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Designing new corrosion resistant ferritic heat resistant steel based on optimal solid solution strengthening and minimisation of undesirable microstructural components

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ABSTRACT

Solid solution strengthening can play a very important role in the performance of heat resistant steels, not only because of its substantial strengthening effect as such, but also because of the fact that the effect that solid solution strengthening is, by definition, time independent. In the present study a computational alloy design approach is presented to explore the chemical composition of high strength ferritic heat resistant steel designed to have an optimal solid solution strengthening, while minimising the presence of undesirable microstructural components. Alloy compositions covering eleven elements are considered in the calculations. The chemical composition and the associating optimal annealing temperature are optimised simultaneously via a genetic algorithm. To validate the approach, the solid solution strengthening contribution in existing commercial ferritic stainless steel was calculated using the same computational procedures, and it is shown that the documented relative experimental performance of the reference alloys agrees very well with the model predictions. According to the predictions results, the newly designed alloys have a substantially higher solid solution strengthening than found in existing alloys.

1. Introduction

Ferritic heat resistant steels have been widely used in high temperature components in power plant applications. One of the main advantages of ferritic steels is its lower thermo-expansion coefficient compared to that of austenitic steels leading to a better thermal fatigue resistance [1]. However, the relatively low strength of ferritic grades at high service temperatures significantly limits their application. Design of new ferritic heat resistant steels with an intrinsically higher strength can significantly expand their application and increase their relevance for the construction of next generation power plants.

Precipitation hardening and solid solution strengthening are two commonly used strengthening mechanism to increase the strength of ferritic steels. Recently Teng et al. have developed a ferritic steel for power plant applications strengthened by NiAl and Ni_2TiAl intermetallics [2,3]. However, for precipitation strengthened alloys, a drop in the strengthening contribution of precipitates is inevitable over very long service time due to the coarsening of precipitates during service. Unlike precipitation strengthening, solid solution strengthening is more stable once the equilibrium state is achieved. Alloys based on a high solid solution strengthening contribution will probably have a combination of a (lower initial) high creep strength but a highly superior stability over very long use times.

Solid solution strengthening arises from the interaction of dislocations and solutes in the solid solution due to the size and modulus misfit of solutes with the solvent. It has been extensively studied both theoretically and experimentally during the last century [4–10]. In recent years, ab initio methods have been used to predict the solid solution strengthening taking into account the size and electronic structure of individual alloying elements [11–15]. In situ observations of the interaction of dislocation with solutes made it possible to investigate the solid solution behaviour at the nano-level [16–18].

Given the existing knowledge on solid solution strengthening and relatively new mathematical tools, computational design of high solid solution strengthened alloys involving many strengthening elements at the same time has become possible. In the present work, a genetic alloy design approach couple with thermodynamics is developed to obtain high strength ferritic heat resistant steels using solid solution strengthening at a service temperature of 650 °C, considering 11 alloying elements. As the final strength of an alloy not only depends on the optimised presence of the strengthening mechanism, but also on the absence of undesirable microstructural components, in the optimisation both the

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desirable and the to-be-avoided components are taken into account. Furthermore, the model also takes into account all relevant microstructural changes at the various heat treatment temperatures.

2. Model description

2.1. Design methodology

The design methodology follows the route from properties to microstructures, and eventually to the composition & processing conditions [19]. Two key conversions are used in this method, as shown in the upper part of Fig. 1: the 'translator' to link the desired mechanical properties to the necessary microstructures, and the 'creator' to link the requested microstructures to alloy composition/heat treatments employing established metallurgical principles [20]. In this study, the required properties of creep resistant steels, such as high strength, good thermal stability and decent oxidation/corrosion resistance, need to be translated into microstructural features using known microstructure–property relationships. For the ferritic creep resistant steel grades studied in the current work, only solid solution strengthening is considered and maximised to safeguard the intrinsic stability of the alloy. The target matrix microstructure is defined as being Ferritic (not martensitic) in combination with a limited precipitate volume fraction (since some precipitates are unavoidable). Subsequently, the creator links the tailored microstructural features to a specific composition and related heat treatment parameters by employing various quantitative criteria related to thermodynamic and kinetics considerations. Finally, all qualified solutions are ranked according to a properly defined solid solution strengthening factor. Considering the large space of the pre-defined compositional domain, a Genetic Algorithm is employed to make sure the solution space is searched effectively and efficiently.

2.2. Defining the go/no-go criteria

To obtain the desirable microstructure (a fully ferritic matrix with maximal solid solution strengthening, a minimal precipitation volume fraction and the absence of detrimental phases), various go/no-go criteria are defined. Following the conventional heat treatment route of existing ferritic heat resistant steels, candidate solutions are first evaluated at the annealing condition by performing the thermodynamic equilibrium calculation at the annealing temperature T_{Anneal}. Two go/no-go criteria are imposed in this step, being

(1) The equilibrium ferrite volume fraction at homogenisation temperature should be larger than 99%.
(2) No presence of liquid phase.

After homogenisation, the alloy is cooled down to room temperature before its service at high temperature e.g. 650 °C. Unlike annealing in the austenitic state, a fully ferritic matrix at the end of the annealing temperature will not undergo a phase transformation during cooling to room temperature, yet during service, the thermodynamic equilibrium may vary and some precipitates may form. Therefore, the second set of thermodynamic calculations is performed at the intended service temperature, i.e. 650 °C. Two additional go/no-go criteria are enforced:

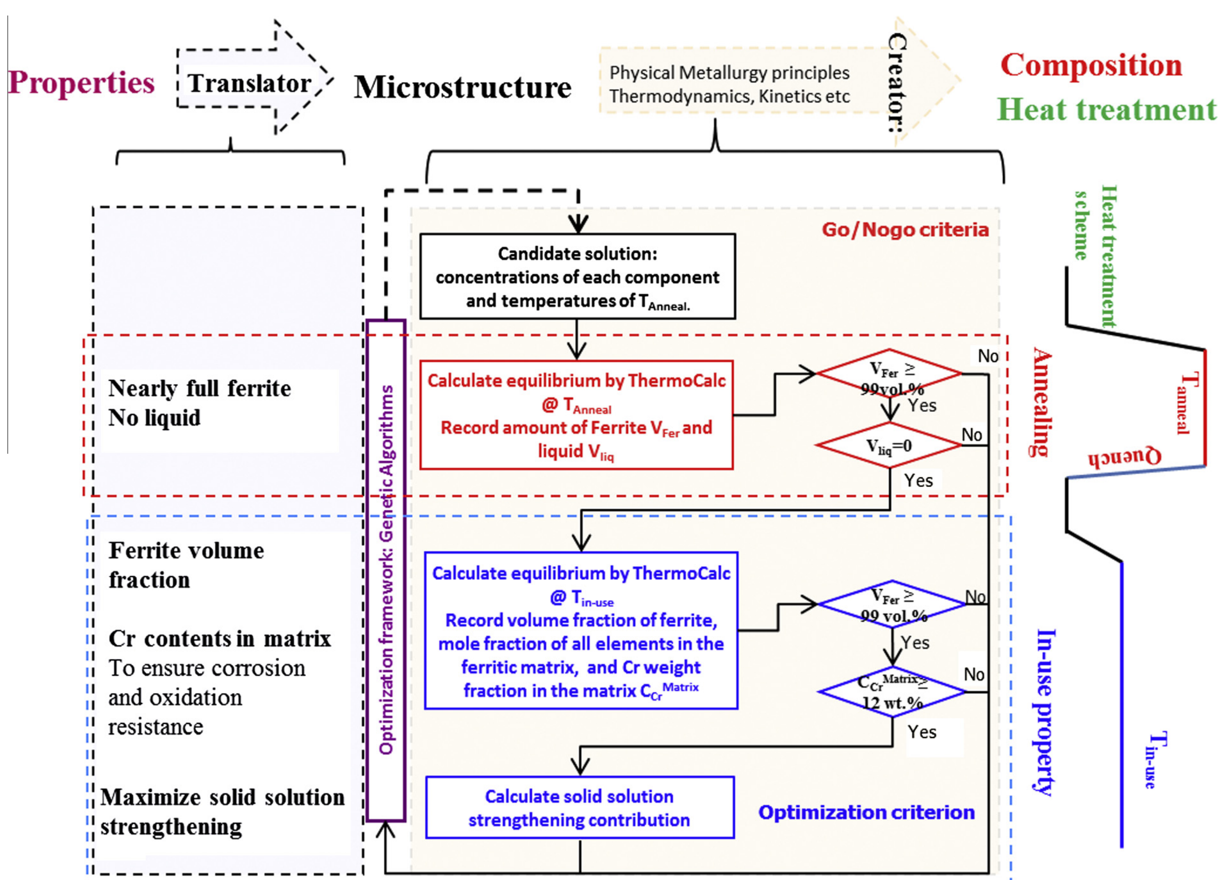

Fig. 1. Alloy design strategy and criteria evaluation of high solid solution strengthening ferritic heat resistant steels.