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Constitutive modeling of dynamic strain aging in niobium

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Abstract. As the temperature rises, metals should lose strength. However, under some combinations of strain rate and temperature, they show a dramatic increase in strength due to the interaction of impurity/solute atoms with the dislocations, a phenomenon known as dynamic strain aging (DSA). Thermomechanical stress-strain curves have been modeled using a variety of numerical approaches, but accurately modeling DSA activation remains a challenge. The activation free energy for dislocation movement rises during DSA, as there are more solute atoms concentrated at the local barriers. As a result, we see an increase in strength. This work modifies the physical parameters-based VA model for commercially pure bcc Niobium, which is known to display DSA at low strain rates and elevated temperatures, in order to create a constitutive model that can accurately capture DSA.

Introduction

Constitutive model development aims for wide applicability and complicated material response. Successful models capture material static and dynamic behavior and obtain model constants from limited experimental data. Furthermore, metals with different crystal structures have been extensively researched for thermomechanical response over a wide strain rate and temperature range. JC [1], ZA [2], Nemat Nasser [3], and VA model [4] are some of the models devised by researchers to capture the thermomechanical response of materials. These models very well evidence the regular thermomechanical response. But when it comes to simulating dynamic strain aging (DSA), which is a sudden increase in the strength of a material at certain configurations of temperature and strain rates, these models have not yielded satisfactory results.

Applied stress causes shear in the material along with a movement of dislocations that is discrete in nature as the dislocations stop for a certain amount of waiting time (t_w) at every obstacle. During this time, a dislocation core atmosphere is formed, in which solute atoms diffuse into the mobile dislocations and create pinning effect. Breaking past this pinned dislocation barrier requires higher stress, thus increasing material strength known as DSA [5]. This is usually seen as a unique response, and it has been observed in many studies [6, 7]

The model must depend on microscopic constituents because solute atoms interact with dislocations to induce DSA. As discussed before, thermomechanical response is well-described by many models but they cannot capture DSA [1-4, 8-10], and have been modified in numerous works to model DSA. One such example is the recent work reported by Devotta et al. [11]. They modified the JC model for a ferritic-pearlitic C45E steel using a second-degree polynomial fit to account for the DSA. However, this approach was not adopted due to the empirical nature of the JC model.

Cheng and Nemat [12] presented a dislocation trough model for titanium and a constitutive model for predicting DSA by developing a relationship between the overall activation free energy, and the solute atom concentration. However, their model is only applicable at higher strain rates

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and is inapplicable at lower strain rates, whereas DSA is generally reported at lower strain rates [13, 14]. In contrast, the VA model is applicable over a wide range of temperatures and strain rates [4, 15-17]. It is a constitutive model based on physical parameters. However, it has been reported that the model could not be tested for DSA [4, 16, 17] as it does not consider the dependence of activation free energy (G_o) on the concentration of solute atoms at local obstacles. The solute concentration has a direct effect on the activation energy at local barriers and is responsible for the activation of dynamic strain aging in metals under thermomechanical loading conditions, and therefore, the VA model is modified in the current work to simulate DSA in commercially pure Niobium at low strain rates, as detailed later in this work.

In the Numerical Model Section, the VA model and its dependency on physical parameters are discussed. Later, the modification in the model is detailed. The application of the modified VA model to capture DSA in Nb is described in the Application, Comparisons and Discussion Section. In the same section, a brief description of how to obtain the various parameters for the modified VA model is provided, followed by the results and discussions. Finally, the study is concluded in the last section.

Constitutive Model

Voyiadjis-Abed (VA) Model. During plastic deformations, the movement of dislocations is constrained by either long- or short-range obstacles, resulting in an increase in the material's strength. Depending on the nature of obstacles, these can be overcome with or without thermal assistance. For bcc metals, if the barrier is long-ranged, thermal assistance is not necessary, but if it is short-ranged, it cannot be overcome without thermal influence. Plasticity in a metal is the flow of dislocations through both these long-range and short-range obstacles. VA model for bcc metals is developed considering these phenomena of flow stress by decomposing it into two components i.e. the athermal stress (σ_{ath}) component (based on long range obstacles) and the thermal stress (σ_{th}) component (based on short range obstacles) [4, 16] as shown in Eq. (1):

$$\sigma = \underbrace{Y_a + B\varepsilon_p^n}_{athermal\ stress} + \underbrace{\hat{Y}\left(1 - \left(\beta_1 \mathrm{T} - \beta_2 \mathrm{T} \ln\dot{\varepsilon_p}\right)^{\frac{1}{q}}\right)^{\frac{1}{p}}}_{thermal\ stress} \quad (1)$$

In athermal stress component (σ_{ath}), (Y_a) is the temperature-insensitive yield strength of the material, and B and n are temperature-insensitive thermal hardening constants. On the other hand, $\hat{Y}$ in the thermal stress component (σ_{th}) represents the minimum stress necessary to breach the Peierls barrier at 0 K. T is the operating temperature, whereas β_i is essentially the thermal activation parameter that depends on Boltzmann's constant (k), reference strain rate ($\dot{\varepsilon}_{po}^{i}$), and activation free energy (G_o). $\dot{\varepsilon_p}$ represents the desired strain rate. (1)The physical dependence of all the material parameters given in Eq. (1) on different micro and nano structural quantities (including grain size, dislocation densities and burgers vector) is detailed in the works by Abed et al. [4, 16, 18].

Dynamic Strain Aging. As discussed so far, the VA model falls short in detecting DSA activation because it does not account for the effect of dislocation's pinning due to variations in solute atom concentration on the activation free energy.

As noted previously, dynamic strain aging is caused by the interaction between impurity/solute atoms and dislocations. The diffusion of solute atoms impedes the mobility of these dislocations, resulting in an increase in the needed waiting time. To overcome these obstacles, a higher activation energy is required, resulting in an increase in the strength of the metal. In a metallic structure, the impurity elements such as C, N, and O are scattered in minute amounts throughout

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the available interstitial spaces of the structure. Due to a scarcity of available space, these atoms are under pressure, and they will always seek a larger site to minimize their energy whenever possible.

When stressed, metals shear. The deformation creates new sites that impurity atoms quickly occupy and pins down the moving dislocations. Consequently, the dislocation waiting time and the activation energy increase. Thus, under specific combinations of strain rate and temperature, a higher strength is observed.

In light of the preceding, the VA model has been modified to accommodate the DSA. It has been found that the thermal activation energy remains unaltered in the absence of DSA [4], whereas DSA enhances the thermal activation energy [12]. Cheng and Nasser [12] linked the binding free energy (G_B) per unit length to the activation free energy (G_o) as follows:

$$G_o \propto \sqrt{G_B G_D} w \tag{2}$$

The model states that the activation free energy is directly affected by the trough's effective width (w) and dislocation free energy per unit length (G_D)., the trough's effective width (w) and the free energy per unit length of dislocation (G_D) directly effects the activation free energy. However, we are interested in how binding free energy (G_B) depends on the concentration of solute atom (C). Cheng and Nasser represented this dependence as a product of the strength of interaction for each solute atoms (G_{BO}) with C as shown in Eq. (3).

$$G_B \propto G_{BO} C \tag{3}$$

Keeping all other parameters constant in Eqs. (2) and (3), it is evident that increasing solute concentration increases the activation free energy. The higher activation free energy, the greater the stress needed to displace dislocations. So, due to impurity/solute concentration, DSA is observed. A modification in Eq. (1) is utilized in the current work to capture DSA using this concept. The VA model modification captured DSA that was not captured when the total activation energy was constant. Next section explains this.

Applications, Comparisons and Discussions

The constitutive model from the previous section is compared to Nemat-Nasser and co-workers' experimental data for commercially pure Niobium [14]. The evaluation of model parameters is discussed first in this section. Later in this section, application of the model for estimating the flow stress and comparisons to experimental results is presented for Niobium.

Model parameters evaluation. Thermomechanical experimental data from Nemat Nasser and coworkers [14] determines all the parameters in Eq. (1). Generally, an increase in temperature decreases material strength until a critical temperature is reached, beyond which the strength becomes insensitive to temperature and the athermal stress component is defined at this temperature. Afterwards, the thermal hardening component is determined at a lower temperature where DSA is not observed. The details to find these parameters is given in the works by Voyiadjis and coworkers [4, 13, 15, 16, 18]. The dependency of the change in activation energy with the temperature and strain rates is beyond the scope of current work due to limited data available. The values for different parameters of VA model is given in Table 1.

Application and Comparisons. The VA model modification was verified by the thermomechanical modelling of Niobium (Nb), a silvery bcc metal, which is utilized to strengthen alloys in carbon and alloy steels. Nemat Nasser [14] and Voyiadjis et al. [4] successfully modeled Nb at higher strain rates in the absence of DSA but their model was incompatible at lower strain rates where DSA was observed.

Table 1 tabulates the parameter values for Niobium. As mentioned, to capture DSA, the total activation energy changed with temperature at the strain rate (0.001/s) as shown in Table 2. The activation free energy increased in the DSA range, rising till the peak position, and decreasing afterwards due to high temperature's assistance in dispersing solute atoms from dislocation core. Figure 1 shows the impact of this activation energy change. VA model could not reflect DSA, but the modification made it successful in doing so.

Table 1 Model parameters for Niobium.

Parameter	**Y_a [MPa]**	**B [MPa]**	**n**	**$\hat{Y}$ [MPa]**	**p**	**q**	**$\dot{\varepsilon}_{po}^{i}$ [s^{-1}]**	**β_2 [K^{-1}]**
Value	25	300	0.23	1450	0.36	1.84	7.07×10^{6}	5.49×10^{-5}

Table 2 Thermal Activation Energy (G_o) for the VA model to capture DSA at $\dot{\varepsilon}_p$ = 0.001/s

Temperature [K]	**293, 400 and 800**	**500**	**600**	**700**
G_o Value [eV]	1.57	2.2	3.4	2.8

Figure 2 (a-f) displays the results of a comparison between the experimental data and the numerical models with and without the influence of DSA. It is evident that the VA model does not account for the activation of DSA between 500 and 700 K. But when the proposed modification was accounted for, the model successfully predicted DSA activation (Figure 2 (c-e)). The proposed modification captured DSA activation quite well for Nb, as evidenced by the comparison given.

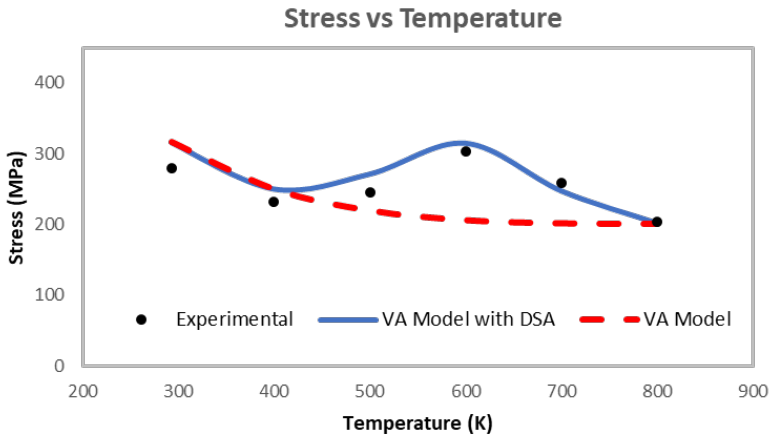

Figure 1. Stress-temperature experimental results compared to VA and modified VA model.

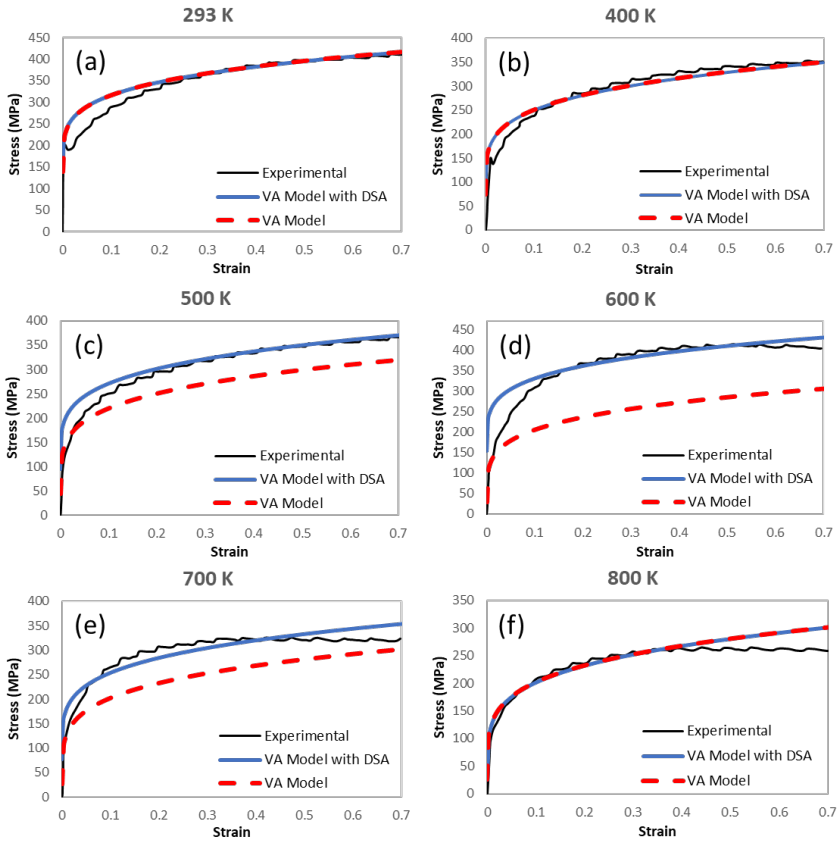

Figure 2. VA model, modified VA model, and experimental stress-strain curves at $\dot{\varepsilon}_p$ = 0.001/s and T = (a) 293 K, (b) 400 K, (c) 500 K, (d) 600 K, (e) 700 K, and (f) 800 K.

Figure 2 shows that VA model results fitted experimental data when DSA was not activated. On the other hand, the modified VA model with DSA inclusion captures DSA inactivation and activation for commercially pure Niobium at low strain rates very efficiently.

Conclusions

This article proposes a VA model modification to capture DSA in commercially pure Niobium using experimental data from Dr. Nemat Nasser. The highlights include:

- An accumulation of solute atoms at local barriers slows down dislocation motion. To get around this, more activation energy is needed, leading to DSA.
- Dislocations pin at thermal stress controlling short-range obstacles in bcc metals and activate DSA.
- Niobium showed DSA at 500–700 K and $\dot{\varepsilon}_p$ = 0.001/s.
- During DSA, activation energy rises as temperature rises, reaching a maximum at the temperature at which the effect is most pronounced. Then, it begins to decline as the higher temperatures facilitate the dispersion of solute atoms from the obstacles.

The modified VA model accurately predicted the stress increase necessary to break through the pinned dislocation-solute atmosphere barrier during DSA. With the model's eventual incorporation into commercial finite element software, it will be possible to forecast a wide variety of scenarios using DSA, greatly increasing the field's potential applications.

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