Physical Modeling of dislocation creep in high temperature steels

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Summary

In modern thermal power plants, there is a permanent request in increasing efficiency to fulfil the demand of power and environmental safety. Service temperatures of 600°C and stress levels up to 100 MPa are currently the typical requirements on critical components. High creep and oxidation resistance are the main challenges for a lifetime 10+ years in steam atmosphere.
New materials may fulfill these requirements; however, the save prediction of the creep resistance is a difficult challenge. In the past, a wide range of different creep models have been developed for prediction. Most of them use a set of fit-parameters to describe and predict the creep behavior of one specific material at one specific condition. Once a set of parameters is found in good accuracy to the experimental data, the calculation of the deformation rate and hence the extrapolation of the final lifetime is possible. One must be aware that the found model parameters are only valid for the specific case they have been adapted for. Due to this restriction, an estimate of the creep behavior is only possible in a small range of material and system parameters.
A strategy to bypass these restrictions is the development of models which consider mechanistic phenomena within the material. As soon as a model considers actual physics and does not rely on fit parameters but measureable physical quantities, one has the chance to improve the model capabilities with respect to variations of the material and the system parameters. In addition, the model provides insight into the underlying mechanisms behind the creep process. This work aims at giving an overview of already existing models on dislocation creep, state of the art modelling and considerations about the future developments. Main focus is laid on the necessary ingredients and requirements for such a model.

Key Words

Creep modelling, creep strength estimation, dislocation glide, physical modelling, microstructure evolution, damage parameter, cavitation

Introduction

In the past few decades, a huge variety of creep resistant steels have been developed. In parallel, multiple modelling concepts on creep deformation and estimation of component lifetime have been suggested in literature. The predominance of phenomenological power laws in creep modelling suggests that applicability of mechanistic models may still have some potential for improvement [1].
Within this situation, the improvement and save prediction of the creep resistance remains the most difficult challenge. A wide range of potentially applicable creep models are available; most of them work with a set of fit-parameters. As soon as these parameters are set with good accuracy, a calculation of the deformation rate and the final lifetime of a component is possible.
In general, a model with parameters adapted to a specific case works only within tight restrictions, e.g. small range of temperatures, stresses, starting microstructures and a specific creep mechanism. As soon as system parameters (or creep mechanisms) differ significantly from these pre-settings, the reliability of a creep models can be limited, and high safety margins have to be applied to the predicted results. In addition, models with fit-parameters adapted for a specific situation cannot be used for the development of new materials or production techniques, but only for interpolation of already existing results.
It is necessary for these reasons to build creep models on a solid mechanistic background. As soon as a model takes into the consideration the actual phenomena leading to creep deformation, it can potentially not only predict deformation rates and lifetimes, but also indicate the underlying mechanisms. This paper aims at giving an overview on the necessary ingredients for such a model.

Overview of current creep model approaches

Basically, two families of creep models can be found in literature:

- Extrapolation and phenomenological methods
- Semi-physical creep models

In some cases, a creep model cannot be classified clearly, but shows characteristics of both groups.

Phenomenological models usually do not consider specific creep mechanisms, but are built on analytic functions describing the creep rate or ultimate lifetime of a material. These functions have been found convenient and supported by the results of macroscopic creep tests. However, they rely heavily on experimentally determined fit-parameters. The predictivity of these models is usually limited, since the fit-parameters may not be constant but depend on temperature, stress, material type and material history. Nevertheless, they turn out to be useful as long as these parameters stay close to the initial experimental conditions.

Extrapolation methods are the most widely used models for predicting the creep life of alloys. They can be applied very simply and straightforwardly as soon as the according fit-parameters are assessed. However, like for all phenomenological models, their application should be limited to cases similar to the condition for which the assessment has been carried out. Generally, the assessment is carried out for short-term creep experiments (up to some 10^3h), the extrapolation is then applied to long-term conditions (up to some 10^5h). This extrapolation always includes the risk of the change of microstructure or creep mechanisms. In both cases, the method will produce systematic errors. Most well-known extrapolation methods have been developed by Monkman and Grant [2] in 1956 and Larson and Miller [3] in 1952. Since the scatter in the result of creep experiments is usually high, a significant number of creep tests has to be carried out in order to assess the material constants properly, see e.g. Haney et. al in a study on steel T91 at temperatures from 500 to 625°C [4]. However, one has to be aware of the limitations and inherent assumptions of the model.

Monkman-Grant, Larson-Miller and its combination indicate the material's ultimate lifetime. Other phenomenological models indicate either the strain or the strain rate at a specific point of time. Some of these models specialize on a specific creep regime: Graham [5], Phillips [6], McVetty [7] and Conway [8] are valid for the primary creep regime, Norton [9] and Nadai [10] focus on the secondary regime and McHenry [11], Robotnov-Kachanov [12] and Sandström-Kondyr [13] are valid up to the tertiary regime. Holdsworth et al. collected the most widely used phenomenological creep models in a seminal paper in 2008 [14]. According to Holdsworth, the most suitable phenomenological creep models for application on P91 steel are the Modified Graham-Walles Model [14], the Bolton Characteristic Strain Model [15] and the MHG Model [16]–[18]. As it is evident especially for the case of the MHG model, where functions can be chosen freely in order to describe the creep strength, these models are rather suitable for fitting already quantified creep curves and not for extrapolating creep behavior to longer running times. As a consequence, they can be used as numerically inexpensive models for implementation in finite element simulations of components. All these models are mostly empirical and bear little microstructural or micromechanical information. As a consequence, their application is limited to cases where the experimental conditions are very similar to those where the assessment of the material parameters took place.

Semi-physical models can potentially include all these parameters (material, microstructure, stress, temperature etc.) into the model description by describing the microstructure, the microstructural evolution and the link between microstructure and macroscopic properties. Thus the predictivity reaches further compared to phenomenological models. As a consequence, semi-physical models are the only option for understanding the impact of starting microstructure on creep properties. This altering starting microstructure may stem from different chemical compositions, heat treatments or other processing steps such as welding or post weld heat treatment. If set up correctly and reasonably complete in terms of creep phenomena, a semi-empirical model can potentially consider these effects. However, there are two disadvantages of these models: first, the microstructure can only be included incompletely due to its vast complexity. Therefore, a semi-physical model can only be an approximation. Second, computing time is considerably higher compared to phenomenological models.

Approach in this work

The current approach in this work is the hybrid model from Yadav et al. [19]. The model combines a physical approach for primary and secondary creep with a continuum damage mechanics (CDM) approach in the tertiary creep regime, since no entirely mechanistic model has been available for the latter regime so far.

The mechanistic aspects of the model are based on the work of Ghoniem et al. [20] whereas the CDM approach adapts work from Basirat et al. [21].

Basirat introduced his CDM model in 2012 specifically for application in martensitic 9-12% Cr steels and applied it to grade 91 material. Contrary to Ghoniem, not only dislocations are considered, but also coarsening of $M_{23}C_6$-type precipitates, solid solution depletion due to the formation of Laves phase and the formation of creep voids. Each of these three processes is quantified in damage parameters. In addition to the damage evolution, Basirat considers

the evolution of (mobile) dislocations according to previous works of Blum [1]. Unfortunately, Basirat does not provide sufficient information on the details of his dislocation model.
Yadav therefore combines the detailed dislocation model of Ghoniem and the damage model of Basirat. Within the combination, following simplifications and extensions have been considered:

- Since the equilibrium fraction of Laves phase is usually reached within a few days and then remains constant throughout the entire creep process, Laves phase formation is not considered as damage. The remaining contributions are carbide coarsening and the formation of creep voids, which are included according to the strategy of Basirat.
- The emission of dislocations from the subgrain walls was found to have extremely low effect on the evolution of dislocation densities and was therefore neglected to improve computational time.
- Nucleation of new subgrains was found to have a negligible effect on the subgrain size evolution and was therefore not considered to improve computational time.
- Whereas the model of Ghoniem assumes all precipitates having equal radius, Yadav extended the model to potentially include precipitate size distributions. This option is not yet utilized, but keeps the door open for a coupling with results from precipitation kinetic software.

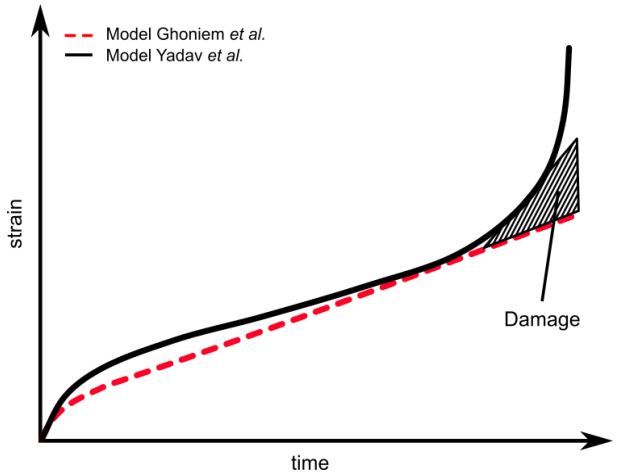

Figure 1: Schematic illustration of the difference between the model of Ghoniem et al. and the hybrid model of Yadav

Figure 1 demonstrates the effect of combining the two models of Ghoniem and Basirat. Whereas Ghoniem is able to include first and secondary creep stage, the addition of Basirat's damage model is necessary to describe the third creep stage as well.
The model itself contains rate equations for elongation, dislocation densities and subgrain size. The evolution of each microstructural constituent is coupled with the status of each other constituent. Please see Table 1 for an overview on the governing equations.

The rate equation of the strain (eq. 1) is basically Orowan's-equation extended with damage parameters stemming from precipitates and cavities. The evolution of the mobile dislocation density (eq. 2) combines the formation of mobile dislocation from Frank-Read sources and the reduction of its number due to formation of subgrain wall, climb recovery and dynamic recovery. Equation 3 describes the evolution of dislocation dipoles considering immobilization of mobile dislocations, static recovery and dynamic recovery. The evolution rate of boundary dislocation density (eq. 4) is governed by the transformation of dipole dislocations into boundary dislocation minus two annihilation terms due to the loss of dipoles while transforming into boundary dislocations, and the formation of new subgrain interfaces. The coarsening of subgrains to minimize the elastic energy of the system is described in equation 5. According to Ghoniem, the average glide velocity increases, once an external load at high temperature is applied (eq. 6). The approach of cavitation softening (eq. 7) has been adapted from sources [21] and [22]. For a more detailed description, see Yadav et. al. [19].

Table 1: List of equations of the dislocation creep model of Yadav

Creep Strain rate

$$\frac{d\varepsilon}{dt} = \frac{b \cdot \rho_m \cdot v_g}{M \cdot (1 - D_{ppt})(1 - D_{cav})} \quad (1)$$

Mobile dislocation density

$$\frac{d\rho_m}{dt} = v_g \cdot \rho_m^{3/2} - \frac{v_g}{2 \cdot R_{sbg}} \cdot \rho_m - 8 \cdot \rho_m^{3/2} \cdot v_c - d_{anh} \cdot (\rho_m + \rho_{dip}) \cdot \rho_m \cdot v_g \quad (2)$$

Dipole Dislocation density

$$\frac{d\rho_{dip}}{dt} = \frac{v_g}{2 \cdot R_{sbg}} \cdot \rho_m - 8 \cdot \frac{v_c}{h_b} \cdot \rho_{dip} - d_{anh} \cdot \rho_{dip} \cdot \rho_m \cdot v_g \quad (3)$$

Boundary dislocation density

$$\frac{d\rho_{dip}}{dt} = \frac{v_g}{2 \cdot R_{sbg}} \cdot \rho_m - 8 \cdot \frac{v_c}{h_b} \cdot \rho_{dip} - d_{anh} \cdot \rho_{dip} \cdot \rho_m \cdot v_g \quad (4)$$

Growth of subgrains

$$\frac{dR_{sbg}}{dt} = M_{sb} \cdot \left[P_{sb} - 2\pi \cdot \left(\sum_{i=1}^{m} r_{mean,i}^2 \cdot N_{v,i} \right) \cdot \gamma_{sb} \right] \quad (5)$$

Dislocation glide velocity

$$v_g = a_1 \cdot e^{-\frac{Q}{kt}} \cdot \frac{\Omega}{kT} \cdot \sigma_{eff} \quad (6)$$

Damage parameter for cavities

$$\dot{D}_{cav} = \mathrm{A} \cdot \varepsilon \cdot \dot{\varepsilon} \quad (7)$$

Figure 2 indicates a flow chart for the calculation of the microstructural evolution, the damage and the creep deformation. As starting condition, the microstructural condition has to be initialized (orange). In each iteration step, the mobile dislocation density ρ_m and the actual glide velocity v_g have to be updated according to the rate equations indicated above. With this updated data the creep rate $\dot{\varepsilon}$ is calculated. Finally, the damage with respect to cavities is updated, as long with ε, ρ and r_{sub} before starting the next iteration.

The main focus of the model lies on the mechanistic description of the microstructure evolution. Nevertheless, two input parameters have to be adapted to the result of creep experiments: a multiplicative constant concerning the velocity of mobile dislocations (a_1), and an according constant determining the damage evolution (A). Both constants have to be optimized with respect to the experimental creep curves and their quantities are specific for each experiment.

With these two parameters the creep simulation and hence the creep curve can be manipulated in a wide range. The idea is to train the model in combination with evaluated creep experiments and subsequent to predict a creep strength in a certain range of parameters. Final goal is to find the dependency of the two fit parameters with respect to temperature, stress and material condition, which is going to help interpreting their physical nature and finally replace them by an underlying physical concept.

One of the main advantages of the model is the insight into the microstructural evolution, which is produced in parallel to the calculation of the creep deformation. This feature actually enables a second reference to the validity of the model. Figure 3 demonstrates this capability on the example of P92 at 600°C. Exemplarily, the evolution of the dislocation density is plotted in addition to the evolution of the creep strain. This evolution can be the compared with experimental data generated by e.g. XRD or positron annihilation experiments. Other model outputs are the evolution of subgrain size or precipitate radii which can be tested against experimental data as well.

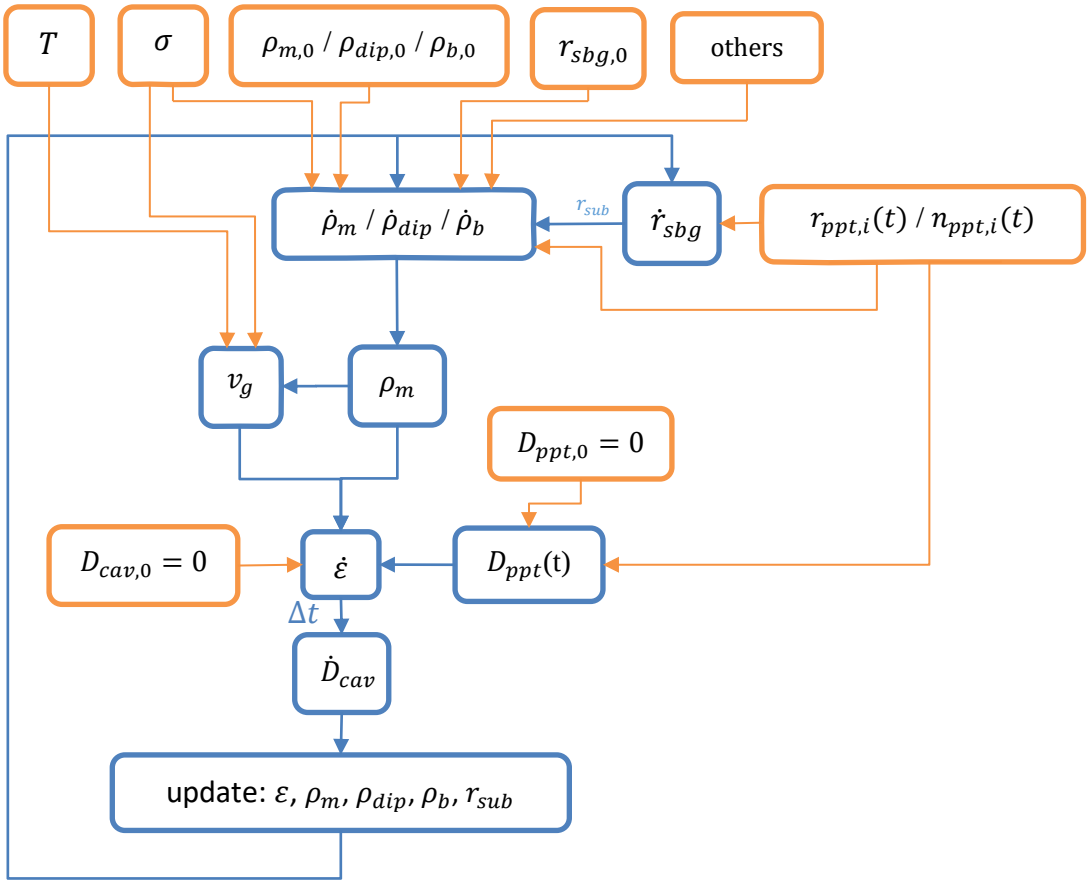

Figure 2: Schematic illustration of main process in the creep model

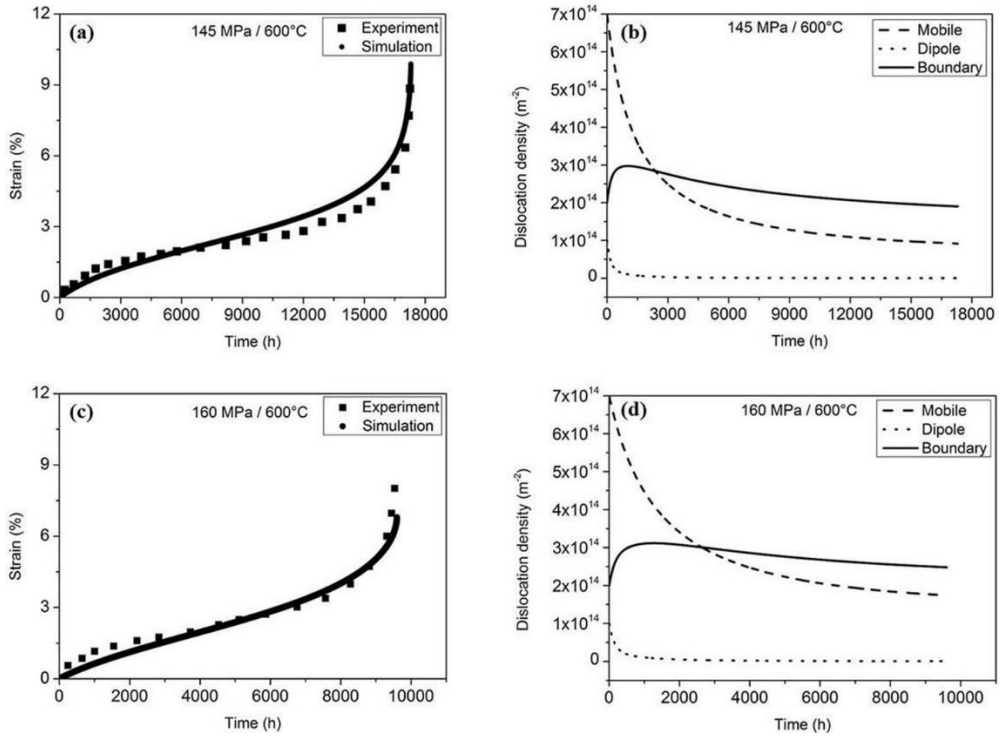

Figure 3: Modelled vs. experimental creep curves at 600°C (P92) and two different stress levels (a)(c); and the corresponding evolution of the three types of dislocation densities (b)(d) [19]

Discussion

In principle, the model is capable of reproducing creep curves with high accuracy. However, like every other model on this topic, the concept contains some flaws which have to be discussed. In literature, not one single concept is available which is able to predict creep deformation without fit parameters which have to be determined by comparing the model results with experimentally produced creep curves. In our case, two fit parameters have to be set, which is a low number compared to other models containing predictions on all three creep regimes.
The two fit parameters in our model A and a_1,depict material damage containing voids, necking and cracks, and a multiplicative constant on the velocity of mobile dislocations, respectively. At this stage, there is no clear and detailed physical interpretation on the nature of these two parameters as well as the impact of the material condition on their actual quantity.

In order to discuss the nature of the damage parameter D_{cav}, a comparison of the elongation rate $\dot{\varepsilon}$ (eq. 1) in this model with Norton's power law (eq. 8) is convenient [9] for identifying the stress dependence of the damage evolution.

$$\dot{\varepsilon} = B \cdot \sigma^n \tag{8}$$

The effective stress can be found by normalizing the applied force to the effective cross section of a sample. This leads to the expression:

$$\sigma_{eff} = \sigma_0 \cdot \frac{1}{1 - f_{cav}} \tag{9}$$

where f_{cav} is the phase fraction of cavities (or the reduction of the cross section due to necking) and σ_{eff} is the effective stress on the material. By comparison of parameters one finds following relation between the fraction of pores f_{cav} and the actual damage parameter D_{cav} (eq. 10).

$$1 - D_{cav} = (1 - f_{cav})^n \tag{10}$$

According to Norton, the creep exponent *n* is specific for different creep mechanisms. As a consequence, the definition of the damage parameter D_{cav} seems to include the nature of the specific creep mechanism and cannot be determined directly from a microstructure, even if all microstructural data are completely available. Consequently, the damage parameter does not represent a real quantity solely related to the material microstructure, but must be seen as theoretical model parameter as a matter of principle. In other words, the damage parameter cannot be measured directly without knowing the creep deformation rate, which the model claims to predict in the first place. The situation is thus similar to other phenomenological models where the description of the creep curve can only be achieved by fitting the model parameters to measured creep curves.
However, equation 10 indicates a solution to the problem: if the Norton creep exponent *n* can be derived from the evolution equations of the mechanistic part of the model, the cavitation fraction f_{cav} can be converted into the damage parameter D_{cav}. This should be one of the next steps for improving the predictability of the model and linking the model parameters to actually measurable observables.

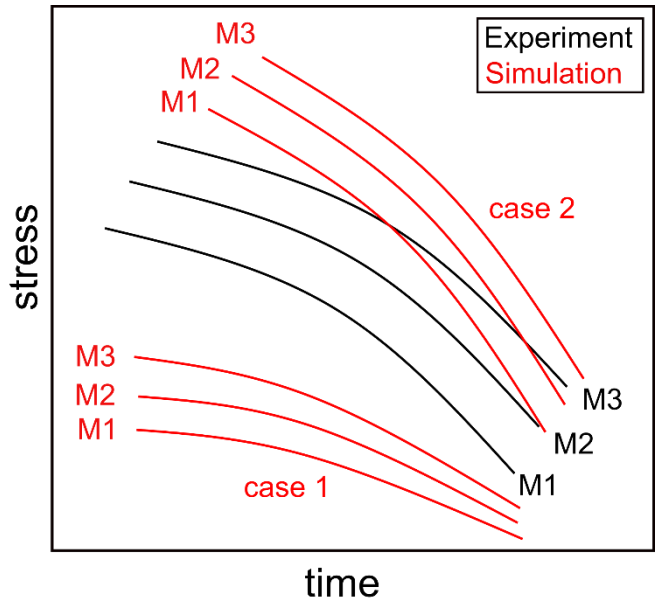

Figure 4: Possible variances of simulation compared to experiment

The interpretation of the multiplicative pre-factor of the glide velocity is simpler; it considers any unknown effect of stress, temperature and microstructure on the dislocation velocity. Accordingly, it may be replaced by an improved mechanistic model at a later stage. Currently, the model has to be trained with sufficient data in order to determine the pre-factor with the necessary accuracy. If this task is not carried out properly, model predictions lead to an over- or underestimation of the final lifetime. The effect is quite clear – an overestimation of the glide velocity leads to an underestimation of the lifetime and vice versa. In any case, the model is still able to compare the lifetime of different material status' relative to each other, as indicated in Figure 4. As a consequence, the model remains practical for predicting trends of component lifetime depending on varying starting microstructures, which is valuable input for material development and interpretation of material degradation.

Conclusion & Outlook

At the present stage, the hybrid model of Yadav seems to be applicable to predict primary, secondary and tertiary stages of creep mostly by mechanistic processes with a low number of fit parameters in the phenomenological part of the model. At least two parameters have to be further investigated: the parameter quantifying the cavitation damage, and the multiplicative pre-factor on the glide velocity of dislocations. Both parameters depend on stress, temperature and microstructure and currently have to be fitted to experimentally determined creep curves, which limits the predictability of the model. However, the model still contains the ability of directly compare the creep rates of different material conditions relative to each other, which is significant output.

It has to be mentioned at this point that a physical model can never be assumed complete, but only convenient until a better model is available. In this context, "better" refers to either (i) more accurate, (ii) same accuracy, but simpler or (iii) applicable to a wider range of cases without changing the model. "Simpler" refers to the number of a-priori unknown fit parameters. With this interpretation, the current model can be considered a valuable contribution to the topic.

Future developments have to address an improvement in the parts of the model, in which the aforementioned fit-parameters are involved. This should happen by replacing the parameters by mechanistic concepts including measurable observables. With this strategy, the number of fit-parameters is going to be reduced, and the model might be improved to a point where a prediction of the final lifetime is possible entirely by the parameters stress, temperature and starting microstructure. On this account the model offers the opportunity to cross-check the predictions not only with creep experiments, but including the microstructural evolution as second reference.

Abbreviations

Variable	Meaning	Unit
A	fitting parameter for cavitation damage	[-]
a_1	fitting parameter for glide velocity	[ms^{-1}]
b	burger vector	[m]
c_{dip}	weight factor	[-]
d_{anh}	annihilation length for dislocations	[m]
D_{cav}	cavitation - damage parameter	[-]
D_{ppt}	precipitation - damage parameter	[-]
h_b	dislocation spacing within subgrain walls	[m]
k	Boltzmann constant	[JK^{-1}]
M	Taylor factor	[-]
M_{sb}	mobility of subgrains	[$mPa^{-1}s^{-1}$]
N_v	number of density of precipitations	[m^{-3}]
P_{sb}	subgrain pressure	[Pa]
Q	activation energy for dislocation glide	[J]
r	mean radius of precipitations	[m]
R_{sbg}	subgrain radius	[m]
T	temperature	[°C]
t	time	[s]
α	dislocation interaction constant	[-]
γ_{sb}	surface energy	[Jm^{-2}]
ε	strain	[-]
$\dot{\varepsilon}$	strain rate	[s^{-1}]
ζ	fraction constant for dislocations	[-]
ρ_b	boundary dislocation density	[m^{-2}]
ρ_{dip}	dipole dislocation density	[m^{-2}]
ρ_m	mobile dislocation density	[m^{-2}]
v_c	climb velocity	[ms^{-1}]
v_g	glide velocity	[ms^{-1}]
Ω	atomic volume	[m^{-3}]
σ_{eff}	effective stress	[Pa]
σ_0	nominal stress	[Pa]
f_{cav}	phase fraction of cavities	[-]
B	material constant	[-]
n	power law exponent	[-]

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