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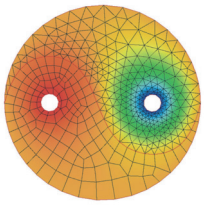

THE STRUCTURE OF A GENERAL MATERIALS GENOME APPROACH TO THE DESIGN OF NEW STEEL GRADES FOR SPECIFIC PROPERTIES

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Abstract

In this work we review and reformulate a general alloy design methodology based on thermodynamic and kinetic principles, employing the genetic algorithm as the optimization scheme. The new approach relies on two key concepts: the 'translator' and the 'creator'. The 'translator' is the conversion of the desired (thermo-)mechanical properties into required microstructures using known microstructure-property relationships. The 'creator' translates quantifiable microstructural parameters into metallurgical and economical parameters, i.e. composition, heat treatment parameter and cost, again employing established metallurgical principles. In the case of well defined 'translator' and 'creator' functions the model allows simultaneous, human intervention free optimization of alloy composition and key heat treatment parameters, i.e., austenitization temperatures and ageing temperatures, so as to fulfill multiple design criteria and eventually to achieve the desired microstructure. The elementary version of the model, not defining the 'translator' or 'creator' modules explicitly has applied to the design of ultra high strength (UHS) stainless steel and was validated by experiments on prototype alloys. The model was subsequently extended to take into account the alloying cost by adding a cost factor to various alloying elements, and is shown to provide valuable guidelines to the design and modification of alloy compositions and has the capacity to optimize strength and material cost in an integrated manner. In this manuscript the new conceptual approach to alloy design is reformulated in a more generic and abstract manner and new extensions of the model to the design of high temperature resistant steels (both creep steels and fire resistant steels) and abrasion resistant steels are discussed, and some preliminary results are shown.

Key words: alloy design; genetic algorithm; ultra high strength (UHS) steels; creep resistant steels; abrasion resistant steels; material genome initiative

1. INTRODUCTION

Alloy design normally requires systematic considerations of all relevant parameters: from an input point of view, alloy composition and proper heat treatment conditions are of paramount importance in achieving a desired combination of properties. On the other hand, the output, i.e. the total set of mechanical, thermal and chemical properties of the new alloy, often requires making a trade-off between conflicting requirements between the various properties and alloy costs etc. With the increased number and complexity of alloying elements involved in creating high performance alloys, the conventional 'trial and error' approach has become a costly and time inefficient route. Inspired by persistent demands to design new alloys faster, at lower cost and via more consistent routes, various efforts have been made by both academia and industry to develop a more efficient approach, stimulated by many governments via programs such as the Materials Genome Initiative (National Science and Technology

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council, 2012). In specific cases, modern versions of the conventional experimental approach (Springer & Raabe, 2012), may lead to relatively fast screening of new steel solutions (composition and treatment parameters), at a reasonable cost. .However, due to the more quantitative understanding of correlations among thermodynamics, microstructures and properties, computational thermodynamics supplementing and replacing the experimental approach (Würzinger et al., 2004; He et al., 2005; Michaud et al., 2007) has become a more efficient and powerful tool in providing guidance for alloy design (Campbell & Olson, 2000; Trabadelo et al., 2005) and process development (Agren, 1994; Lee et al., 1998; Klotz et al., 2008). Other approaches, such as artificial neural networks (ANN), may also be an aid in guiding both (Bhadeshia, 1999; Hodgson et al., 1999; Guo & Sha, 2004; Brahme et al., 2009). However, ANN based approaches are statistically rooted, and cannot supply compositions and/or processing parameters outside the data ranges employed to train the network. On the other hand, the ultimate bottom-up design approach based on *ab initio* calculations, has also demonstrated the capability in designing new alloys (Vitos et al., 2003; Hao et al., 2004). Nevertheless, the ab initio approach requires great simplifications of the system and hence its applications to date are limited to simple matrices containing well defined and validated precipitates.

Recently, a theory-guided general computational alloy design model has been presented and applied successfully to the design of new UHS stainless steel grades (Xu et al., 2008a, b; Xu et al., 2009a; Xu et al., 2009b), in which alloy compositions and heat treatment parameters (austenitization and ageing temperatures) are simultaneously optimized applying genetic algorithm, so as to obtain desirable microstructural components and avoid undesirable phases considering the entire heat treatment process. In genetic algorithms all information of a steel such as its composition and critical process temperatures are coded as short binary numerical strings, which can be regarded as the genes for that particular parameters. All genes are then concatenated to form a chromosome which represents the specific steel solution. The genetic algorithm provides an efficient search engine to sample the multi (n>15) dimensional search space with a high accuracy and to identify regions of optimal properties. Characterizations of prototype alloys based on these model optimizations confirmed the presence of the intended precipitates, and the new alloys showed very high mechanical and corrosion resistant properties comparable to those of successful industrial grades with a long optimization history (Xu et al., 2010a; Xu et al., 2010b). It is important to point out that, once the microstructural optimization parameter and the (multiple) constraints are properly set, the optimization process itself does not require any expert user intervention.

In the present work, the general design approach coupling the physical metallurgical principles and employing the genetic algorithm as the optimization scheme is reviewed and reformulated. The crucial role of the two key transition steps, 'translator' and 'creator' are addressed in detail and new insights are presented. The extension of the concept to the design of other steel grades, e.g. creep resistant and abrasion resistant steels, is discussed and some preliminary results are shown. The current examples focus on steel grades in which grain size is not so important. For steel grades in which the grain size plays an important role in the approach presented here the 'creator' is to be extended with a dedicated thermomechanical module

2 GENERAL DESIGN METHODOLOGY

Following the chain model of goal/means oriented alloy design methodology proposed by Olson (Olson, 1997), the alloy design involves three chains linking the performance, properties, microstructures and eventually the composition/processing. The chain model starts with the first chain of defining a set of target properties following an analysis of the intended applications. In the second step, the required property combination has to be translated to metallurgical variants, i.e. microstructural features, as illustrated in the flow chart figure 1. The translator is based on existing knowledge to describe the effects of various microstructural components/ features on different properties. This knowledge comes from the numerous experimental investigations and alloy design experiences throughout the development of metallurgy. For example, the matrix (austenite, martensite or bainite) volume fraction and their morphology, the presence of precipitates and their distribution etc. together determine (thermo-) mechanical properties of a steel. The rule of the translator is to quantitatively formulate the desirable microstructures according to required (thermo-) mechanical properties, based on known metallurgical knowledge. A detailed example will be given in the next section. The last chain, attaining the tailored

microstructures with (optimal) alloy composition and associated heat treatment condition, is the key and most sophisticated process in the goal/means alloy design strategy. The desired microstructure features have to be created based on the implicit and complicated correlations between the microstructure and alloy composition, heat treatment or processing parameters. The creator module is to build quantifiable and verifiable mathematical formulations between the quantitative description of target microstructures and quantities representing the steel solution (composition and treatment parameters), via employing various physical rooted metallurgical principles, e.g. phase transformation model and precipitation model etc. Therefore, the alloy composition and heat treatment condition can be numerically calculated and optimized employing an appropriate algorithm. However, the desired microstructure is often composed of multiple microstructural components/features, aimed to achieve a desired combination of properties. Those different microstructural requirements are often competing or even conflicting with each other, and hence the combination of properties often requires making choices and achieving a global compromise. In such a case, an algorithm with the capacity of handling multiple criteria optimization is of crucial importance in achieving a solution in an efficient manner. Moreover, some extended factors, such as the property/cost ratio, can be obtained, or even employed as the optimization factor, as demonstrated in figure 1.

We will now present three design studies for steel grades of increasing complexity. The first case is that of Ultra High Strength stainless steel. These steels are to have a relatively simple microstructure (tempered martensite) and the required properties (strength and corrosion resistance) are defined for room temperature only and are therefore time independent. For this case the 'translator' is well defined and relatively simple and the 'creator' function is also relatively straightforward. Without any increase in model complexity the properties can be optimized in an absolute or in cost driven manner.

The second case is that of high temperature resistant steels, i.e. creep resistant and fire resistant steels. Again, the microstructure is relatively easy but the properties are now temperature and time dependent, creating additional complexities in defining the 'creator' function properly. The strength determining precipitates should not only be of the right type, quantity and dimension, but should also maintain their key parameters for defined periods of time. In the case of fire resistant steel grades the time to maintain the high strength is relatively short and some coarsening is allowed provided the alloy has a good initial strength. In creep resistant steels this exposure time is very much longer and the required extremely low precipitate coarsening rate leads to rather different alloy compositions.

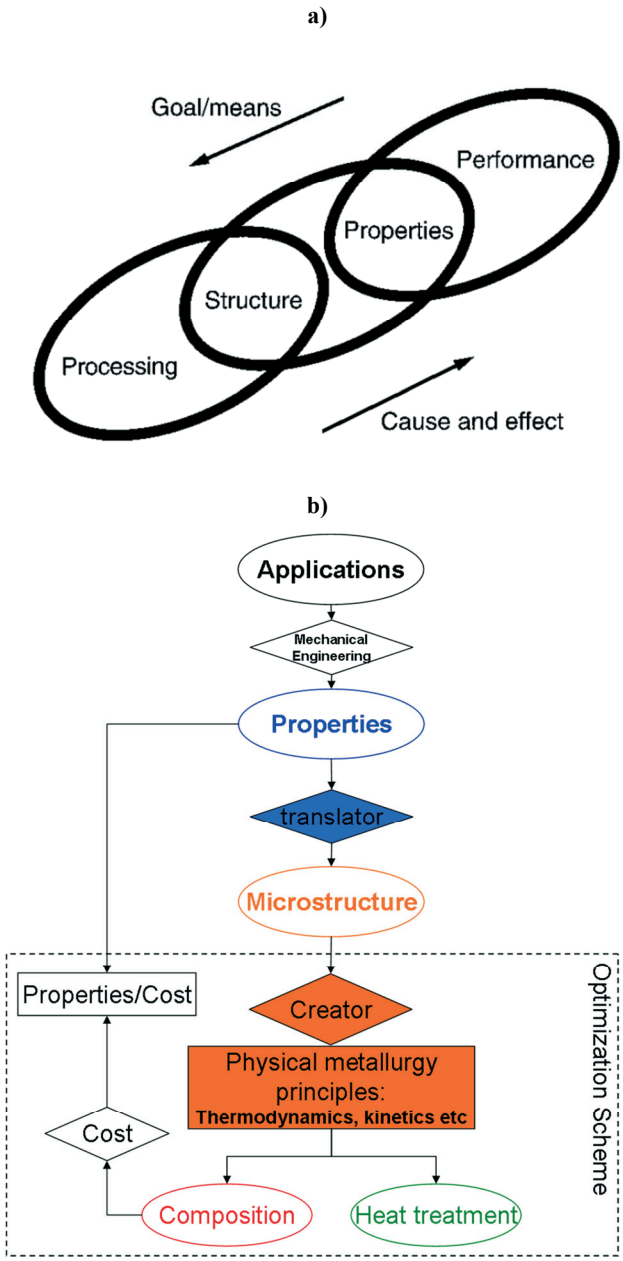

Fig. 1. *(a) Three-link chain model of the central paradigm of materials science and engineering[20], (b) Flow chart of the general alloy design methodology following the goal/means orientation.*

The third case concerns abrasion resistant engineering steels commonly used in the mining and transportation industries where three parties abrasion is the predominant wear mechanism and generate gradually a materials loss. A detailed literature study has shown that for these steels the 'translator' func-

tion is very hard to define as there are no general rules linking intrinsic material properties to abrasion resistance and that processing determined microstructural dimensions also plays a role. For such a more complex design challenges the choice of subsystems with well defined microstructures may offer, at the moment, the best way forward.

3. DESIGN OF ULTRA HIGH STRENGTH STAINLESS STEELS

3.1. Translator: from properties to microstructure

In general, the combination of UHS and good toughness can be realized via a uniform dispersion of nano-sized precipitates in a fine lath martensite matrix. This microstructure can be obtained via a two-step heat treatment as demonstrated in the right hand side of figure 2: firstly a solution treatment followed by quench and secondly an ageing treatment for precipitation. The targeted microstructures at each stage during the process are described below and also shown in figure 2:

(A) The solution treatment is aimed at dissolving precipitates/inclusions formed preceding the austenitization treatment and obtain a homogeneous austenitic matrix. Depending on the alloy composition, various phases can be presented in the as-cast or as-rolled condition, e.g. various primary carbides and δ-ferrite. The presence of phases other than austenite is generally detrimental to the final mechanical properties and therefore it is desirable to start from a (nearly) pure austenitic matrix.

(B) The hardenablity of the homogenized austenite determines its decomposition product upon quenching, which is eventually controlled by the alloy composition and Ms temperature. A fully martensitic matrix with its high potential precipitate nucleation site density is required in order to achieve the high strength level as such a structure with many lattice defects promotes the subsequent precipitation during an ageing process.

(C) The precipitation strengthening is considered to be the most effective and commonly applied strategy in the design of UHS stainless steels and therefore a fully martensitic matrix is the best starting structure to be further strengthened by an ageing treatment, which promotes the formation of desirable precipitates, e.g. MC carbide, Cu clusters and

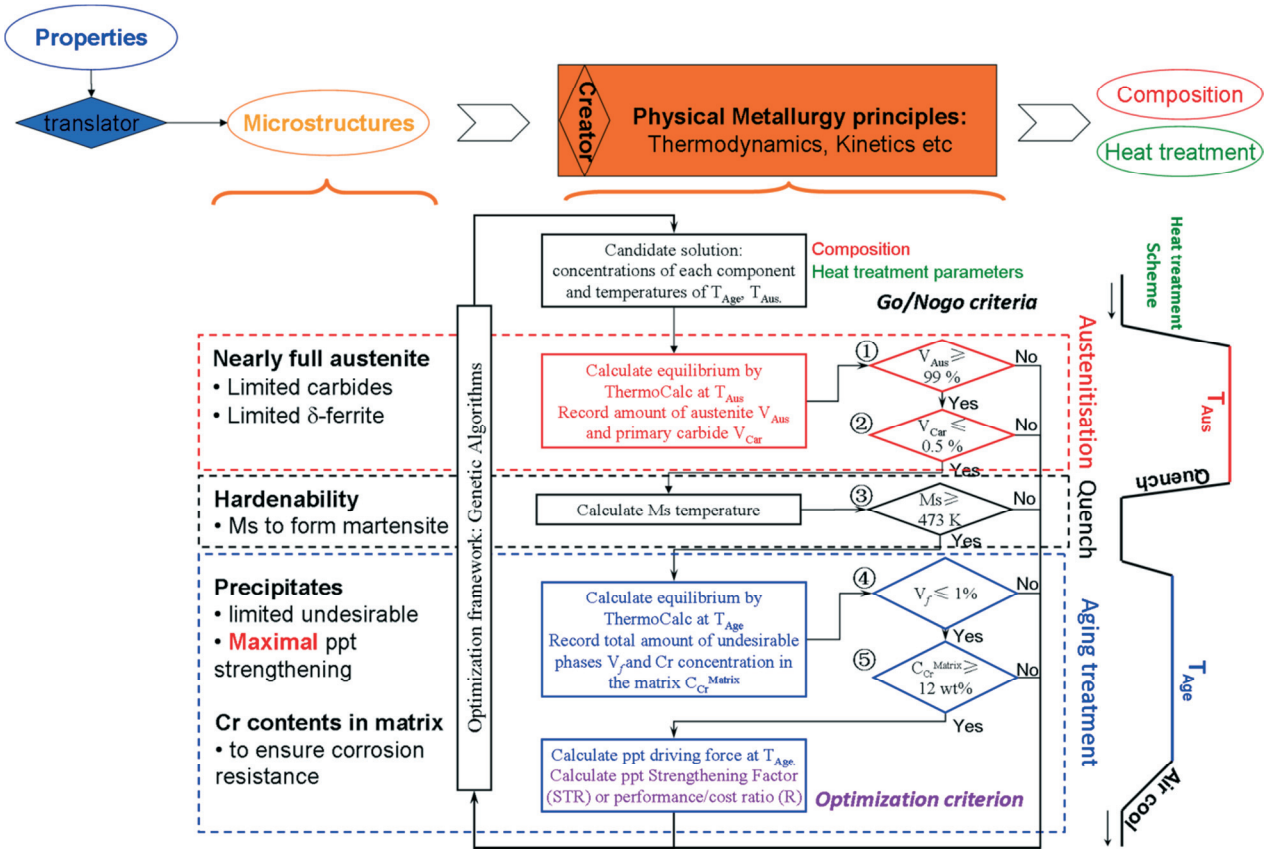

Fig. 2. Detailed alloy design strategy and criteria evaluation of UHS stainless steels.

Ni_3Ti intermetallics, with the desired dispersion of a dense network of nanosized particles (Servant et al., 1987; Stiller et al., 1998; Campbell & Olson, 2000; Raabe et al., 2009). Furthermore, a good corrosion resistance can be achieved by ensuring a sufficient Cr concentration (i.e. > 12 wt%) in the matrix upon the completion of precipitation. Furthermore, while fostering the formation of desirable microstructures, the formation of phases limiting strength or toughness, e.g. δ-ferrite and primary carbides during austenitization and $M_{23}C_6$, M_6C and M_7C_3, cementite, μ and χ phases upon ageing, should be prevented (Padilha & Rios, 2002).

3.2. Creator: converting microstructure to quantifiable criteria

In order to create targeted microstructures described above, the next step in the alloy design process is to convert the targeted microstructures into multiple quantifiable criteria representing the metallurgical essences of each microstructural consideration. In the design of UHS stainless steels, as demonstrated in figure 2, various criteria are built in and quantified via thermodynamic calculations, and classified as go/no-go criteria and optimization criteria in the following manner (all specific details can be found elsewhere (Xu et al., 2008a, b; Xu et al., 2009a; Xu et al., 2009b)):

(A) The composition and heat treatment parameters are decoded from the chromosome and the thermodynamic equilibrium calculation is performed at the austenitization temperature T_{Aus}. Two go/no-go criteria are imposed subsequently being (1) the equilibrium austenite volume percentage larger than 99% and (2) the maximum level of primary carbides limited to 0.5% in volume.

(B) The key factor of martensitic transformation, the martensite start (Ms) temperature is calculated with the composition of austenite at austenitization temperatures taking into account the solute depletion by the formation of undesired phases. The criterion is enforced as a go/no-go criterion that the Ms temperature is above 473 K to ensure the formation of fine lath martensite with a volume fraction of over 95% (Ishida, 1995).

(C) Thermodynamic equilibrium is calculated at the ageing temperature T_{Age} using composition of the austenite at the austenitization temperature and two go/no-go criteria are enforced: (4) the maximum allowed volume fraction for all unavoidable undesirable phases together was arbitrarily set at 1% and (5) a minimum of 12 mass% Cr in the matrix upon completion of the precipitation reactions is required so as to form the Cr-rich corrosion resistant film.

(D) For candidate solutions which fulfill all go/no-go criteria (1)–(5), the precipitation-strengthening contribution (STR) of desired species is calculated as $f_v^{1/2}r^{-1/2}$, where f_v is the equilibrium volume fraction of the precipitate at the aging temperature and r is the critical precipitate nucleus size, which is inversely proportional to the thermodynamic driving force for the precipitation. This strengthening estimation is based on a mixture of shear and bypass precipitate strengthening mechanisms and was justified in an earlier work (Xu *et al.*, 2008b).

3.3. Optimization framework

Having defined multiple competing/conflicting criteria, the alloy composition optimization has to balance in a systematic manner the weight percentages of different alloying elements, find a compromise between the positive and negative effects of each component, and evaluate their influences on forming the desirable microstructures while suppressing undesirable influences. Moreover, in addition to the alloy composition, key heat treatment parameters, i.e. austenitization and ageing temperature, are also of determinative importance and have to be simultaneously optimized. To deal with the extremely huge solution space and multiple objectives, a computational alloy design model embedded in a genetic algorithm has been developed and published elsewhere (Xu et al., 2008a, b; Xu et al., 2009a; Xu et al., 2009b). This approach allows a simultaneous optimization of alloy composition and the austenitization and ageing temperatures in a very efficient manner, so as to achieve the maximum precipitation-strengthening contribution while fulfilling all go/no- go criteria along the entire heat treatment cycle as described before.

3.4. Model applications and results

The model described above was applied to design UHS stainless steels utilizing strengthening precipitates of MX carbide and Ni based intermetallics (Ni_3TI/NiAl), named alloy CAR and NiTi, respectively. Steel compositions containing up to 13 alloying elements (C, Cr, Ni, Ti, Mo, Al, Cu, Co, Nb, N, V, Mn and Si) were considered. The cost and concentration ranges of each alloy element are shown in table 1. The concentrations of all alloying

elements were allowed to vary in ranges as recommended for the facilitation of alloy production on an industrial scale. Each component was allowed to take 32 potential concentrations by dividing the predefined compositional range for each element in 31 equal steps. The ageing temperature and austenitization temperature were allowed to vary within the range of 693-848 and 1223-1533 K with intervals of 5 and 10 K, respectively. Thermodynamic calculations were performed by ThermoCalc coupled with the TCFE6 database and a tailored database for Ni/Ti-based precipitates. Diffusion coefficients were obtained from MOB2 database for the composition considered. Characterizations have validated presences of targeted strengthening precipitates of Ti(Nb)C(N) and Ni_3Ti, as shown in figure 3 and the mechanical properties achieved the state of the art of ultrahigh strength stainless steels optimized through decades by empirical approaches (Xu et al., 2010a; Xu et *al.*, 2010b).

Table 1. *Ccost of alloying elements and composition ranges employed in the design exercises of UHS stainless steels.*

	C	Cr	Ni	Ti	Mo	Al	Cu	Co
Cost	–	2,79	12,6	3,14	23,33	-	4,5	35,23
Min	0,01	12,00	1,00	0,01	0,50	0,01	0,5	0,01
Max	0,30	20,00	15,00	2,00	10,00	2,00	2,00	2,00
	Nb	N	V	Mn	Si	Fe	TAge	TAus
Cost	29,09	–	34,38	0,75	1,27	-	-	-
Min	0,01	0,01	0,01	0,50	0,3,	Bal,	693	1223
Max	1,00	0,01	1,00	0,50	1,00	Bal,	848	1533

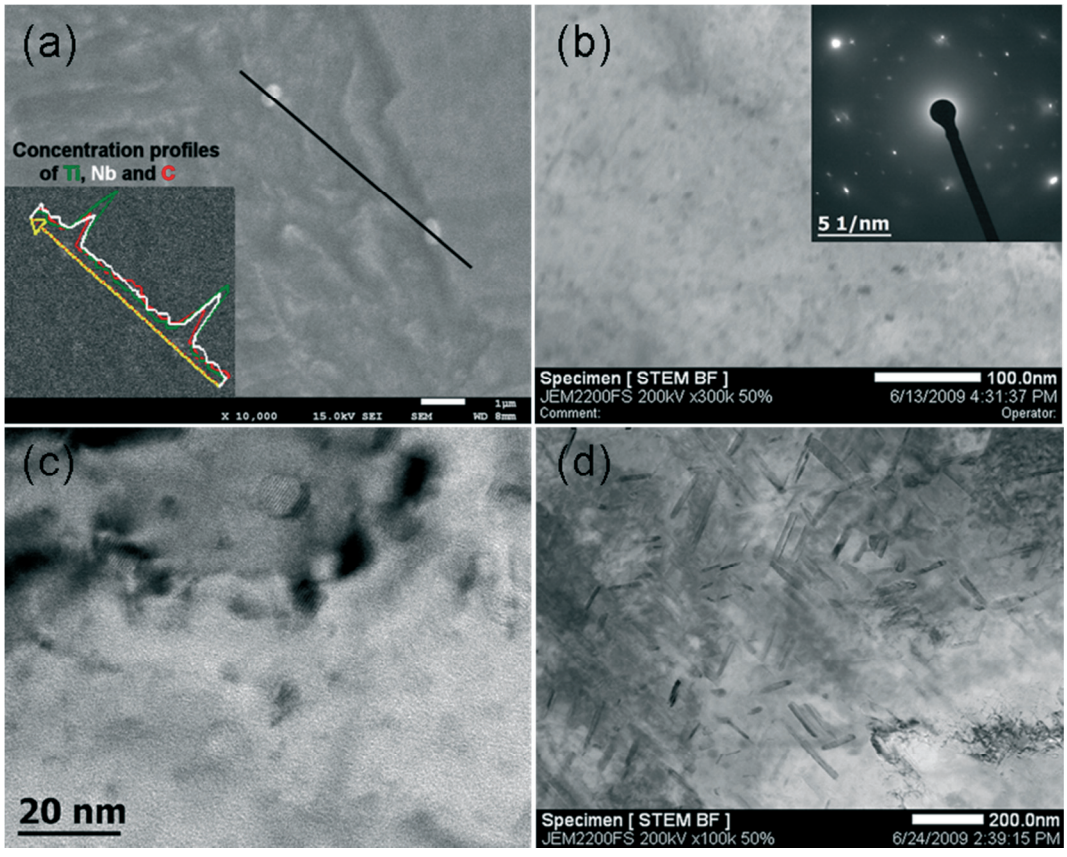

Fig. 3. *Electron microscope images of strengthening precipitates: SEM micrographs (a), TEM image with diffraction pattern (b) and HRTEM image (c) of Ti(Nb)C(N) in alloy CAR (Xu et al., 2010b), and HRTEM image of Ni_3Ti precipitates in alloy NITI (Xu et al., 2010a).*

To demonstrate the effects of all criteria on alloy composition optimization, alloy CAR was taken as the baseline to explore the binary compositional effects of C-Ti (keeping the levels of all other elements as found by the optimization scheme) as

shown in figure 4 (Xu et al., 2009b). The color contour of the background in these figures indicates the degree of strengthening contribution obtained upon precipitation at 773 K. The black vertical patterns superimposed on the color coded background display the forbidden composition domains where Ms temperature is below 473 K; the horizontal black patterns mask the forbidden area in which the total amount of undesirable phases is over 1% in volume and the forward slash region shows the (forbidden) domain where Cr concentration is below 12 wt% after the completion of precipitation. In the composition domain the region where the austenite volume fraction is less than 99% at 1473 K is masked by white horizontal lines and the area where the primary carbides volume fraction at 1473 K exceeds 0.005 is indicated by the vertical white line pattern. The scattered black spots reflect compositions where ThermoCalc equilibrium calculations could not performed successfully, due to numerical imperfections in the original databases used by ThermoCalc. The undashed areas in figures 4(a) and 5(a) unveil the compositional domain in which the precipitation strengthening factor is maximized, while meeting all constraints mentioned above. The solid star shows the concentration value of alloy CAR, which is located exactly at the maximum strengthening level in the uncovered area of the searching domain.

3.5. Cost analysis

New alloy design not only requires good combination of mechanical properties, and also the cost price is of prime importance. Therefore, an analysis of the alloying cost efficiency was made, again taking the alloy CAR as a baseline. In figure 5, results of cost analysis is presented based on alloy CAR and only compositions fulfilling all go/nogo criteria are shown. The closed symbols represent concentrations within the searching window while open symbols correspond to extended concentrations either below minimal or up to three times of the maximal as shown in table 1, if the optimal concentration is exactly on the searching boundary. All points to the left of alloy Car correspond to CAR-like new alloys with slightly lower strength values but with slightly reduced concentrations and a reduction of the total alloying costs. From the figure it is clear that both Ti and Nb are very cost effective for precipitation strengthening and their concentrations, especially that of Ti, should not be decreased. On the other

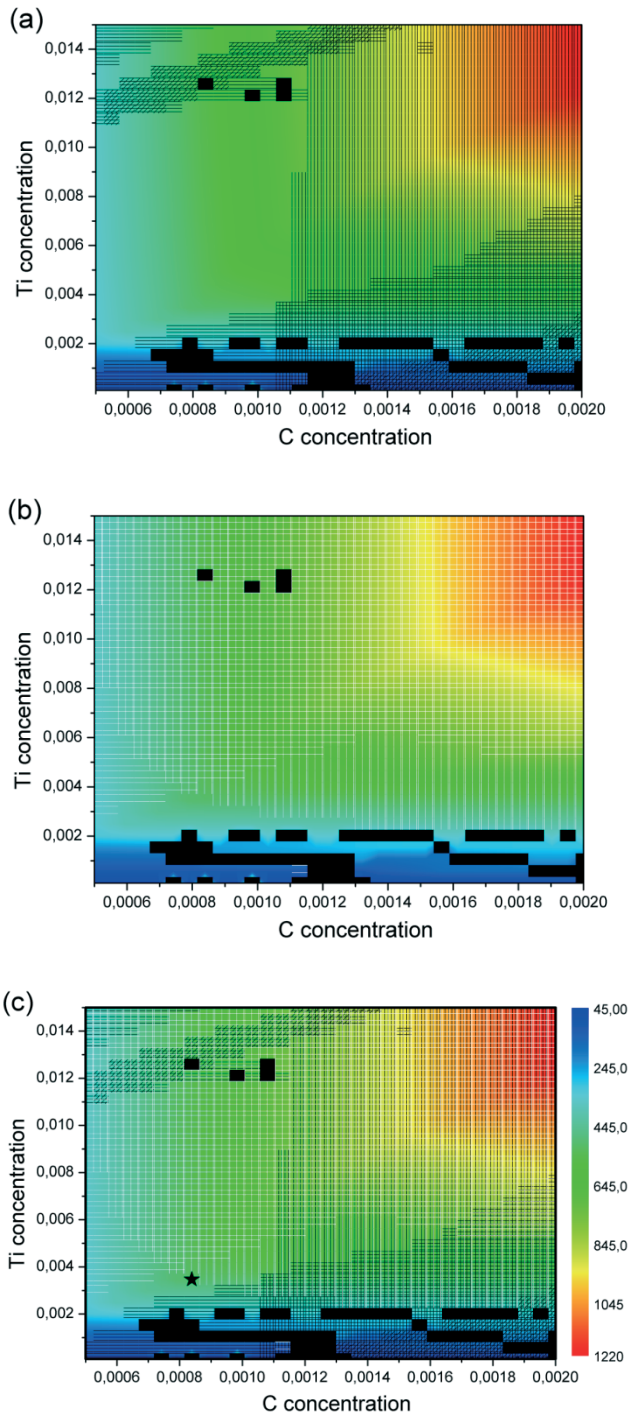

Fig. 4. *Binary compositional effects of C-Ti based on alloy CAR.*

hand, reductions of Ni, Cu and especially Co will clearly reduce the total extra alloying cost without significantly sacrificing the precipitation strengthening contribution. The analysis also shows that if the lower limit of Cr concentration is reduced to 11 wt%, the alloying cost drop significantly but the precipitate strengthening effect is increased while all other go/no-go criteria, including the adjusted minimum Cr level, are met. The figure also shows that increasing the Ni concentration will yield higher cost

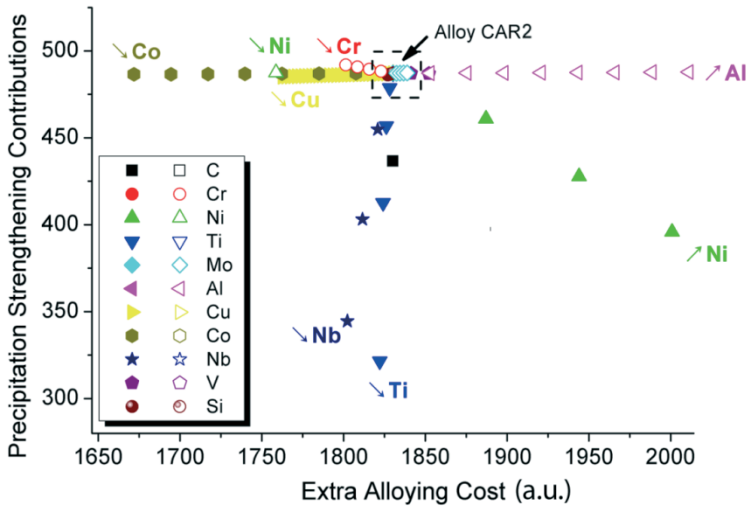

Fig. 5. Compositional effects of each alloy element on extra alloying cost and precipitation strengthening contribution.

creases the driving force to form TiC. Increasing the Al level will slightly increase the strengthening but is not cost effective. For alloying elements other than those discussed above, their contribution to strength or cost is small or their approved concentration windows is thus narrow, that one or more of go/nogo criteria are no longer fulfilled. The best solution resulting from figure 5 is to reduce the Co concentration from 2.0 to 1.6 wt%, which results in a reduction of alloying cost from 1830 to 1670 without sacrificing a notable amount of strength.

The single component analysis demonstrated the cost effectiveness of alloying v.s properties. However, a combination of adjustment of concentration levels of mul-

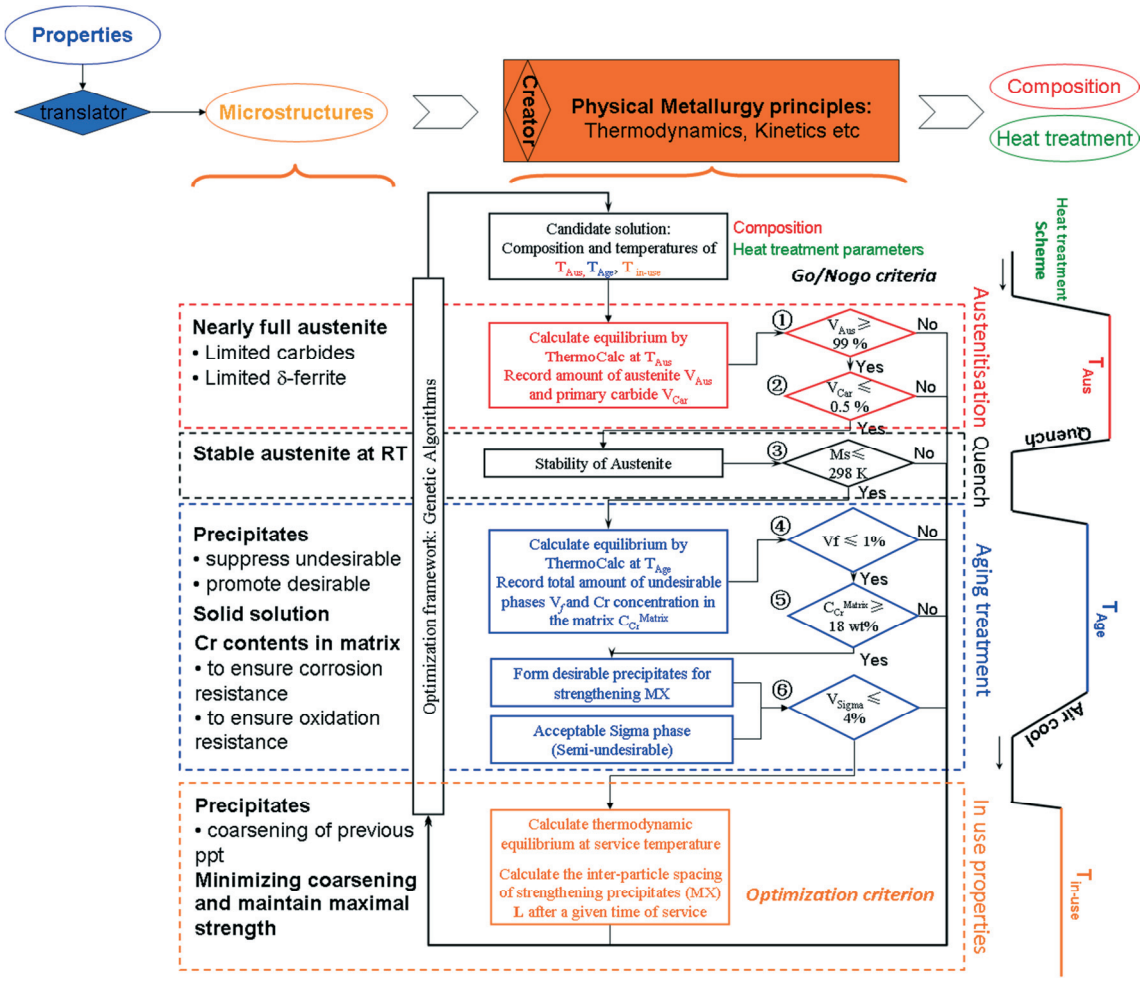

Fig. 6. Alloy design strategy and criteria evaluation of high strength creep resistant steels.

while significantly decreasing the precipitation strengthening contribution due to its effect on the thermodynamics of the system, e.g. Ni depletes Ti in the matrix by forming Ni3Ti intermetallics and de-

tiple components may lead to an even better compromise. For this reason, the alloy design model was extended to take into account the total alloying cost by employing the ratio of strengthening contribution

to alloying cost as the new optimization factor. Redesigned alloys displayed significant cost reductions without significantly sacrificing the strength (Xu & van der Zwaag, 2011).

4. DESIGN OF AUSTENITIC CREEP RESISTANT AND FIRE RESISTANT STEELS

Required by specific applications at elevated temperatures, e.g. power plant, various kinds of creep resistant steels have been developed over a period of many years by the conventional experimental approach leading to several families of creep resistant steels which can be mainly classified into ferritic (martensitic) and austenitic steels. The austenite family predictably contains high amounts of austenite stabilizer, Ni, and various alloying elements which were added in order to strengthen the alloy by precipitation and hence to maintain a high strength level at the high service temperature. In addition to requirements of high strength and creep resistance, other properties, such as corrosion resistance, oxidation resistance etc are also required depending on the nature of final applications.

Following the general design strategy as presented in figure 1, a dedicated design chart for austenitic creep resistant steels and associated heat treatment are presented in figure 6. Starting from the property requirements as discussed above, the 'translator' function indicates that the most appropriate microstructure is a stable fully austenitic matrix without detrimental precipitates, to be subsequently strengthened by precipitation of particular precipitates formed at a dedicated tempering temperature, or directly at the final use temperature. An intrinsic critical requirement of creep resistant steels is a tight control of the coarsening of precipitates at the high temperature as this is highly detrimental to the strength and the long term stability of the material.

4.1. Translator: from properties to microstructure

Following the discussion above, an ideal solution for a creep resistant (austenitic) steel should possess the following microstructural features simultaneously:

(A) During the austenitization, a homogenous austenite matrix with moderate grain size without significant amounts of detrimental phases such as primary carbides and δ-ferrite.

(B) The stability of austenite should be controlled such that it remains a stable austenite throughout the entire heat treatment including service life, i.e., no decomposition upon quenching and during service, and no transformation due to the deformation.

(C) The as-quenched austenite can be strengthened by selected desirable precipitate (e.g. MX carbides or N_3Ti intermetallics) at corresponding temperature, while suppressing the formation of undesirable species. The tempering temperature should be higher than or equal to the in-use temperature of it applications so that the precipitation strengthening is not lost significantly during the service.

(D) The strengthening precipitates formed during tempering or at early stage of the service should remain stable and not undergo significant coarsening and subsequent strength lost during exposure to the operating temperature.

(E) The Cr concentration upon precipitation should be sufficient high so as to obtain a desired corrosion and oxidation resistance.

4.2. Creator: converting microstructure to quantifiable criteria

To create the desirable microstructure throughout the entire process as described above, corresponding criteria are developed and illustrated figure 6. For simplification, the ageing temperature and service temperature are considered the same as 923K. This assumption is also in agreement with common practice that existing commercial alloys employing MX carbides for strengthening don't need a specific tempering treatment prior to serve at a high temperature.

(A) The austenitization resembles the case of UHS stainless steel design. The thermodynamic calculation is performed at the austenitization temperature T_{Aus}. Two go/no-go criteria are imposed subsequently, being (1) the equilibrium austenite volume percentage larger than 99% and (2) the maximum level of primary carbides limited to 0.5% in volume.

(B) The austenite should remain stable upon quenching to room temperature and stay unchanged during its operation , therefore, a go/nogo criterion of (3) $Ms \leq 298$ K is imposed.

(C) Thermodynamic calculation is performed at the ageing and service temperature T_{Age}, and three go/no-go criteria are enforced: (4) the maximum allowed volume fraction for all unavoidable undesir-

able phases (Sigma phase excluded) together was arbitrarily set at 1 vol%, (5) a minimum of 18 wt% Cr in the matrix upon completion of the precipitation reactions is required for corrosion and oxidation resistances considerations, and (6) due to the common presence, the maximal allowed Sigma phase (not a strengthening precipitate) is given as 4 vol%.

(D) For candidate solutions which fulfill all go/no-go criteria (1)–(6), the degradation of precipitation strengthening due to coarsening of precipitate should remain minimal at the given design temperature and time, and hence keep the highest strength level. The strength lose due to precipitation coarsening can be estimated according to the time dependent average inter-particle spacing (Kelly, 1958; Cahn & Haasen, 1996; Agren et al., 2000):

$$\sigma_{ppt} \propto 1/L = \sqrt{f_p}/r = \sqrt{f_p}/\sqrt[3]{r_0^3 + Kt} \quad (1)$$

in which

$$r_0 = 2\gamma/\Delta G_v \quad (2)$$

and

$$K = 8\gamma V_m^{\ p}/9\sum_{i=1}^{n}\frac{(x_i^p - x_i^{mp})^2}{x_i^{mp} D_i/RT} \quad (3)$$

where L is the average inter-particle spacing, f_p is the equilibrium volume fraction of the strengthening precipitate at the service temperature, r_0 is the critical precipitate nucleus size, which is proportional to the matrix-precipitate interfacial energy (γ) and inversely proportional to the thermodynamic driving force for the precipitation ΔG_v. K is coarsening rate and t is time exposing to high temperature. x is interface concentration at equilibrium on both matrix (m) and precipitate (p) sides. V_m^p is the molar volume of precipitate. T is service temperature and D is corresponding diffusion coefficient. For interfacial energies, a value of 1 J/m^2 for all types of precipitates is chosen. In principle it would be possible to make more precipitate specific choices but at present there is insufficient justification to do so. Thermodynamic information and diffusion coefficients for a given composition are obtained from TCFE6 and MOB 2 databases, respectively.

4.3. Alloy design exercises

Preliminary design exercises utilizing MX carbide as strengthening precipitates and employing identical temperature for tempering treatment and service at 923K are performed. Two alloys are designed for optimal precipitate strengthening factors (Eq. 1) after serving for 10 hours, i.e a fire resistant steel grade(Alloy A) or for 100,000 hours, i.e. a regular creep resistant steel (Alloy B) respectively. The composition ranges of all alloying element, design parameters and resulting optimal compositions of alloy A and B are summarized in table 2. With the resulting optimal alloy compositions, the alloy softening due to coarsening of precipitates at 923K as a function of service time is calculated according to Eq. 1 for both alloys and results are presented in figure 7. It is immediately clear that alloy A is designed for optimal service for a period of only 10 hours, and therefore the initial strengthening at 10 hours is high, but it rapidly and continuously decreases after 10 hours. While for alloy B, which was optimized to remain high precipitation strengthening after 100,000 hours, the initial strength at 10 hour is lower than that of alloy A, but it decreases slowly until 1000 hours and then accelerates to certain extent, but is still considerably slower than alloy A, and hence results in a much higher strength level at 100,000 hours comparing to alloy A.

The design exercises clear demonstrate the models capability of designing high temperature resistant steels for a dedicated times and temperatures. To qualitatively compare the model prediction of the time dependent creep strength, experimental results of creep strength of a commercial austenitic creep resistant steel 347H at 923K, are also plotted in fig-

Table 2. *Search ranges of composition (in wt%), austenitisation temperature T_{aus} (in ^oC), service temperature (in ^oC) and different coarsening time (in hours) employed on the design exercise. Optimal compositions of alloys A and B are indicated.*

	C	Cr	Ni	Ti	Mo	Cu	Nb	N	Mn	Si	Fe	T_{aus}	$T_{age}=T_{ser}$	Service/coarsening time
MIN	0,01	15.00	8.00	0,01	0,10	0,01	0,01	0,01	1.00	0.50	Bal.	1000	650	10/100,000
MAX	0,15	25.00	25.00	1.00	3.00	5.00	1.00	0,15	1.00	0.50		1250		
Alloy A	0.041	15.97	21.16	0.20	0.10	0.42	0.39	0.069	1.00	0.50	Bal.	1250	650	10
Alloy B	0.047	16.61	18.97	0.20	0.10	0.26	0.01	0.064	1.00	0.50	Bal.	1217	650	100,000

ure 7 (NRIM Creep Data Sheet, 2001). The experimental data clearly suggests two segments, the first stage is relative flat without much strength loss, while the second stage displays continuously and fast strength losses due to coarsening of strengthening precipitates. The strength degradation formula applied in the alloy design exercise is very capable of capturing this two stage feature and it also well describes the fast degradation stage. A more comprehensive and quantitative justification of the model and the design results will be published elsewhere.

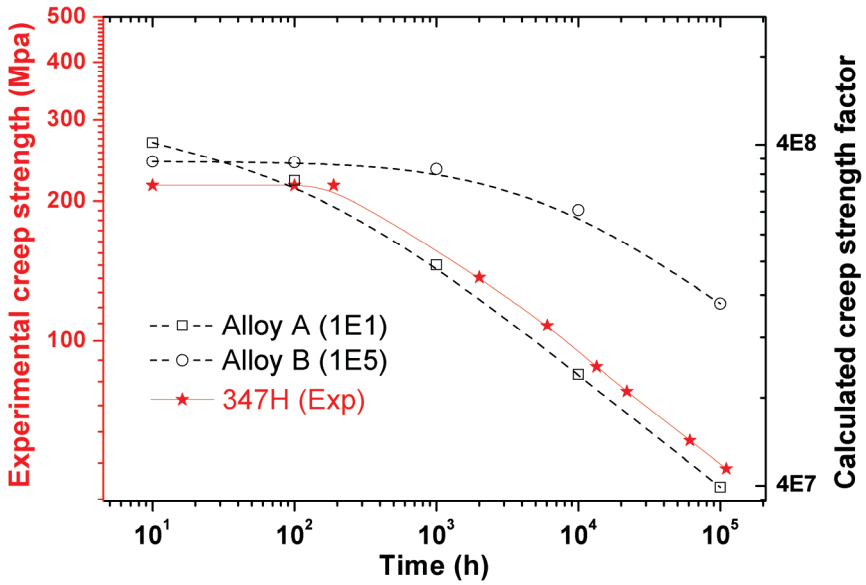

Fig. 7. *Evolution of precipitation strengthening factor as a function of service time at 923K due to coarsening of MX precipitates, for both alloy A (designed for 1E1 hours) and alloy B (designed for 1E5 hours). The experimental observation of strength decrease of austenitic creep resistant steel (347H) utilizing MX carbides is also demonstrated (NRIM Creep Data Sheet, 2001).*

5. DESIGN OF SELF-REINFORCING ABRASION RESISTANCE STEELS

Abrasion resistant steels combining high abrasion resistance, good cold formability and superior impact toughness are in highly demand for applications subjected to harsh abrasive environments, e.g. mining, mineral, and agricultural and earth moving industries etc. Since the abrasion process itself is very complex and abrasion resistance is a (tribo-) system response rather than a material property, it is impossible to derive a simple and general 'translator' function. For a particular family of steel grades (for instance martensitic steels, bainitic steels and multiphase steels) there are some general trends linking for instance a higher hardness to a better abrasion resistance (Wang & Danninger, 2001; Luo & Bai 2010; Wang & Li, 2011), but the relationships are by no means transferable. Hence, a high hardness martensitic steel may have a lower abrasion resistance than a softer multiphase steel grade (Sundstrom, A. et al., 2001; Jha et al., 2003).

Therefore, according to the general design model in figure 1(b), formulating a translator function for the translation of abrasion resistance into the most appropriate microstructures, remains the first and most challenging task, and this is one major difference to previous design applications in UHS stainless and creep resistant steels where the creator, from well defined microstructures to quantifiable metallurgy criteria, is the most difficult step. Although the desirable microstructure can not yet be well established for abrasion resistant steels, a qualitative hypothesis of desirable microstructures could be a balanced microstructure composing of a soft phase, e.g. ferrite and hard components e.g. martensite or bainite, in which the soft phase can provide support and impart compatibility and the hard phase can share the load and resist the destructive action of abrasive particle. In addition to the dual-phase matrix, a considerable amount of retained austenite could further enhance the abrasion resistance, the cold formability and toughness owing to its significant strain hardening capability via the TRIP effect upon abrasion. In such a manner, the relative soft matrix offers good toughness and processibility while the self-reinforcing surface provides superior abrasion resistance. Dedicated experiments are being carried out in order to obtain more detailed insight into the process of material removal during abrasion and most of all to achieve a quantitative description of the desirable microstructure. Once these key microstructural parameters are defined, proper 'creator' functions for specific steel grades may be defined and an alloy optimization cycle involving composition and tailored heat treatments during the steel production can be executed. Fortunately, the microstructure of abrasion resistant steels in itself is time invariant, slightly simplifying the optimization parameters in the 'creator' design.

6. CONCLUSIONS

The paper presents a summary of a reformulated computational alloy design model following the goal/mean design philosophy, based on physical based metallurgical principles and coupled with genetic optimization scheme, which allows the composition and heat treatment conditions to be designed and optimized simultaneously. From design exercises in UHS stainless steels, high temperature resistant steels and abrasion resistant steels, the following general conclusions can be drawn:

1. The developments of 'translator' and 'creator' functions, responsible for the conversion of desired mechanical properties to required microstructure, and the conversion of quantified microstructural parameters to alloy composition and heat treatment parameters are the crucial components in this design approach. Sufficient physical and metallurgical understanding and knowledge is essential to build such translator and creator. Once these 'translator' and 'creator' functions are properly defined, the actual optimization does not require human expert intervention.
2. The model is successfully applied to the design of UHS stainless steels and proven to be able to achieve the exact matrix and intended strengthening precipitates, and the state of the art mechanical properties and corrosion resistance.
3. With a slight modification of the optimization criterion, the model is also capable to take into account the alloying cost as an optimization consideration. The most and least cost efficient alloying element can be identified and hence the properties can be optimized while minimizing the cost.
4. The preliminary design exercise to creep resistant steels has demonstrated its potential to design creep resistant steels for a given conditions of service time and temperature. The calculated creep strength degradation is well capable in capturing the two stage feature observed in real steel grades.
5. Application of the model in advanced abrasion resistant steels design, particularly for a complex phase microstructure employing retained austenite so as to achieve a self-reinforcing gradient abrasion resistant steel, requires further quantitative descriptions of the desirable microstructure before can be converted to quantifiable criteria by corresponding creators. More understanding of precise effects of microstructure characteristics on abrasion resistance are required for developments of both translator and creator.

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STRUKTURA OGÓLNEGO PODEJŚCIA MATERIAŁOWEGO DO PROJEKTOWANIA NOWYCH GATUNKÓW STALI O SPECJALNYCH WŁASNOŚCIACH

Streszczenie

W pracy omówiono metodę projektowania stopów wykorzystującą zasady termodynamiki i kinetyki i stosując algorytmy genetyczne w procedurze optymalizacyjnej. Metoda polega na zastosowaniu dwóch głównych pojęć: translatora i kreatora. Translator jest zamianą wymaganych własności termomechanicznych na wymaganą mikrostrukturę, wykorzystując znane zależności między tymi parametrami. Kreator stosuje ustalone zasady metalurgiczne i zamienia ilościowe parametry mikrostruktury w parametry metalurgiczne i ekonomiczne, tzn. skład chemiczny, parametry obróbki cieplnej i koszty. W przypadku dobrze zdefiniowanych funkcji translatora i kreatora model pozwala na równoczesną optymalizację, z interwencją człowieka,dla składu chemicznego oraz dla parametrów obróbki cieplnej, tzn temperatury austenityzacji i temperatury starzenia. W ten sposób spełnione są różne kryteria projektowania i ostatecznie uzyskiwana jest wymagana mikrostruktura. Podstawowa wersja modelu, która nie definiuje modułów translatora i kreatora w sposób jawny, została zastosowana do projektowania stali nierdzewnych o podwyższonej wytrzymałości (ang. Ultra High Strength - UHS). Otrzymane wyniki zostały zweryfikowane doświadczalnie. Następnie model został rozszerzony i uwzględniono koszt dodatków stopowych poprzez wprowadzenie czynnika kosztów dla różnych pierwiastków stopowych. W ten sposób uzyskano cenne wskazówki dla projektowania i modyfikacji składu chemicznego i możliwość optymalizacji w sposób zintegrowany wytrzymałości materiału i kosztów jego wytwarzania. W niniejszej pracy to podejście zostało dalej uogólnione i stworzono nowe rozszerzenie modelu dla projektowania stali żaroodpornych, stali odpornych na pełzanie w wysokich temperaturach i stali odpornych na zużycie ścierne. Zamieszczone zostały wstępne wyniki uzyskane z nowej wersji modelu.

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