A continuous dynamic recrystallization model to describe the hot deformation behaviour of a Ti5553 alloy

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Abstract. A physical based model is developed to describe recrystallization phenomena of titanium alloys during hot working of the β phase. Continuous dynamic recrystallization is attributed as the restoration mechanism based on the progressive transformation of low angle boundaries (subgrains) into high angle boundaries (grains). The model describes both, the microstructure, and the flow stress evolutions during hot deformation with large strains. The microstructure is conceived as being formed by three different populations of dislocations, and high as well as low angle grain boundaries. Evolution rates of all microstructural features are determined based on the effects of generation, interaction and annihilation of dislocations during deformation due to dynamic recovery, continuous dynamic recrystallization and static recovery. Continuous dynamic recrystallization is modelled and is considered to occur homogeneously within the microstructure. The model is able to predict the formation of subgrains from a fully annealed microstructure and the progressive formation of high angle grain boundaries. The subgrain and grain sizes are also obtained as output of the model. The model was applied to describe the hot compression behaviour of a Ti5553 alloy deformed between 880°C to 920°C and strain rates from 0.001 s⁻¹ up to 10 s⁻¹. The model is validated with flow curves and microstructural characterisation of hot deformed, and with microstructural information of non-deformed samples. The critical strain rate increases with increasing strain rate and decreasing temperature, similar to the discontinuous dynamic recrystallization phenomenon. The model can be implemented to simulate the microstructure and predict flow stresses of titanium alloys in industrial processes.

1. Introduction
The plastic deformation of high stacking fault energy (SFE) alloys at high temperatures involves dynamic recovery (DRV) [1] that can be followed by continuous dynamic recrystallization (CDRX) at larger strains [2]. The microstructures of hot deformed samples are not homogeneous with increasing the strain rate and the formation of boundaries in the interior of the grains are observed after some deformation. Moreover, after 50% deformation with low strain rate (0.01 s⁻¹) serrated grain boundaries are present in the microstructure and two complementary mechanisms have been proposed to explain this behaviour. The conventional lattice rotation leads to the development of geometrically necessary dislocations forming subgrains that migrate and evolve to high angle grain boundaries. Furthermore, a heterogeneous distribution of dislocations near the prior β grain boundaries results in the formation of substructures that are arranged in bands allocated in one side of β grain boundaries because of
heterogeneous deformation. Progressive deformation can eventually cause the merging of such substructures, forming new high angle grain boundaries, parallel to prior β grain boundaries. The hot deformation behaviour of a similar alloy, the Ti-5Al-5Mo-5V-3Cr-1Zr, was also systematically investigated [3]–[5]. Warchomicka et al. [5] observed that near the prior β grain, CDRX occurs by progressive rotation of the lattice in the β phase at high strain rates. At low strain rates and large strains, geometric dynamic recrystallization (GDRX) is observed. The elongated prior β grain boundaries are pinched off leading to the formation of new small grains with similar size compared to the subgrains. The occurrence of GDRX during hot deformation of Ti-5Al-5Mo-5V-3Cr-1Zr was also observed by Dikovits et al. [4] at low strain rates. Furthermore, at high strain rates CDRX plays a role above β transus temperature. However, it has been observed that dynamic recovery (DRV) of the β phase is the dominant mechanism during deformation over a wide range of temperatures and strain rates. Instabilities have been attributed to the formation of deformation bands (DBs). A continuous misorientation change towards the grain boundaries has been attributed to be the major origin of the formation of the deformation bands at moderate and higher strain rates.

Physical models based on the evolution of internal variables such as the dislocation density have been developed for Ti alloys. Alabort et al. [6] proposed a mesoscale physical model to predict the hot tension behaviour of an equiaxed Ti-6Al-4V alloy during superplastic behaviour. The developed model is based on internal state variables and could predict the grain size, dislocation density and void fraction. A mesoscale model for hot deformation behaviour of a Ti-6Al-4V alloy was also developed [7]. The stress has been proposed to follow Taylor’s assumption. The internal state variables to predict the flow stress and the microstructure evolution are the dislocation density and the vacancy concentration.

Although several attempts have been made to model both the flow stress, as well as microstructure evolution during deformation of Ti alloys, most of them consider discontinuous dynamic recrystallization as the deformation mechanism. In this work we developed a model to predict not only the flow stress but also the microstructure evolution during hot deformation of a cogged Ti5553 in β phase field based. The internal variables are three different populations of dislocations, high and low angle grain boundaries, and boundary misorientation angle distribution. The evolution rates of the microstructural features are determined based on dynamic recovery, continuous dynamic recrystallization and static recovery.

2. Experimental procedures
A cogged commercial Ti-5Al-5V-5Mo-3Cr with large prior β grains elongated in the cogging direction, and globular α phase was used in this investigation. The β transus temperature of this material lies around 850°C. Cylindrical samples of 10 mm diameter and 15 mm length were compressed using a Gleeble® 3800 device in the single β phase field at 880, 900 and 920°C at 5 strain rates between 0.001 and 10 s⁻¹, and up to a total strain of 0.9. The specimens were heated up at 5 K s⁻¹, held for 15 min before deformation, and subsequently in situ water quenched. The high cooling rate did not allow any static restoration of the β phase or diffusion-controlled phase transformation after deformation.

Specimens for metallographic characterization were ground with SiC abrasive papers from P320 to P2000, polished with 1 µm diamond suspension, followed by polishing with OPS suspension. Finally, vibro-polishing for 24 h using an acidic suspension of Alumina was performed. Scanning electron microscopy (SEM) was conducted using a Tescan Mira3 SEM equipped with a Hikari Electron Backscattered Electrons (EBSD) camera. EBSD measurements were performed for an area of 500 µm x 500 µm using a step size of 0.5 µm. The data treatment was performed using the OIM Analysis® software. A confidence index standardization was performed considering a grain with minimum size of 10 points and grain boundary misorientation tolerance angle of 12°. Finally, the neighbour confidence index correlation was utilized to re-index the data-points with confidence index lower than 0.75. A subgrain is defined as a region within grains where at least 2 points share a similar orientation with a boundary misorientation less than 15° but greater than 2°. In order to access the local microstructural features, kernel average misorientation (KAM) was calculated from the EBSD measurements [8], [9]. The density of geometrically necessary dislocations or GNDs was also calculated.
A maximum misorientation of 5° is considered and the misorientation is calculated according to the first nearest neighbours.

3. Modelling description

The representative microstructure entity is considered as a grain. Within a grain, LAGBs are produced as result of dynamic and static recovery. The dominant recrystallization mechanism is assumed to be continuous dynamic recrystallization (CDRX) and experimental evidence is also shown. In CDRX, the progressive increase in misorientation of the LAGB occurs due to subgrain rotation or accumulation of dislocations along a subgrain boundary. The progressive increase in misorientation of the LAGBs gradually forms new HAGBs. When the steady state is reached, a fully recrystallized microstructure is obtained.

The dislocation populations are separated into three different ones: mobile, immobile and walls. The mobile dislocation density is considered as the average density of dislocations that are moving along the slip systems causing plastic deformation. The wall dislocations are spaced and organized so that a boundary misorientation is observed in the microstructure. The immobile dislocation density is considered as the average density of dislocations that do not glide and are located at the grain interiors, such as forest of dislocations, pinned dislocations within the slip systems, and dipoles.

The total stress is calculated as a sum of three components (Equation (1)): an athermal or internal stress ($\sigma_{\text{ath}}$) related to the strain field caused by the dislocations, a thermal or effective stress ($\sigma_{\text{th}}$) attributed to the activation energy for the movement of dislocations in the lattice, and a Hall-Petch component ($\sigma_{\text{HP}}$) to account for the effect of the subgrain and grain sizes on the total stress.

$$\sigma = \sigma_{\text{ath}} + \sigma_{\text{th}} + \sigma_{\text{HP}}$$

The athermal stress is a function of the different dislocation populations, equation (2).

$$\sigma_{\text{ath}} = M\alpha G b \sqrt{\rho_i + \rho_m + f \rho_w}$$

where $M$ is the Taylor factor, $\alpha$ is the Taylor constant and considered 0.1, $G$ is the shear modulus, $b$ is the Burgers vector, $\rho_i$ is the immobile dislocation density, $\rho_m$ is the mobile dislocation density, $\rho_w$ is the wall dislocation density, and $f$ is a factor that varies from zero for well-organized LAGB (observed at low strain rates), to 1 for dislocations piled up at the boundaries due to localized deformation, progressive lattice rotation, etc. (usually the case at high strain rates).

The evolution of the microstructural components is modelled taking into account recovery and CDRX. The rate equations to account for the dislocation densities evolution as well as the equations used to compute the glide and climb velocities are based on the work of Ghoniem et al. [11]. The description of continuous dynamic recrystallization was proposed by Montheillet et al. [12]. Finally, the dynamic as well as static restoration phenomena are considered for the evolution of the dislocation densities, equation (3).

$$\frac{\partial \rho_x}{\partial t} = \left(\frac{\partial \rho_x}{\partial t}\right)_{\text{dynamic}} + \left(\frac{\partial \rho_x}{\partial t}\right)_{\text{static}}$$

where $m, i$ and $w$ corresponds to mobile, immobile and wall dislocations densities, respectively.

Figure 1: Inverse pole figure map of Ti5553 annealed at 920°C for 15 min.
4. Results and Discussion

The microstructures of the samples before the hot compression exhibits a fully static recrystallized microstructure as shown in figure 1 for the heat treatment performed at 920°C for 15 min.

Figure 2 shows the inverse pole figures and the kernel average misorientation (KAM) maps of the Ti5553 deformed at 920°C at 0.001 s⁻¹ (a and b, respectively) and 1 s⁻¹ (c and d, respectively). The β phase shows notable substructure formation. Subgrains were surrounded by low and high angle boundaries, in agreement with works on similar alloys and the CDRX mechanism. The amount of LAGB formed is larger at 1 s⁻¹, as highlighted by the local misorientation in the KAM map in figure 2(d). The substructure was homogeneously distributed for the deformation at 0.001 s⁻¹ (figure 2(a)), while some regions within the grains are observed with large misorientation accumulation along the grain and not visible subgrain formation at 1 s⁻¹ (figure 2(c)). Despite of this localization of the plastic deformation inside a grain, no indication of discontinuous dynamic recrystallization was observed for the investigated Ti5553. The degree of recrystallization is very low for 920°C. In figure 2(a) the substructure formation seems to be completed for the microstructure but only a low amount new high angle boundaries is observed.

![Figure 2: Inverse pole figure maps and kernel average misorientation (KAM) maps of the typical microstructure of the Ti5553 samples deformed at: (a), (b) 920°C and 0.001 s⁻¹; (c), (d) 920°C and 1 s⁻¹, respectively. Black lines indicate high angle grain boundaries (misorientation > 12°) and white lines indicate low angle grain boundaries (2° < misorientation < 12°); CD is the compression direction and TD is the transversal direction.](image)

Figure 3 shows the results of the simulated and experimental flow curves for the investigated deformation conditions. A good agreement between the measured and simulated flow curves is found. The model is able to predict the nearly constant flow stress. The formation of HAGB from LAGB must lead to flow softening at much larger strains. The localization of the deformation, as shown in figure 2 (c), is attributed to the deviation between simulated and measured flow stress for the deformation at high strain rates (10 s⁻¹).

![Figure 3: Measured (M.) and simulated (S.) flow curves: (a), (b) 880°C and 920°C, respectively.](image)
Figure 4 exhibits the simulated and the measured results for wall dislocation density and subgrain size for different deformation conditions. The measured wall dislocation density is considered as the GND density obtained from the EBSD measurements. A large deviation is observed between the measured and simulated data when comparing the results of the low strain rate. The large initial grain size and the non-homogeneous deformation would require notably larger areas to be measured with EBSD to obtain satisfactory statistic data although the trend shows almost always an overestimation of the model.

![Graph](image)

Figure 4: Comparison of: (a) measured (M.) and simulated (S.) wall dislocation density for different deformation temperatures and strain rates of 0.001 s$^{-1}$ and 1 s$^{-1}$; (b) average subgrain diameter for the strain rate of 1 s$^{-1}$ for different deformation temperatures.

To illustrate the capability of the proposed model to predict the microstructure evolution for larger strains, figure 5 shows the subgrain, grain sizes and fraction of HAGB evolution for strains up to 10 at 920°C. A decrease in subgrain size, which reaches a minimum, is predicted until the formation of new HAGB is pronounced. The steady state grain size corresponds to the grain size when CDRX is finished. The proposed model predicts larger steady state grain size for lower strain rates. The formation of the initial substructure from a fully recrystallized microstructure is shown by the decrease of HAGB until the minimum. After that, the onset of CDRX is pronounced leading to a recrystallized microstructure. The fraction of HAGB is considered as the fraction of recrystallization. The HAGB fraction (thus, the recrystallization fraction) is higher for lower strain rates for a given strain. Therefore, the onset of CDRX is delayed with increasing the strain rate for a given temperature.

![Graph](image)

Figure 5: Simulation results of the developed model. The evolution of subgrain and grain sizes as well as fraction of high angle grain boundary (HAGB) are shown for a strain up to 10 and deformation at 920°C.
5. Summary and conclusions
A physically based model was developed for predicting the microstructure evolution and the flow stress of a Ti5553 alloy. The model is able to predict the grain size, subgrain size, boundary misorientation and dislocation densities evolution during deformation. The production, annihilation and conversion of one type of dislocation population into another are modelled. Moreover, glide and climb velocity can be determined. CDRX and DRV are considered as the major restoration mechanisms for the microstructure evolution. In this case, a progressive increase in boundary misorientation and the progressive formation of new subgrain boundaries are the proposed mechanisms for CDRX.

The proposed models were able to predict the investigated microstructure. Subgrain formation from a fully recrystallized microstructure is predicted and the subgrain size decreases with increasing strain rate. The investigated hot deformed microstructures show the presence of subgrains and new high angle boundaries in the vicinity of low angle boundaries, evidencing the role of CDRX. Smaller subgrains are formed for higher strain rates, while the size of the subgrains increases with increasing temperature due to higher HAGB mobility and faster CDRX. A more homogeneous microstructure is observed for low strain rates, while a notable degree of heterogeneity in the microstructure is found for high strain rates. Regions with intense misorientation spread are found for hot compression at high strain rates, which can be considered as regions with a notable pile-up or entanglement of dislocations. This localization of deformation is not considered in the model and assumed to be the reason for the observed deviations.

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