Design of abrasion-resistant alloys using data mining and thermodynamics

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Among different wear-resistant alloys, Stellites (Co-Cr-C alloys) occupy an exceptional place. Yet, their main disadvantage comes from the presence of cobalt, an expensive and strategic element, that is necessary to avoid in any nuclear applications due to the ^{60}Co activation. Several alloys have been developed to replace Stellites, without a real success. In this work, a set of models to predict microstructure, hardness and wear resistance as a function of composition, is created using machine learning and thermodynamics and exploited by a genetic algorithm to design new groups of alloys to replace Stellites. Several so-designed alloys were successfully elaborated (at laboratory scale) and are being tested in different experimental conditions.

Keywords (from 3 to 5 max): Nuclear application, alloy design, machine learning, abrasion-resistant coatings

1. Introduction

In order to prevent the activation of ^{60}Co cobalt particles in the primary circuit of nuclear reactors, it is necessary to replace cobalt-based alloys of the Stellite type, used as abrasion-resistant coatings, with cobalt-free alloys. Several materials, including commercially iron- or nickel-based alloys, have been tested in the past, but none of them has equivalent characteristics to those of Stellites. The objective of this project is to design complex concentrated alloys resistant to abrasion using data mining, thermodynamic models and genetic algorithm optimisation, following a method that has already been applied on other alloy categories [1].

2. Methods

2.1. Data mining models

Using data mining tools, such as pairwise comparison algorithms or Gaussian processes, models could be established to relate alloy composition to various properties like Vickers hardness and abrasion resistance.

2.2. Computational thermodynamic

With the CALPHAD method (Calculation of Phase Diagrams), the microstructure of an alloy can be predicted for a given composition and preparation conditions. Constitution of each phase can also be used to calculate thermodynamic variables such as martensite-start temperature, free chromium content or some processability criteria.

2.3. Alloy design by multi-objective optimisation

The genetic algorithm used in this study is a non-sorting genetic algorithm (adapted from NSGA-II [1]) with multiple objectives and constraints. These criteria are calculated from data mining and thermodynamic models.

3. Results and discussion

Gaussian process models for hardness (Fig.1) and abrasion resistance allow them to be predicted from the composition of an alloy.

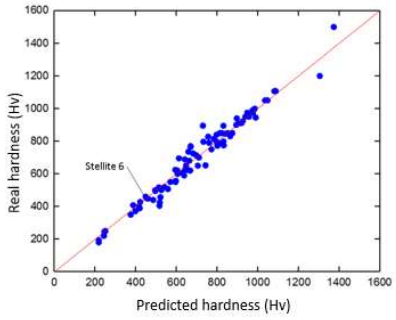

Fig.1 Real hardness as a function of predicted hardness calculated from Gaussian process model.

The comparison of real and predicted microstructures shows that the welding-type deposition processes fairly match to a structure calculated according to the Scheil-Gulliver solidification model. The average composition of the austenite provides information on the content of free chromium - to ensure corrosion resistance - and enables the calculation of empirical quantities such as martensite-start temperature, for which a certain range of values is expected to yield a TRIP effect, which seems beneficial to wear resistance [2].
Different combinations of objectives and constraints have been tested to obtain various types of composition, among which two have been elaborated to be tested.

4. References

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