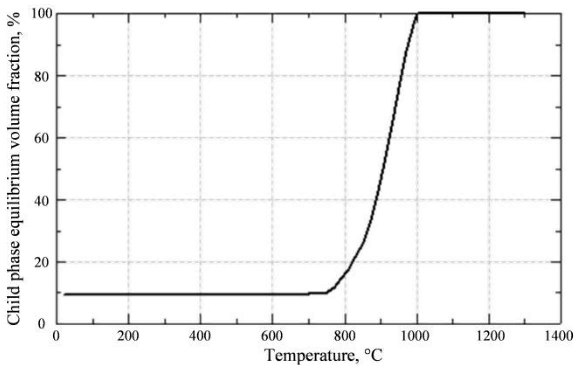

***Fig. 10**. α-β phases equilibrium curve (Ducato et al., 2014).*

There are two major transformations take place in Ti-6Al-3.5Mo-1.5Zr-0.3Si during quenching: diffusional polymorphic transformation β → α and diffusionless martensitic transformation. The main goal of quenching after solution treatment is to prevent loss of supersaturation of the solid solution and thus reduction of the maximum amount of dispersed hardening particles phase that can be formed during aging.

Polymorphic transformation during quenching was simulated by Johnson-Mehl-Arvami-Kolmogorov model, in which a volume fraction of a new phase (ξ) is calculated as:

$$\xi = 1 - \exp\left(-bt^{m}\right) \qquad (3)$$

where: b, m – parameters to be automatically calculated using two points on TTT diagram (figure 11) at every temperature.

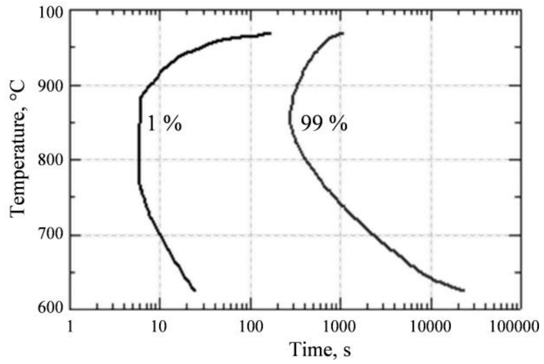

***Fig. 11**. TTT diagram for β → α transformation (Ducato et al., 2014).*

Martensitic transformation was simulated using Lee – Van Tyne equation (Lee, Van Tyne, 2012).

Next step of heat treatment is aging. The Avrami-type equation was used to describe the kinetics of dissolution of supersaturated solid solution. Approach used for simulation was similar to our previous work (Biba et al., 2018). During the aging of the alpha-prime phase, the complex «alpha-prime aged» phase is obtained. Alpha-prime aged phase is a fictive phase consists of α and β-phases formed during dissolution of α' martensite. Parameters of Johnson-Mehl-Avrami-Kolmogorov equation have been determined automatically from TTP curves that have been obtained from experiments (figure 14).

With increasing temperature or time of aging the strength or hardness increases, reaches a maximum, and finally diminishes. This phenomenon is known as overaging. By overaging the alpha-prime phase, a fictive «alpha-prime overaged» phase is obtained. This transformation was simulated by Leblonde-Devaux model with coefficients derived by inverse analysis.

As a result, transformations, which take place during heat treatment of Ti-6Al-3.5Mo-1.5Zr-0.3Si, can be summarized using scheme shown in figure 12.

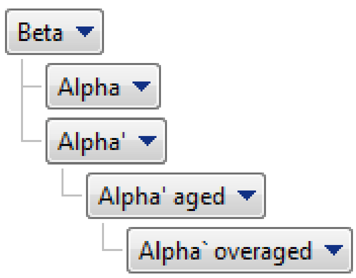

***Fig. 12**. The scheme of transformations during Ti-6Al-3.5Mo-1.5Zr-0.3Si heat treatment.*

3.6. Experimental study of aging

Effect of aging time and temperature on hardness of Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy has been studied experimentally. Vickers hardness after annealing heat treatment at 960°C was 312. Aging treatments at temperatures of 450, 500, 550, 600 and 650°C were applied to specimens for 1, 2, 4 and 6 hours. Changes in Vickers hardness during aging at different temperature are shown in figure 13.

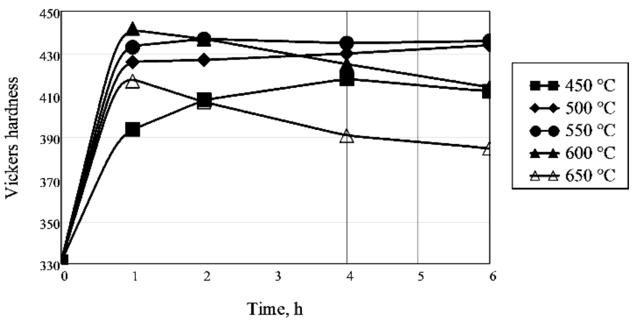

***Fig. 13**. Changing of hardness with aging time for different temperatures.*

The data can be rearranged to contour plot of Vickers hardness dependence on aging time temperature (figure 14). This plot is often called Time-Temperature-Property diagram. As we can see, the highest hardness can be obtained by aging during 4-6 hours at 500-550°C.

3.7. Simulation of heat treatment

Simulation of Ti-6Al-3.5Mo-1.5Zr-0.3Si heat treatment consists of solution treatment, quenching and aging. The goal of simulation is to investigate what increase of hardness can be achieved by utilizing the water quenching instead of air cooling.

Volume distribution of α-phase after water and air quenching are shown in figure 15. It can be seen, that volume fraction of α-phase after air quenching is higher than after water quenching. It means, that certain amount of β-phase has been transformed diffusionally to α–phase, thereby volume fraction of α'–phase has been decreased.

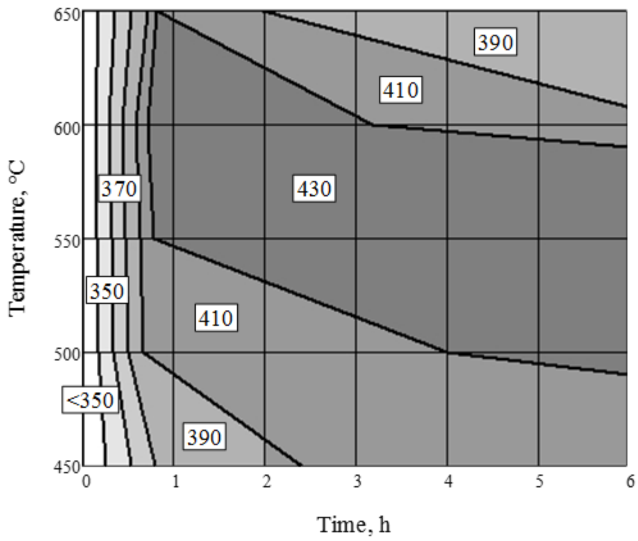

***Fig. 14**. Time-Temperature-Property diagram for aging of Ti-6Al-3.5Mo-1.5Zr-0.3Si.*

As we can see from figure 16 average volume fraction of α'–phase after water quenching was 78.71 %, while after air quenching only 50.5 %.

Average volume phase composition and hardness after different heat treatment simulations have been summarized in table 1.

During air cooling 13.56% of α'–phase transformed to α' aged, reflected in an increase of hardness from 331.65 to 344.02 compared to water quenching. But after aging during 4 hours at 550°C it led to a decrease of hardness from 412.61 to 402.19.

Simulation of water quenching and aging during 4 hours at 650°C was performed to show the effect of overaging. As you can see, there is a decrease of hardness due to overaging from 412.61 to 397.47.

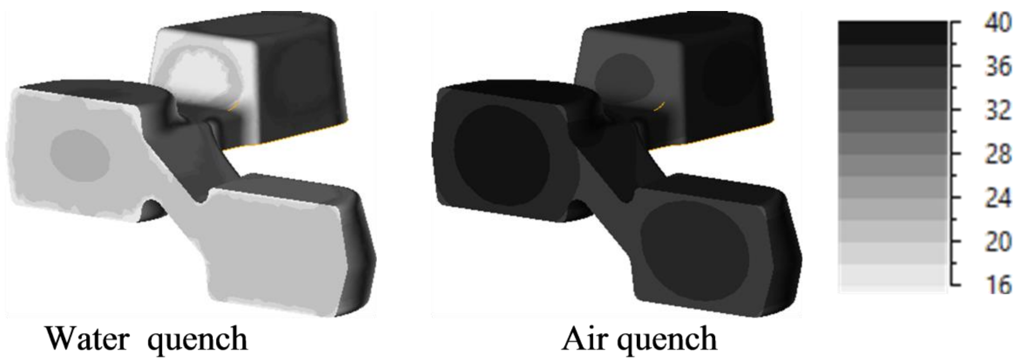

***Fig. 15**. α-phase volume fraction after quenching (in percents).*

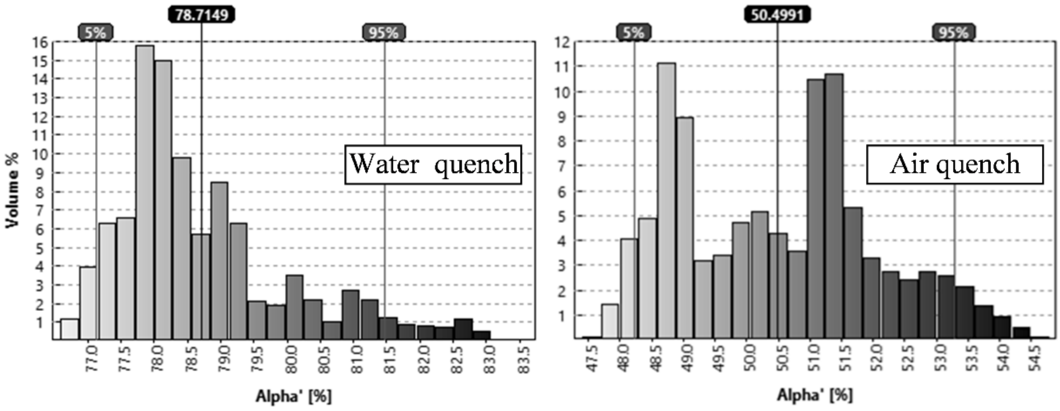

***Fig. 16**. α'-phase volume distribution histogram after quenching.*

***Table 1.** Average volume phase composition and hardness after different heat treatments.*

Phase	Water quench	Air quench	Water quench + aging 550°C 4h	Air quench + aging 550°C 4h	Water quench + aging 650°C 4h
α	20.49	35.91	11.89	27.12	10.15
β	0.00	0.00	9.63	9.62	9.61
α'	78.71	50.50	0.40	0.32	0.39
α` aged	0.80	13.56	78.08	61.89	46.27
α` overaged	0.00	0.03	1.12	1.02	33.58
HV	331.65	344.02	412.61	402.19	397.47

It can be seen, that hardening heat treatment is suitable to raise Vickers hardness from 312 in annealed state to 412.61 by water quenching and aging during 4-6 hours at 500-550°C. Replacement of quenching in water for cooling in air results in 402 HV after aging during 4-6 hours at 500-550°C.

4. CONCLUSIONS

1. The model of microstructure evolution of Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy has been developed and implemented in FEM code QForm.
2. Predicted distributions of recrystallized volume fraction of α-phase are in a good agreement with the experimental data.
3. Effect of aging time and temperature on mechanical properties of Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy has been experimentally studied.
4. The model of heat treatment of Ti-6Al-3.5Mo-1.5Zr-0.3Si titanium alloy has been developed and implemented in FEM code QForm. The model is capable to predict phase composition and hardness during and after arbitrary heat treatment within studied range.
5. The highest hardness of Ti-6Al-3.5Mo-1.5Zr-0.3Si can be obtained by aging during 4-6 hours at 500-550°C.

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SYMULACJA ROZWOJU MIKROSTRUKTURY PODCZAS KUCIA I OBRÓBKI CIEPLNEJ STOPU TYTANU Ti-6AL-3.5Mo-1.5Zr-0.3Si

Streszczenie

Na podstawie badań doświadczalnych opracowany został model dynamicznej rekrystalizacji stopu Ti-6Al-3.5Mo-1.5Zr-0.3Si. Model został zaimplementowany w programie MES QForm. Kinetykę rekrystalizacji symulowano wykorzystując równanie JMAK (Johnson-Mehl-Avrami-Kolmogorov). Zbadano wpływ czasu (1-6 h) oraz (temperatury (450-650^{o}C) starzenia na własności mechaniczne stopu. Opracowano model obróbki cieplnej stopu Ti-6Al-3.5Mo-1.5Zr-0.3Si, który również został zaimplementowany w programie QForm. Model przewiduje skład fazowy i twardość stopu po dowolnym zabiegu obróbki cieplnej w zakresie przeprowadzonych badań. W pracy wykazano, że największa twardość stopu może być uzyskana po starzeniu przez 4-6 h w temperaturze 550^{o}C, poprzedzonej wyżarzaniem w 960^{o}C.

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