Engineering Applications of Artificial Intelligence 37 (2015) 103–114

Contents lists available at ScienceDirect

Engineering Applications of Artificial Intelligence

journal homepage: www.elsevier.com/locate/engappai

A new holistic systems approach to the design of heat treated alloy steels using a biologically inspired multi-objective optimisation algorithm

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ARTICLE INFO

Article history:
Received 21 March 2014
Received in revised form
7 August 2014
Accepted 31 August 2014
Available online 29 September 2014

Keywords:
Multi-objective optimisation
Fuzzy modelling
Artificial Immune Algorithm
'Right-First-Time' production of alloy steels

ABSTRACT

The primary objective of this paper is to introduce a new holistic approach to the design of alloy steels based on a biologically inspired multi-objective immune optimisation algorithm. To this aim, a modified population adaptive based immune algorithm (PAIA2) and a multi-stage optimisation procedure are introduced, which facilitate a systematic and integrated fuzzy knowledge extraction process. The extracted (interpretable) fuzzy models are able to fully describe the mechanical properties of the investigated alloy steels. With such knowledge in hand, locating the 'best' processing parameters and the corresponding chemical compositions to achieve certain pre-defined mechanical properties of steels is possible. The research has also enabled to unravel the power of multi-objective optimisation (MOP) for automating and simplifying the design of the heat treated alloy steels and hence to achieve 'right-first-time' production.

1. Introduction

As stated in the Steel Industry Technology Roadmap: Barriers and Pathways for Yield Improvements (Energetics, Inc., 2003) "making the steel and internal products correctly the first time minimises waste oxide generation, in-plant returns and, most importantly, customer rejects". Nearly 1% of all production is returned from the customers because it does not meet certain specifications, and in-house scrap represents another 8 million tons per year that must be reprocessed. Both types of scrap represent significant yield loss since the energy consumed in the production of these is lost (Energetics, Inc., 2003). Faced with increasing competitive markets and economic demands, metal producers are forced to 'rethink' their short and long term strategies when it comes to producing metal in order to meet tighter customers' specification and to more efficiently provide steels with more consistence and higher quality. Therefore, more research work is required to improve microstructure control and reduce defects.

The properties of the end product can be improved mainly through: (a) heat treatment process and, (b) thermomechanical processing. In this paper, we will focus on the first method which involves using specialist heat treatments to develop the required mechanical properties in a range of alloy steels. Traditionally, a heat treatment metallurgist would attempt to balance these factors using their metallurgical knowledge and experience in a bid to obtain the desired mechanical properties. However, due to the increasing complexity of the underlying system, this may still prove difficult even for the metallurgists to tune these parameters. Given the lack of mathematical models which can account for these complex systems and a large amount of available industrial process data associated with the systems, data-driven modelling becomes more and more vital for assisting the metallurgist to predict the mechanical test results without actually doing it. Based on these models, further operations of optimisation of the heat treatment process can also be developed, which is envisaged to be able to automate the steel design process and reduce the experimental costs (Chen, 2009).

Abbreviations: Abs, antibodies; AIS, artificial immune systems; Al, aluminium; BEP, back-error-propagation; C, Carbon; Cr, chromium; FRBS, fuzzy rule-based systems; IMOFM, an immune inspired multi-objective fuzzy modelling approach; Mn, manganese; Mo, molybdenum; MOP, multi-objective optimisation problems; Ni, nickel; PAIA2, a modified population adaptive immune algorithm; RMSE, root mean square error; ROA, reduction of area; *S*, Sulphur; Si, silicon; UTS, ultimate tensile strength; V, vanadium

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http://dx.doi.org/10.1016/j.engappai.2014.08.014
0952-1976/

In the light of the above considerations, finding out a suitable optimisation framework, which is more flexible to accommodate multiple objectives and more effective in search towards the new optimal design methodology is key to steel design. A more holistic framework is proposed to deal with these problems, which is based upon a modified Population Adaptive Immune Algorithm (PAIA2) (Chen, 2009; Chen and Mahfouf, 2006). An Immune inspired Multi-Objective Fuzzy Modelling (IMOFM) approach (Chen and Mahfouf, 2012) for prediction of steel properties is also devised based on PAIA2. The elicited mechanical property models are then incorporated into the framework of PAIA2 to automate and simplify the design of the heat treated alloy steels. The overarching aim of this research is to unravel the powers of multi-objective optimisation for automating and simplifying the design of the alloy steels and hence to achieve 'right-first-time' production. The work was part of the research activities which were previously carried out in the Institute for Microstructural and Mechanical Process Engineering: The University of Sheffield (IMMPETUS).

The paper is organised as follows: Section 2 introduces PAIA2, which gives the basis and framework for further alloy design tasks; also in this section, PAIA2 is applied to multi-objective fuzzy modelling for prediction of steel properties; Section 3 is devoted to the optimal design of heat treated alloy steels in a multi-objective optimisation sense; experimental results relating to the prediction of mechanical properties, such as Ultimate Tensile Strength (UTS) and Reduction of Area (ROA) of the end product, are presented; with such a knowledge and PAIA2 in hand, simultaneous optimisation of several conflicting objectives, such as the strength, the ductility of steels and the costs of the heat treatment process, is carried out; finally, discussions and conclusions are given in Section 4.

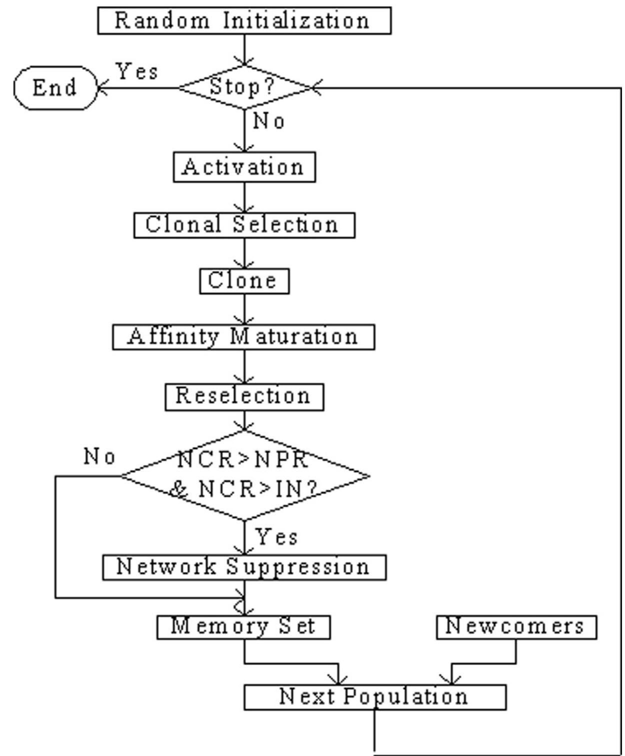

Fig. 1. Main stage of PAIA2 for MOP solving (NCR: the number of current non-dominated Abs; NPR: the number of non-dominated Abs in the last iteration; IN: the initial Abs size; Stop: at least one iteration step is executed).

2. Bio-inspired multi-objective optimisation and modelling

The increasing interest in applying biological inspired optimisation to real engineering problems lies in the fact that the apparently simple structures and organizations in nature are capable of dealing with most complex systems and tasks with relative ease. Compared to classical optimisation techniques which aim at exact optimal solutions, bio-inspired (heuristic) search methods propose instead to locate the near optimal solutions and do not rely on availability of analytical models. The flexible structure of such a search mechanism can not only handle different knowledge representations in a single framework, but can also provide pragmatic solutions in a more efficient way. Given the fact that optimal alloy design problem requires different types of models to fully describe the whole process and is more often than not of a multi-objective nature, a heuristic search method represents a salient tactic to fuse different models and produce Pareto solutions. Among many biological optimisation paradigms, Artificial Immune Systems (AIS), as a relatively new research area dating back to Farmer and Packard (1986)'s paper, lends itself to represent a viable candidate to the problems investigated in this paper for its more flexible structure and enhanced search power.

2.1. A modified population adaptive immune algorithm (PAIA2)

In (Chen, 2009; Chen and Mahfouf, 2006), Chen and Mahfouf proposed a modified Population Adaptive Immune Algorithm (PAIA2) for Multi-objective Optimisation Problems (MOP). The algorithm is the synthesis of the four human immune metaphors for the creation of novel solutions to real world problems, which are the Clonal Selection Principle (Burnet, 1959); the Network Hypothesis (Jerne, 1974; Perelson, 1989); the adaptive antibody's concentration (Chen and Mahfouf, 2006), and the vaccination and the secondary response (Chen and Mahfouf, 2006). The main stages of PAIA2 are shown in Fig. 1.

Two types of fitness evaluation methods (Activation) are used in PAIA2 so that the algorithm receives environmental information from both the objective space (through non-dominated sorting) and the decision variables space (through the distance measured in the variable space between the two chosen solutions). Such information combined with the density information in the decision variable space provides adequate selective pressure to effectively advocate the most promising and evenly distributed solutions into the next iteration. On the one hand, the Clonal Selection and Clone prefer good solutions by providing them with more chances to be cloned so that they always dominate the whole population. On the other hand, the Clone itself contributes significantly to the diversity of the population. Affinity Maturation includes hypermutation, receptor editing and recombination. The former two increase the diversity of the population so that more objective landscape can be explored. The hypermutation rate of the cloned solutions decreases when the optimization process evolves so that a more focused search is introduced in the later iterations. This decreasing rate can be controlled through a predefined Dirac's parameter. The Simulated Binary Crossover (SBX) (Deb and Agrawal, 1994) is utilised as the recombination operator which efficiently uses the information contained in the solutions so that fine search can be executed in the late stage of the optimization. Reselection ensures that good mutants are inserted into the memory set and bad solutions *apoptosis*. Network Suppression regulates the population so that it is adaptive to the search process. Newcomers are used to further increase the diversity of population. For more details of the implementation of PAIA2, readers are referred to (Chen, 2009; Chen and Mahfouf, 2006).

As argued in (Chen, 2009, ch. 3), an ineffective search could be introduced in the MOP context due to many search attempts being