Modelling of the thermomechanical behaviour of FCC metals under various conditions

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ABSTRACT. The main objective of this study is to propose a physics-based modelling adapted to describing the thermomechanical behaviour of metal alloys (specifically FCC metals). This approach takes into account the prominent phenomena generated by plastic deformation. Because of its specific mechanical and physical properties (ductility, lightness, etc.), this study is conducted on 1050 aluminium sheets widely used in sheet metal forming sector. The effect of two opposite and simultaneous physical phenomena on plastic deformation has been highlighted: the strain hardening rules that occurs because of dislocation movements and dislocation multiplication within the crystal structure of the metal and the dynamic recovery governed by thermal activation at intermediate temperatures (T≥0,4Tm). The evolution of two internal state variables (dislocation density and subgrain size) under different loading conditions was investigated. A Fortran program was used to identify the constitutive model parameters. To validate the present model, the curves obtained by numerical method were compared with those obtained by experimental traction data derived from literature.
In a wide range of strain rates and temperatures, the obtained results show that the proposed model is effective in predicting the thermomechanical behaviour in traction for FCC metals due to the good agreement between calculated and experimental data. The results show that the strain hardening decrease significantly with increase in temperature and/or decrease in strain rate which explains dominance of dynamic recovery at elevated temperatures.
Based on research conducted in the field, some proposals were introduced in the study to contribute to the improvement of numerical results and attempt to expand the use of the model for other types of loading (creep for example whose study is underway).

RÉSUMÉ. L'objectif principal de cette étude est de proposer une modélisation phénoménologique à base physique adaptée à la description du comportement *thermomécanique des alliages métalliques (en particulier les métaux CFC). Cette approche prend en compte les phénomènes dominants générés au cours de la déformation plastique. En raison de ses propriétés mécaniques et physiques spécifiques (ductilité, légèreté, etc.), le métal retenu pour cette étude est l'aluminium 1050 utilisé souvent dans le secteur de mise en forme des tôles métalliques. L'effet de deux phénomènes physiques antagonistes et simultanés sur la déformation plastique a été mis en évidence : l'écrouissage qui est dû aux mouvements et multiplication des dislocations au sein de la structure cristalline du métal et la restauration dynamique gouvernée par l'activation thermique à des températures intermédiaires (T≥0,4Tf). L'évolution de deux variables internes (densité de dislocations et la taille de sous-grain) sous différentes conditions de sollicitation a été étudiée. Un programme Fortran a été utilisé pour identifier les paramètres du modèle constitutif. Pour valider le modèle actuel, les courbes de traction obtenues par une méthode numérique ont été comparées à celles obtenues expérimentalement qui sont dérivées de la littérature.*

Sur une large gamme de température et de vitesse de déformation, les résultats obtenus montrent que le modèle proposé permet de prédire efficacement le comportement thermomécanique des métaux CFC en traction en raison d'un bon accord entre les courbes calculées et expérimentales. Les résultats montrent que l'écrouissage diminue significativement avec l'augmentation de la température et / ou la diminution de la vitesse de déformation, ce qui explique que à des températures élevées la restauration dynamique est prédominante.

Sur la base des travaux menés dans ce domaine, de maintes propositions ont été introduites dans l'étude pour améliorer les résultats et tenter d'élargir l'utilisation du modèle à d'autres types de chargement (fluage par exemple dont l'étude est en cours).

KEYWORDS: *dislocation density, dynamic recovery, strain hardening, subgrain size, thermomechanical behaviour.*

MOTS-CLÉS: *densité de dislocations, restauration dynamique, écrouissage, taille de sous-grain, comportement thermomécanique.*

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1. Introduction

The development of sheet metal forming processes requires use of numerical computation and simulation tools such as FEA. In this case, it is very important to define accurately the constitutive model for the mechanical behaviour of material under various conditions. Widely used so far, the phenomenological models have their limitations especially when confronted with cases of complex thermomechanical loading. Knowing that, the metal deforms elastically under the influence of small forces, the mechanical response is linear and can be characterized by two physical constants: Young's modulus and Poisson's ratio which can be derived by simple tensile experiments. Once the load exceeds a threshold, the material does not return to its original shape but there is a permanent and irreversible deformation. At the microscopic scale, the plastic deformation corresponds to the motion of large numbers of dislocations; it may also have the effect of multiplying the dislocations and promoting their entanglement from the Frank–Read source (Shimokawa and Kitada, 2014). These tangles in the microstructure tend to make more difficult the movement of dislocations leading to a hardening of metal. Definitely, the temperature plays an essential role in the microstructural evolution during thermomechanical processing, that promote the mobility of pinned dislocations or their annihilation (Lissel, 2006). In general, the mechanical properties and performance of materials change with increasing temperatures (Jiao, 2014). It is therefore very relevant to use physically based models (PBM) to accurately predict the complex loading effects. The lattice distortion induced by each dislocation produces a shear stress in addition to others at any point of the material; this is the origin of internal stress influenced by thermal changes (Tabourot *et al.*, 2015). Extensive research has been conducted to find reliable relationships between physical properties and mechanical behaviour of materials. PBM have been increasingly developed to accurately describe at the gross and microscopic levels the mechanical behaviour of metals. The counterpart is that a dedicated model is required for every situation (Sene *et al.*, 2016), knowing that the metallic alloys have a very heterogeneous and discontinuous nature that one erases at the level of phenomenological modelling to integrate the framework of continuum mechanics (Haupt, 2000). Dislocations, phases and grains are all discontinuities, thus they are also sources of heterogeneity with effects on material behaviour that are not really well reproduced by a model based on a continuity assessment (Kiritani *et al.*, 2010).

The purpose of this study is to establish a PBM to predict the plastic behaviour of FCC metals in the intermediate temperature range from 390 to 540 K. This physico-mechanical model is carried out by coupled diffusion and an isotropic hardening law.

Numerical tests are carried out on 1050 A specimens which is a popular grade of aluminium for general sheet metal forming where moderate strength is required (AZO, 2005). Two internal variables were introduced in the model to describe the material behaviour in hot tensile testing**.** A comparison between experimental and numerical results was also presented. In this study it was assumed that the metal does not undergo recrystallization, so the grain size remains constant and equal to the initial mean grain size.

Based on research conducted in the field, some proposals were introduced in the study to improve the numerical results obtained from the model.

The paper is organized as follows: section 2 introduces the equations governing the evolution of the flow stress with the internal parameters under various conditions. The obtained results are presented and discussed with reference to the aim of the study in Section 2. Finally, conclusions are drawn and suggestions for future work are presented.

2. Governing equations and constitutive model

At elevated temperatures, the plastic behavior of polycristals show a strong dependency of flow stress to temperature and strain rate according to thermally activated glide of mobile dislocations across short-range obstacles (Priester, 2012). Several studies show that the total flow stress during plastic deformation is decomposed into the internal stress (athermal component σ_μ) and the effective stress (thermal component σ^*) (Martínez *et al.*, 2011):

$$\sigma(\varepsilon,\varepsilon^{\cdot},T)=\sigma_{\mu}+\sigma^{*} \tag{1}$$

For temperatures higher than $0.4T_m$, the effective stress associated with thermally penetrable obstacles becomes negligible (Ouakdi *et al.*, 1998). The internal stress caused by other dislocations present within the grains and in the boundary depends on a number of microstructural variables such as dislocation density and subgrain size. It can be expressed according to Klepaczko relationship (Klepaczko, 1987).

$$\sigma\approx\sigma_{\mu}(X_i,\varepsilon^{\cdot},T)=\alpha_1 Gb\sqrt{\rho}+\alpha_2 G\sqrt{\frac{b}{d}}+\alpha_3 G\sqrt{\frac{b}{D}} \tag{2}$$

X_i denotes the different state parameters.

G =G(T) is the shear modulus.

The two internal state variables ρ and d vary significantly during plastic deformation and are closely dependent on strain rate and temperature.

$$\frac{d\rho}{d\varepsilon}=\frac{1}{b\lambda}-\frac{K_a(\varepsilon^{\cdot},T)}{(\rho-\rho_0)} \tag{3}$$

ρ_0 is the value of ρ before deformation ($\varepsilon = 0$).

K_a is an annihilation constant.

λ is defined as the average distance traveled by a dislocation before being stopped or annihilated. The evolution of λ during deformation is given by the following equation (Ouakdi, 1988):

$$\lambda=\lambda_s+(\lambda_0-\lambda_s)\exp(-K_a^{'}\varepsilon) \tag{4}$$

λ_0 et λ_s represent the extreme values of λ.

K'_a is a rate constant.

In this study, some propositions have been introduced in order to improve the quality of the model. The first proposition is to establish a rate ratio named C between K_a and K'_a as follows:

$$C=\frac{K_a^{'}}{K_a} \tag{5}$$

Approximately, λ represents the average distance of dislocation cells, thus its value is very close to that of the average subgrain size d (Ouakdi and Louahdi, 1996). The Figure 1 shows an example of cells or subgrains formed during plastic deformation.

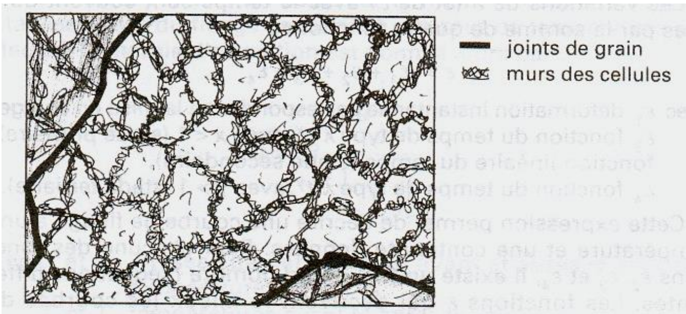


Figure 1. Subdivision of a grain during plastic deformation (Davenport et Higginson, 2000)

Therefore, λ can be substituted by the internal variable *d* in eqs. (3) and (4).

Experimental studies on aluminium alloys show that, for temperatures exceeding $0.4T_m$, the subgrain size decreases rapidly towards its saturation value. So to integrate the relationship (3), the variable *d* was assumed equal to its saturation value d_s. After integration we obtained the following expression:

$$\rho = \rho_s \lfloor 1 - K_i \exp(-K_a \varepsilon) \rfloor \quad (6)$$

ρ_s is the saturation value of the dislocation density;

K_i is the integration constant.

Based on the experimental results obtained by McQueen and Hockett (1970) from compression and extrusion tests on aluminium specimens, an empirical approach has been proposed by Ferron and Ouakdi (1988) to describe the maximum amount of the subgrain size as a function of temperature and strain rate:

$$d_s = d_{s0} + A\left(\frac{\dot{\varepsilon}}{D_L}\right)^{-\frac{1}{n}} \quad (7)$$

The same for the annihilation constant K_a which can be expressed as follows:

$$K_a = K_{a0} + B\left(\frac{\dot{\varepsilon}}{D_L}\right)^{-\frac{1}{n}} \quad (8)$$

A, *B* and *n* are constants; K_{a0} represents the value of K_a at low temperature and/or high strain rate.

D_L represents the self-diffusion coefficient for material, it depends only on temperature (Luthy *et al.*, 1980):

$$D_L(m^2s^{-1}) = 1.7\times10^{-4}\exp\left(\frac{-142}{RT}\right) + 6\times10^{-7}\exp\left(\frac{-115}{RT}\right) \tag{9}$$

From the last two equations, a constant ratio between d_s and K_a can be deducted:

$$r = \frac{K_a}{K_{a0}} = \frac{d_s}{d_{s0}} \tag{10}$$

According to an experimental study carried out on 1050A (Sevillano *et al.*, 1980), a constant ratio can be concluded between the boundary conditions d_0 and d_s:

$$d_0 \approx 3\ d_s \tag{11}$$

Taking into account this proportionality, the equation for subgrain size evolution based on eq. (4) is given by the following expression:

$$d = d_s\left[1 + 2\exp(-K_a^{'}\varepsilon)\right] \tag{12}$$

Taking into consideration the different proposals, the applied stress given by the relationship (2) can be rewritten in the following form:

$$\sigma(\varepsilon,\varepsilon^{\cdot} T) = \alpha_1 G b\sqrt{\rho_s\left(1 - K\exp(-K_a\varepsilon)\right)} + \alpha_2 G\sqrt{\frac{b}{d_s\left(1+2\exp(-K_a^{'}\varepsilon)\right)}} + \alpha_3 G\sqrt{\frac{b}{D}} \tag{13}$$

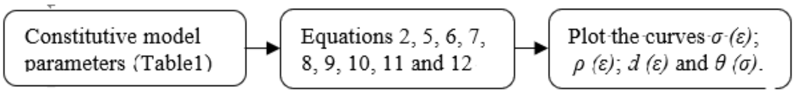
Table 1. The constitutive model parameters.

d_{s0} (m)	D (m)	ρ_0 (m^{-2})	B ($m^{-2/5}$)	b (m)	α_1	α_2	α_3
0.5×10^{-6}	60×10^{-6}	5×10^{12}	7500	$2.863\text{x}10^{-10}$	0.2	0.07	0.08
r	n	C	A($m^{3/5}$)	R(J mol^{-1} K^{-1})			
3	5	40	2500	8.32			

A Fortran program was used to identify the constitutive model parameters (Table 1). To enable accurate comparison with experimental results, two strain rates were chosen for different tensile tests ($\acute{\varepsilon}_1=1.6\times10^{-4}$ s^{-1} and $\acute{\varepsilon}_2=1.6\times10^{-2}$ s^{-1}).

3. Results and discussion

A comparison study was conducted between the numerical results obtained with the model and experimental data derived from the literature (Ouakdi, 1988). the numerical results were obtained according to the following order:



For example, Figures 2 and 3 describe the tensile behaviour of 1050 A specimens under different conditions of temperature and strain rate.

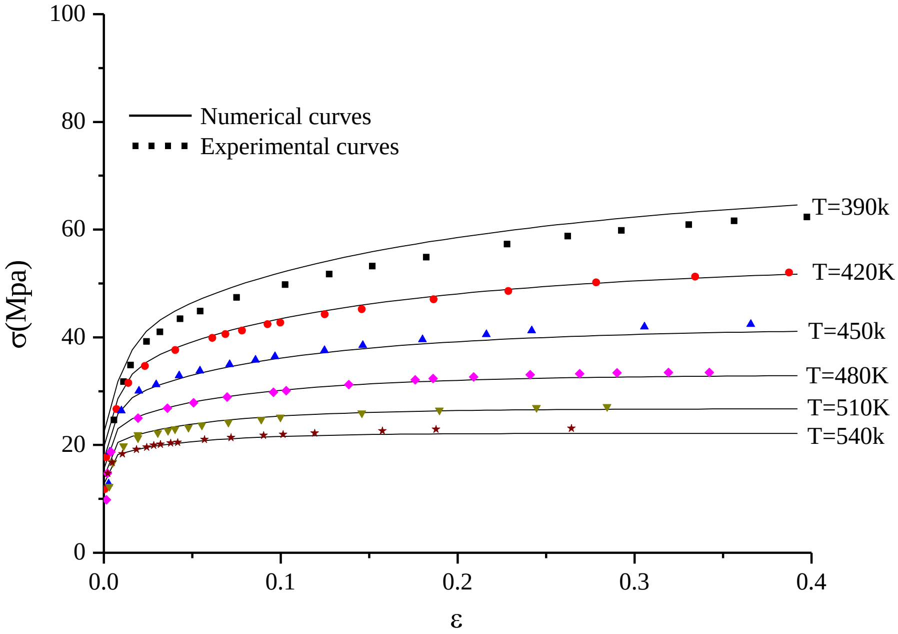


Figure 2. Experimental and numerical traction curves of 1050 A specimens for some temperatures and $\acute{\varepsilon}$1=1.6×10-4 s-1

Therefore, at elevated temperature some of the stored energy due to the accumulation of dislocations is relieved by virtue of the dynamic recovery effect, this leads to decrease in yield strength and an increase in the material ductility. An inverse effect was observed when increasing strain rate as shown in Figure 4.

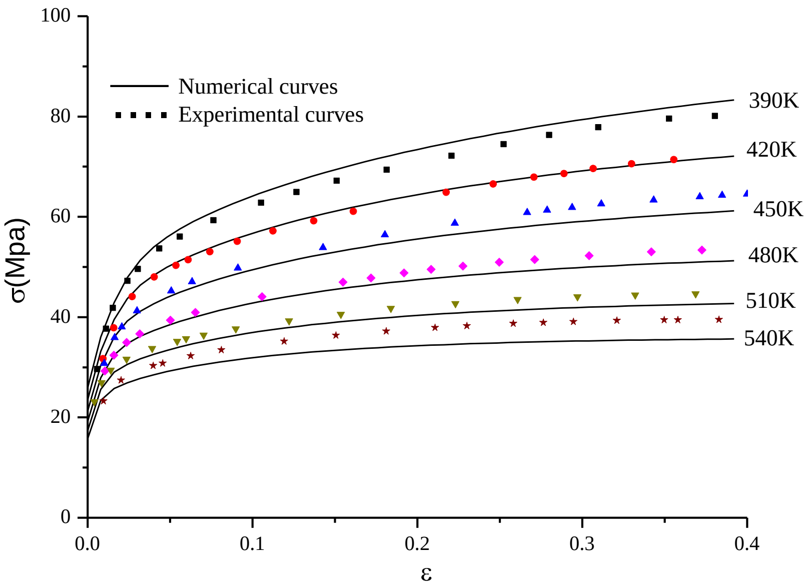


Figure 3. Experimental and numerical traction curves of 1050 A specimens for some temperatures and έ2=1.6×10-2s-1

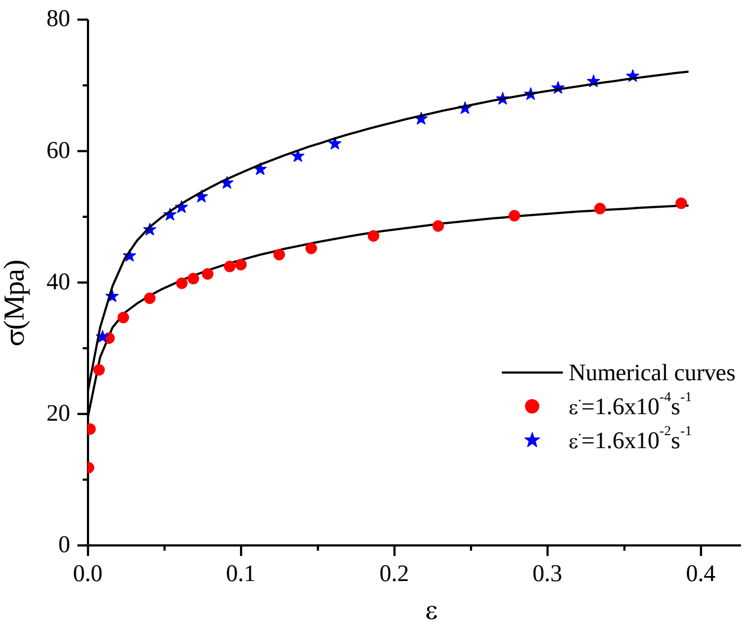


Figure 4. Effect of the strain rate on the stress- strain curve

The strain-hardening rate θ is given by an incremental differentiation of eq. (2):

$$\theta = \left.\frac{\partial \sigma}{\partial \varepsilon}\right|_{\dot{\varepsilon},T} \tag{14}$$

This leads to:

$$\theta = \frac{\sigma_{\rho s} K_i K_a \exp(-K_a \varepsilon)}{2\left[\,1 - K_i \exp(-K_a \varepsilon)\,\right]^{1/2}} + \frac{\sigma_{ds} C K_a \exp(-C K_a \varepsilon)}{\left[1 + 2\exp(-C K_a \varepsilon)\right]^{3/2}} \tag{15}$$

with $\sigma_{\rho s} = \alpha_1 G b \sqrt{\rho_s}$; $\sigma_{ds} = \alpha_2 G \sqrt{\frac{b}{d_s}}$.

As shown in Figure 5, the flow stress and the strain-hardening rate decrease significantly with increase in temperature which indicates dominance of dynamic recovery at elevated temperatures. The evolution of the strain-hardening rate versus flow stress can be expressed in a normalized form as follows:

$$\frac{\theta}{G} = f\left(\frac{\sigma}{G}\right) \tag{16}$$

As shown in Figure 6, the constant C was chosen equal to 40 because this value gives a good curve fit between numerical and experimental results.

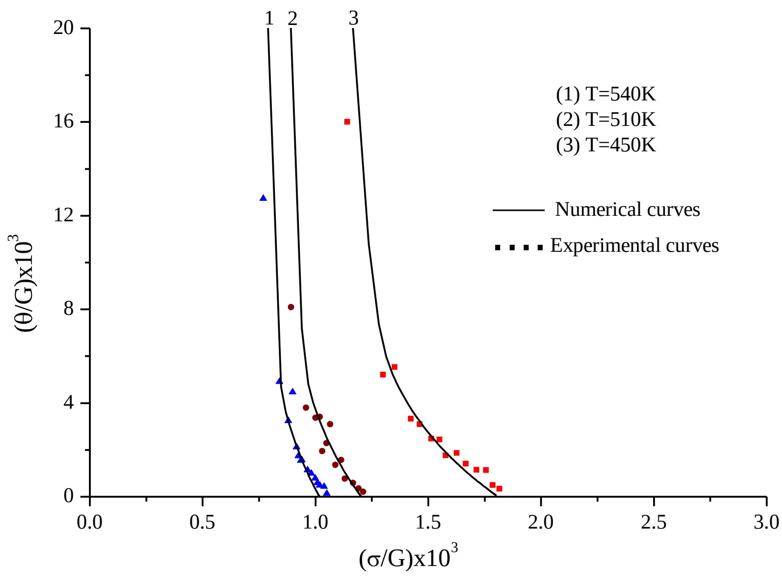


Figure 5. Evolution of the strain-hardening rate versus flow stress at different test temperatures ($\dot{\varepsilon}$=1.6×10^{-4}s^{-1})

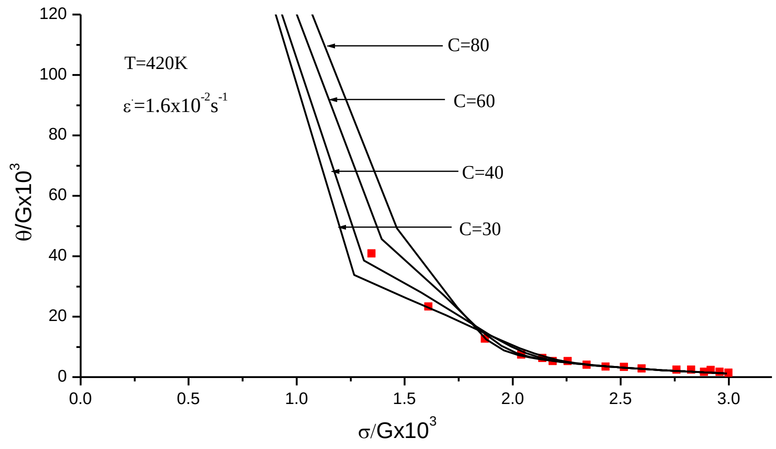


Figure 6. Influence of the constant C on the strain-hardening rate

Finally, the proposed model enables us to describe multiple representations in the course of plastic deformation at the microscopic scale, for example, Figures 7a and 7b depict the dislocation density and subgrain size evolution respectively.

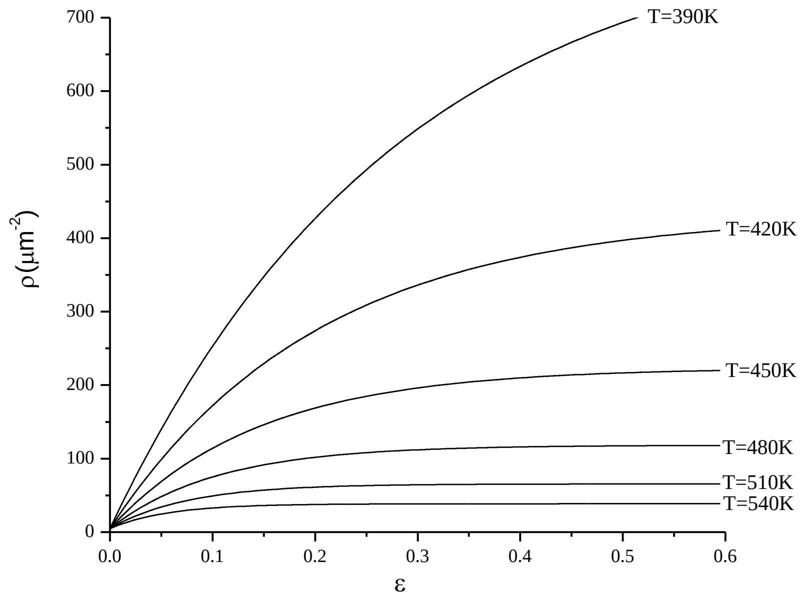


Figure 7a. Dislocation density evolution in the course of plastic deformation ($\acute{\varepsilon}$=1.6×10-4 s^{-1})

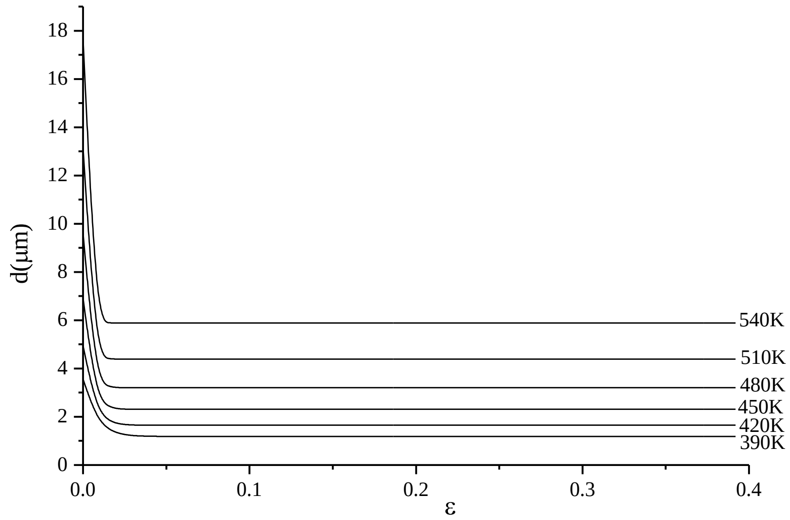


Figure 7b. Subgrain size evolution in the course of plastic deformation

($\acute{\varepsilon}$=1.6×10-4 s^{-1})

As well as subgrain size in the steady state is closely dependent on the term $\acute{\varepsilon}/D_L$ that represents the combined effect of strain rate and temperature (see Figure below).

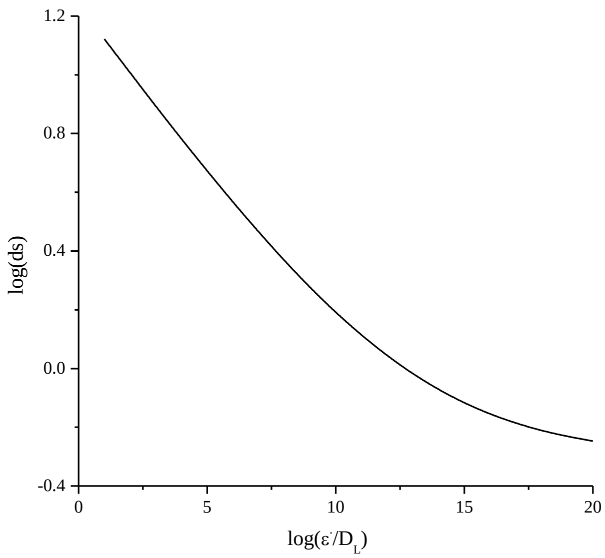


Figure 8. Dependence of the subgrain size on the term $\acute{\varepsilon}$/DL in the steady state (T=420K)

4. Conclusion and perspectives

Although the modelling based on physical principals is more complex than phenomenological modelling, it remains more consistent to obtain more reliable numerical results. The proposed model investigates the evolution of microstructure and flow stress at elevated temperatures during plastic deformation. Two internal variables directly related to the material microstructure that evolve with plastic strain are introduced in this model. The annihilation of dislocation by dynamic recovery is also taken into account in this study. In accordance with experimental results, a good agreement is observed between the experimental and calculated data. Small discrepancies between numerical and experimental results can also be observed because of physical considerations such as:

The effective stress is considered to be negligible compared to the internal stress;

Uncertainties in the values assigned to the model constants; etc.

Finally, it is very interesting to study the possibility of extending the application of the present model to other loading modes such as creep and relaxation tests.

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