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ADVANCED ALLOY DESIGN TOOLS APPLIED TO THE DEVELOPMENT OF VANADIUM NITRIDE STRENGTHENED HIGH-TEMPERATURE STEELS

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Introduction: In order to satisfy more demanding efficiency requirements and to achieve better environmental and economic performance, the modern power generation industry requires a continuous process of improvement. New materials able to outperform present ones in safety, mechanical properties and service temperature are a continuous need in this process. In the past, the process of designing a new material was mostly heuristic, requiring repeated experimental trial and error, but the accuracy of current scientific knowledge in thermodynamics and transformation kinetics enables us to design successful new alloys using minimal empirical feedback. The design process is, however, still somewhat iterative, each stage leading to a more refined definition of the final alloy. The difference from the traditional approach is that most of the process is performed theoretically or computationally, involving the production of only a few essential trial casts to verify the suitability of the product material. The work presented here pretends to demonstrate the feasibility and strength of the present method.

Selected References:

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Step 1

Alloy Design Methodology

Step 1:
General composition and Microstructure

Literature & Industrial "Know-How"

Step 2:
Target properties

Advanced Statistical Methods
Neural Networks on Creep

insufficient properties

Step 3:
Microstructure

Thermodynamic stability of phases
CALPHAD method-based models

undesirable phases

Step 4:
Heat Treatment and Manufacturing

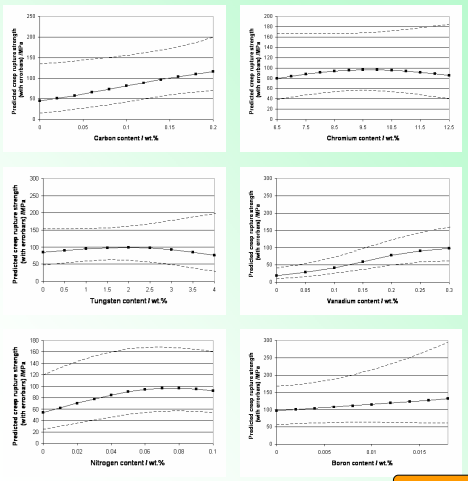
Thermodynamic and kinetics modelling

manufacturing limitations

Step 5:
Assessment of final alloy

Casting and characterisation

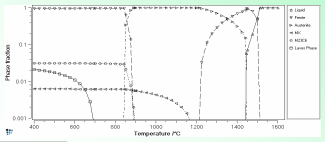
Analysis of composition effects using a Bayesian-based Neural Network



Step 2

Thermodynamic stability of phases

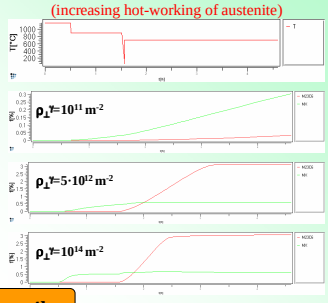
CALPHAD Method



Step 3

Thermo-Mechanical Treatments

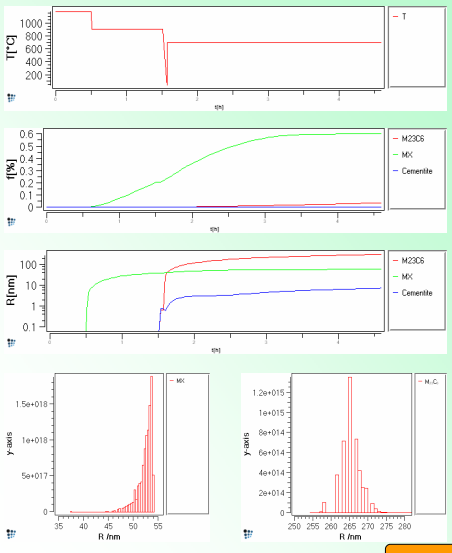
(increasing hot-working of austenite)



Step 4b

Thermodynamics and kinetics of the heat treatment

(density of dislocations/m^{-2}: austenite 10^{12}; martensite 10^{15})



Step 4a

Fe	C	Cr	W	V	N	B	
bal.	0.14	9.5	2.5	0.35	0.07	0-0.1	/wt%

Step 5

Conclusions: The work presented here is a case study on how the current accuracy of thermodynamic and kinetic calculations allow new alloys to be designed to respond to demanding operating conditions, while avoiding most of the experimental trial and error needed in the past. Software tools based on the CALPHAD method and various kinetic models are available, allowing the prediction not only of the feasibility of a target microstructure but also of its evolution during various heat treatments.

In the present study a new reduced activation ferritic/martensitic alloy has been designed that should be able to sustain service temperatures of 650°C. This alloy has been cast and treated and is being characterised microstructurally and in terms of mechanical properties.