Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 64 (2014) 133–143

Acta MATERIALIA

www.elsevier.com/locate/actamat

A strain-based computational design of creep-resistant steels

Q. Lu, W. Xu *, S. van der Zwaag

Novel Aerospace Materials Group, Faculty of Aerospace Engineering, Delft University of Technology, 1.28NB, Kluyverweg 1, 2629 HS Delft, The Netherlands

Received 26 May 2013; received in revised form 1 October 2013; accepted 2 October 2013
Available online 6 November 2013

Abstract

This work reports on a study into the design of creep-resistant precipitation-hardened austenitic steels using an integrated thermodynamics-based model in combination with a genetic algorithm optimization routine. The key optimization parameter is the secondary stage creep strain at the intended service temperature and time, taking into account the coarsening rate of MX carbonitrides and its effect on the threshold stress for secondary creep. The creep stress to reach a maximal allowed creep strain (taken as 1%) at a given combination of service temperature and time is formulated and maximized. The model was found to predict the behaviour of commercial austenitic creep-resistant steels accurately. By means of the alloy optimization scheme, three new steel compositions are presented, yielding optimal creep strength for various intended service times (10, 10^3, 10^5 h). According to the evaluation parameter employed, the newly defined compositions will outperform existing precipitate-strengthened austenitic creep-resistant steels.

Keywords: Alloy design; Strain; Creep-resistant steels; Thermodynamics; Precipitation strengthening

1. Introduction

Creep-resistant steels are widely used in the power plant and aero-engine industries, owing to their excellent properties under demanding conditions, i.e. elevated temperatures, high loads and long service times. During such conditions, the creep strain evolves and shows three stages: primary, secondary/steady and tertiary creep. Of these three stages, the secondary/steady stage is the most important, as it accounts for the largest part of creep life [1]. During the secondary stage, the creep rate is constant and inversely proportional to the creep life, according to the Monkman–Grant relationship [2], Moreover, in industry, the stress that produces a creep rate of $10^{-7}\,h^{-1}$ (or 1% strain for 10^5 h) is taken as the maximum allowable stress.

Design of new creep-resistant alloys by traditional trial-and-error methods is time consuming and expensive. Computational methods have been considered as an alternative way to design novel alloys in recent years. Computational thermodynamics [3–6], artificial neural networks [7–11] and ab initio calculations [12–15] have been developed to predict the optimal alloy composition for specified uses, and to guide and accelerate costly experimental alloy development programmes. More recently, a thermodynamics-based model in combination with a genetic algorithm (GA) was developed and successfully applied to the design of novel ultrahigh-strength stainless steel grades for room temperature application in which the precipitation strengthening is considered to be time independent [16–18]. This alloy design approach was further extended to the design of heat-resistant precipitates strengthened steels [19], and focused on the high-temperature strength evolution by taking into account the development of precipitates. However, in the latter approach, the creep strain during use itself, which essentially determines the creep failure, was not considered. The creep strain can be estimated using constitutive equations, which correlate the strain (rate) to the stress and the temperature. Some constitutive models have been developed based on experimental

* Corresponding author. Tel.: +31 15 278 5218; fax: +31 15 278 4472.
E-mail address: W.XU@tudelft.nl (W. Xu).

1359-6454/$36.00
http://dx.doi.org/10.1016/j.actamat.2013.10.004

observations of strain–stress behaviour [20]. Other models attempt to link creep behaviour with microstructural parameters, such as inter-particle spacing [21–24], leading to microstructure-associated constitutive equations. These constitutive equations can be used either as an assessment of creep rupture life at a given stress or for the prediction of the creep strength for an intended lifetime.

In the present work, the genetic alloy design approach of high-temperature steels is further developed by introducing a new (secondary creep) strain-based optimization criterion and taking the coarsening of the TiX carbonitrides and its effect on the creep threshold stress as the main strength determining microstructural parameter. The model is validated against experimental data for various commercial creep-resistant steel grades. Using the alloy optimization scheme, three new steel compositions are presented, yielding optimal creep strength at 1% allowed strain for various intended service times (10, 10^3, 10^5 h).

2. Model description

2.1. Design methodology

In line with the "chains model" proposed by Olson [25], the design methodology presented here follows the direction from performance to properties, microstructures and eventually to the composition and processing conditions. The method relies on two key conversions, the "translator" for the correlation from mechanical properties to desirable microstructures, and the "creator" to link desirable microstructures to alloy composition/heat treatments employing established metallurgical principles [26]. In the present work, the translator needs to translate the required properties for creep-resistant steels, such as high strength, good stability and decent oxidation or corrosion resistance, into desirable microstructures, using known microstructure–property relationships. The tailored microstructure is chosen to be an austenitic matrix with MX carbonitride precipitates. The compositional and microstructural details of such steels have been reported in a previous study [19]. Then, the creator should link the tailored microstructural features to a specific composition and related heat treatment parameters via employing various go/no-go criteria, which involve thermodynamic and kinetics calculations. All qualified solutions are then ranked according to a properly chosen optimization factor. Considering the large space of the pre-defined compositional domain, a GA is employed to make sure the space is searched effectively and efficiently.

In the previous design study of heat-resistant precipitation-strengthened steels [19], the maximum precipitation-strengthening contribution of MX carbonitrides at the intended time of use was considered as the optimization criterion. While the method yielded interesting suggestions for optimal compositions, it can be argued that the precipitate coarsening rate is an indirect optimization parameter. Hence, it may be more appropriate to take the creep strain development itself as the direct optimization parameter.

Creep behaviour can be divided into diffusional and dislocation creep, depending on the service temperature and applied stresses. According to Frost and Ashby's deformation map for 316 austenitic stainless steel [27], advanced austenitic creep-resistant steels will undergo dislocation creep at the intended service condition, i.e., a service temperature of 650 °C and an applied stress >60 MPa. Various failure models have been proposed for this type of creep mechanism. Some researchers focused on the rupture due to void, grain boundary wedge accumulation [28,29] and tried to correlate the damage with the rupture time/strength in creep-resistant steels [30,31] accordingly. Others focused on investigating the effects of stress and temperature on strain rate and accumulated strain [32,33], especially in the secondary/steady stage [1,34]. The present work follows the latter approach, and the choice of equations to describe strain–stress and other new model features is presented in the following.

Based on numerous experimental results involving various types of pure metals and precipitate-free alloys [1], a power law equation of dependence of strain rate upon applied stress has been proposed and is now commonly accepted for estimating the strain rate during the steady stage [1]:

$$\dot{\varepsilon}_{ss} = C\exp(-Q/RT)\left(\frac{\sigma}{G}\right)^n, \tag{1}$$

where $\dot{\varepsilon}_{ss}$ is the creep rate of the steady stage, C is a constant, Q is the activation energy, R is a gas constant, T is temperature, σ is applied stress, G is the shear modulus, and component n is a constant, normally ranging from 4 to 6. However, in the case of precipitate-strengthened alloys, the creep rate is not properly described by Eq. (1), and a threshold stress σ_{th} has been introduced [35,36]. If the applied stress is lower than the threshold stress, the strain rate is negligible and can be ignored. When it reaches the threshold stress, the strain rate will increase significantly with further increase in the applied stress. Thus, for precipitate-strengthened alloys, Eq. (1) is reformulated as:

$$\dot{\varepsilon}_{ss} = C\exp(-Q/RT)\left(\frac{\sigma-\sigma_{th}}{G}\right)^n. \tag{2}$$

In Eq. (2), the component n will again be in the range 4–6. In the further analysis, a fixed value for n, $n=5$, is imposed.

According to Ref. [1], the threshold stress can be expressed as:

$$\sigma_{th} = \alpha Gb/L, \tag{3}$$

where α is a constant, G is the shear modulus, and L is the average inter-particle spacing. For general dislocation climb, α varies from 0.004 to 0.02, for local climb, $\alpha = 0.19$ [1]. According to the detachment model [37,38], α is not a constant, but changes with the mechanism of dislocations passing the particle. However, as a first-order approximation, α can be taken as being constant and equal for alloys with a common dislocation–precipitate