Neighborhood Hybrid Structure for the Optimization of Mechanical Properties of a Microalloyed Steel Based on its Chemical Composition

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Abstract

This article presents the Iterated Local Search Algorithm (ILS) heuristic with a neighborhood hybrid structure, composed of four different types of adjacent structures. Their effectiveness was evaluated to maximize the microalloyed steels mechanical strength. Tests show that ILS using a hybrid structure has better mechanical strength for the micralloyed steel due to its chemical composition.

1. Introduction

The ultra-high strength steels (UHS) have a very complex microstructure due to several processes involved, including the thermomechanical and heat treatment, which increases the cost. Similar behavior has been found in high strength low alloys (HSLA), which are known as micro alloyed steels. This has made it important to use alternative tools to enable prediction of properties of these steels based on various microstructural parameters. Some studies attempting to obtain a nearly optimal resistance have relied on optimization methods. In [1], [2] and [3], a genetic algorithm is used that is based on chemical composition, which considers 13 steel alloys: C, Cr, Ni, Ti, Mo, Al, Cu, Co, Nb, N, V, Mn and Si. The design and development of the alloys was performed on a computer using optimization criteria based on the principles of thermodynamics, kinetics and mechanics.

The Neighborhood heuristic search techniques have proven to be very efficient in finding solutions. The size and structure are the essence of a good neighborhood structure [4]. The greater the size of the neighborhood, the better the quality will be of the local optimal solutions, as well as the precision of the final solution.

In [5], a comparative analysis of a group of adjacent structures is presented, including a hybrid structure. This structure promotes better exploration and exploitation of the solution space for the Traveling Salesman problem. After testing this Neighborhood Hybrid Structure, experimental results show its improved efficiency over other proposed structures, while maintaining competitive effectiveness.

Hybrid structures have been used in various optimization problems [5], [6], but there has not been an investigation using hybrid structures with the ILS algorithm for the problem of maximizing the microalloyed steel's strength.

The contribution of this paper is the following: when using ILS, the theoretical strength as compared with the experimental strength in the laboratory is improved.

This article is composed of six sections: the introduction, the problem definition, the development of local search iterated, the neighborhood structure, the experimental results using ILS and future work, and finally, the conclusions drawn in this research.

2. The Problem Definition

The microalloyed steels have been positioned as an important class of high-strength structural materials because they have had a major expansion in development and production. The development of these steels includes alloy design, processing and applications. Their development and research span the last four decades, making them indispensable for structural applications [7].

Their ability to respond and obtain final mechanical properties required in engineering applications through controlled rolling and accelerated cooling hot, eliminates the need for costly heat treatment. The yield-strength efforts that can be obtained are between 550 and 660 MPa in order to increase 0.01% of certain elements which are considered microalloying. These elements, Nb, V and Ti, are strong-forming micro-particles (precipitates) carbonitrides with low cost. They significantly increase the strength of steel and are a feature of most of microalloyed steels.

A discovery which allowed a better understanding of physical metallurgy involved in this type of steel, and the role that microalloying plays, was reported by Petch [8]. His early research revealed that it was mainly the formation of fine carbides/nitrides which provided grain refinement. He also studied the role performed by its precipitation. Based on his work, the microalloying elements V, Nb and Ti were established as the most convenient and favorable. For most microalloyed steels, a fine grain size of ferrite provides the greatest contribution in terms of strength requirements. Each of the microalloying elements is capable of inducing the refinement of grain size. Another important role of these microalloying elements is their marked increase in mechanical strength due to precipitation. The most effective hardening is caused by the formation of fine carbides/carbonitrides during or immediately after austenitization of the ferrite. In microalloyed steels, the increase in the tension of precipitation can be substantial, despite the relatively low volume fraction due to the sizes of the fine particles which are often less than 10 nm.

In most steels, V is more soluble than Nb, even when the N content is higher. However, V is the most versatile in precipitation, able to be effective in steels with very different compositions. Often, the addition of multiple microalloying elements has a greater effect on the properties of steel than the sum of the individual effects of every one [8].

Upon analysis of some features of the microalloyed steels, agreement was reached to focus only on the chemical composition of these steels (in order to achieve a grain size and a certain amount of precipitates with microalloying). Another reason for the agreement was the measurement of the steel's strength; only one of the existing computational methods had been applied, Genetic Algorithm. However ILS, when applied, was able to obtain a nearly optimal solution with regard to the steel's strength.

The chemical composition used, as shown in Table 1, is based on typical microalloyed steel for transport of hydrocarbons. From this composition, the weight % of the elements of C through V is randomly generated, while maintaining the remaining elements constant.

Table 1. Chemical composition of the elements in steel (weight %)

Fe	C	Cr	Cu	Mn	Mo	Ni	V	N	Nb	Ti	P	S	Si
98.9	0	0	0	0	0	0	0	0.001	0.001	0.001	0.013	0.002	0.3
0	0.02	0.02	0.2	0.8	0.008	0.02	0	0.001	0	0	0.013	0.002	0.1
98.9	0.08	0.1	0.6	1.2	0.03	0.1	0.15	0.008	0.06	0.02	0.013	0.002	0.3

To obtain the objective function, it was necessary to use the following microstructures as a base:

Microstructures of acicular ferrite and bainitics

These microstructures are based on low alloy steels with high strength: bainitic structural steels, tempered steels, and aus-alloy steels [2]. These steels are used in large sections of pressure vessels and in piping. Bainitic and acicular structures are also found generated in welds and heat affected zones. There have been many measurements of its properties, but little success relating those properties quantitatively to its microstructure. This is the opposite for steels with ferritic-pearlitic structures.

The yield stress

Due to the continuous yield point of these structures, the yield stress σ_y usually refers to 0.2% of the testing effort. The main mechanisms for resistance are due to grain size, dislocation, dispersion of carbides and solid solution. It is well known [9] that the tensile strength increases linearly as the transformation temperature descends, due to the relationship between yield stress/tensile stress, which is approximately 0.7 [9]. The transition temperature is linearly related to the steel composition [10], therefore a linear equation (Eq. 1) can be used to approximate the σ_y:

$$\sigma_y = 170 + 1300(\text{wt.\%C}) + 160(\text{wt.\%Mn}) + 160(\text{wt.\%Cr}) + 130(\text{wt.\%Mo}) + 88(\text{wt.\%Ni}) + 45(\text{wt.\%Cu}) + 270(\text{wt.\%V}) \qquad \text{(Equation 1)}$$

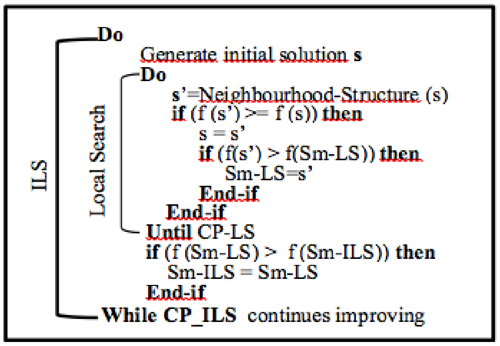
This equation gives the yield stress, which is used as the objective function in this research. The objective function (Eq. 1) is empirical, having determined implicitly the grain size and the amount of precipitates. The solutions obtained with this equation serve as a basis for comparison for the computational structures that comprise a neighborhood structure. By using this equation, we can determine the most ideal neighborhood structure to apply with ILS.

3. Iterated Local Search

For combinatorial optimization problems, very different heuristics methods exist that offer better solutions than are currently available. There is an optimization method called *Iterated Local Search* which is based on a non-deterministic heuristic. In [11], a stochastic local search heuristic is used that iteratively applies local search starting from an initial solution. The initial solution is often randomly generated.

The operation of the local search in the problem of maximizing the mechanical strength in microalloyed steels is the following:

1. Obtain, from the solution space, a steel composition generated stochastically (initial solution *s*). Evaluate *s* with the objective function *f(s)* [4].
2. To the initial solution *s*, apply a perturbation (with some neighborhood structure), which gives rise to a new solution ***s'***. Evaluate the new solution with the objective function *f(s')*.
3. If *f(s') >= f(s)* then $s \leftarrow s'$, otherwise *s* will remain the same.
4. Within the local search, steps 2 and 3 repeat until the stop criterion is met. The criterion is based on the size of the neighborhood defined by the problem.



```
Do
    Generate initial solution s
    Do
        s'=Neighbourhood-Structure (s)
        if (f (s') >= f (s)) then
            s = s'
            if (f(s') > f(Sm-LS)) then
                Sm-LS=s'
            End-if
        End-if
    Until CP-LS
    if (f (Sm-LS) >  f (Sm-ILS)) then
        Sm-ILS = Sm-LS
    End-if
While CP_ILS  continues improving
```

Fig. 1. Iterated Local Search [Cruz-Chávez et al, 2010].

Figure 1 presents the algorithm for ILS, which applies the local search algorithm. It is shown that the local search works iteratively and applies a stop criterion (CP_ILS), which in this case is defined as the average number of iterations obtained when the convergence reaches the value of the objective function. Each iteration of ILS involves the full implementation of a local search, which reaches its stop criterion (CP-LS). ILS [11] allows an escape from local optima, since the algorithm starts with a new randomly generated solution for each iteration.

4. Neighborhood Structures

It is important to understand the problem in order to determine the solution space of the problem, given the problem specifications [12]. This makes it possible to define a solution space with a neighborhood, while firmly maintaining the objective to *maximize.*

The percentages of the elements in the steel are the basis to randomly obtain the first solution. Figure 2 presents a simple example of a neighborhood. The first solution is taken as the starting point ***s***, all solutions that are near that point will be considered in a *neighborhood* represented by a neighborhood structure ***N(s)***, which is represented by a function $N : S \rightarrow 2^S$. The neighborhood size depends on the type of structure which is defined. The solution space in 2D is represented by ***S*** [4] and the starting point is *s*. When another ***s***' is generated to improve the first, it is represented by ***s'***. Thus, the search for a better solution uses neighborhood searches through movement in a function of N(s). Step by step, the solutions improve, each better than the previous one. In this way, the strength of the steel is optimized, according to the Objective Function:

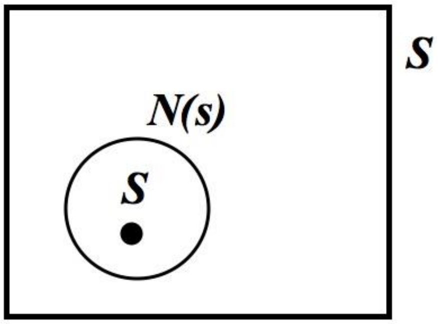


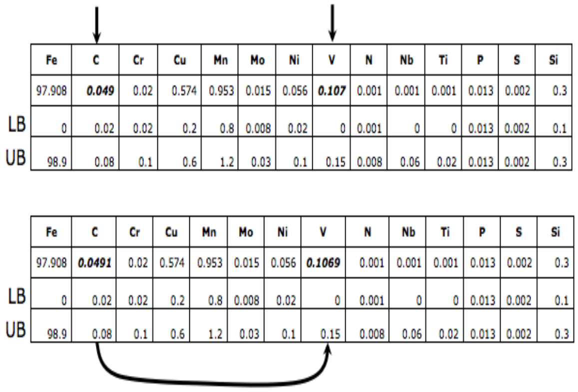
Fig. 2. Representation of a neighborhood structure [Michaelewicz, Z. et al, 2000].

To determine the size of the neighborhood, a perturbation was performed, based on the possible increase (Δ) and decrease (-Δ) of the 7 elements of the microalloyed steel that can vary without harmfully affecting the composition. Fe, which is the element with the highest percentage, contains a range over which the adjustment can be performed. The upper limit of Fe is **98.9** and the lower limit is **0**. The size of the neighborhood is **989,000** and it is obtained by dividing the upper limit by the minimum modification value of **0.0001**.

4.1. Neighborhood Structure using Random Double

For the Random Double neighborhood structure, **s,** an initial feasible solution, is generated. In addition, two random numbers, each one corresponding to a position in the vector that stores the initial solution, are chosen. There are two possible cases:

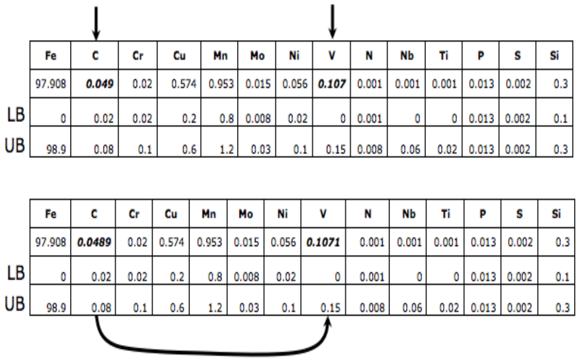
- First case: the first element increases and the second one decreases (Fig. 3).
- Second case: the first element decreases and the second one increases (Fig. 4).



	Fe	C	Cr	Cu	Mn	Mo	Ni	V	N	Nb	Ti	P	S	Si
	97.908	***0.049***	0.02	0.574	0.953	0.015	0.056	***0.107***	0.001	0.001	0.001	0.013	0.002	0.3
LB	0	0.02	0.02	0.2	0.8	0.008	0.02	0	0.001	0	0	0.013	0.002	0.1
UB	98.9	0.08	0.1	0.6	1.2	0.03	0.1	0.15	0.008	0.06	0.02	0.013	0.002	0.3

	Fe	C	Cr	Cu	Mn	Mo	Ni	V	N	Nb	Ti	P	S	Si
	97.908	***0.0491***	0.02	0.574	0.953	0.015	0.056	***0.1069***	0.001	0.001	0.001	0.013	0.002	0.3
LB	0	0.02	0.02	0.2	0.8	0.008	0.02	0	0.001	0	0	0.013	0.002	0.1
UB	98.9	0.08	0.1	0.6	1.2	0.03	0.1	0.15	0.008	0.06	0.02	0.013	0.002	0.3

Fig. 3. Representation of a disturbance in a random neighborhood double structure. First case.



	Fe	C	Cr	Cu	Mn	Mo	Ni	V	N	Nb	Ti	P	S	Si
	97.908	***0.049***	0.02	0.574	0.953	0.015	0.056	***0.107***	0.001	0.001	0.001	0.013	0.002	0.3
LB	0	0.02	0.02	0.2	0.8	0.008	0.02	0	0.001	0	0	0.013	0.002	0.1
UB	98.9	0.08	0.1	0.6	1.2	0.03	0.1	0.15	0.008	0.06	0.02	0.013	0.002	0.3

	Fe	C	Cr	Cu	Mn	Mo	Ni	V	N	Nb	Ti	P	S	Si
	97.908	***0.0489***	0.02	0.574	0.953	0.015	0.056	***0.1071***	0.001	0.001	0.001	0.013	0.002	0.3
LB	0	0.02	0.02	0.2	0.8	0.008	0.02	0	0.001	0	0	0.013	0.002	0.1
UB	98.9	0.08	0.1	0.6	1.2	0.03	0.1	0.15	0.008	0.06	0.02	0.013	0.002	0.3

Fig. 4. Representation of a disturbance in a random neighborhood double structure. Second case

The previously generated random numbers are validated. Not all the components may change in the percentage of their chemical composition. The elements that do change by Δ and -Δ are between C and V, provided that the randomly generated positions are not the same. If this happens again, it is necessary to generate them until they meet the condition.

When the condition is satisfied, a new neighborhood solution ***s'*** is obtained**.** In the case of a Neighborhood Triple, Quadruple and Quintuple, the only difference is that the random numbers generated reflect the number of the neighborhood.

4.2. Neighborhood Hybrid Structure

This neighborhood structure was formed with the four previous ones. A neighborhood structure is randomly selected in each iteration of the ILS (Fig. 5).

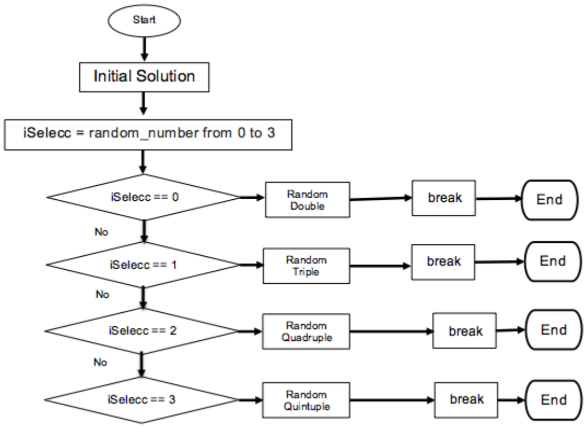


Fig. 5. Flowchart of the Hybrid Structure.

5. Experimental Results

Experimental tests were conducted using a PC with 2.80GHz CPU, 1GB RAM and 160GB HD.

In the tests conducted to evaluate the most efficient neighborhood structure (Random Double, Triple, Quadruple, Quintuple and Hybrid, Figure 6), a stop criterion of **400** for ILS was applied. The local search stop criterion was **989000**, which is the size of the neighborhood. Table 2 presents the results of these tests. The structure that was most effective in obtaining results was the hybrid structure.

This structure was tested with a stop criterion for ILS of 400 and for local. The percentages handled are:

5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90% and 100% from a stop criterion of 989000 (Table 3 and Fig. 7). The best result obtained with the hybrid neighborhood structure was 100%.

Table 2. Results of each of the neighborhood structures. Average of 30 tests of ILS

STRUCTURE	BEST	WORST	BEST AVERAGE	σ AVERAGE
Double	560.7226	560.5687	560.71195	0.038837532
Triple	560.723	559.261	560.7093767	0.041466125
Quadruple	560.7272	560.5694	560.7110967	0.031658928
Quintuple	560.7181	554.7926	560.69919	0.29037762
Hybrid	**562.1482**	**560.5701**	**560.7122467**	0.039025684

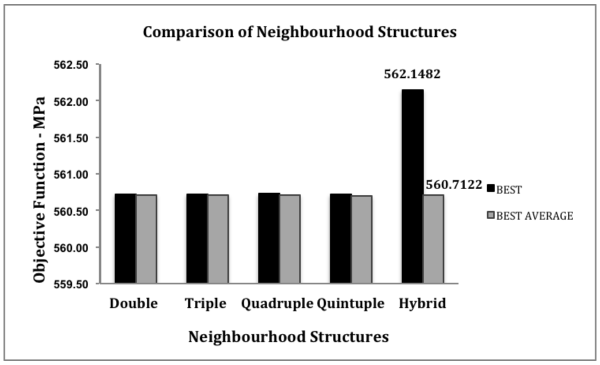


Fig. 6. Results for each neighborhood structure, showing the structure winner.

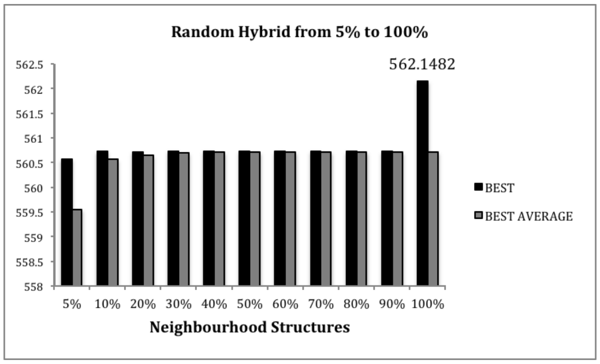


Fig. 7. Comparative results of the random hybrid structure evaluated from 5% to 100%

The best resistance obtained with ILS was 562.1482MPa, which corresponds to the best chemical composition % wt. of the solution s, which is presented in Table 4. The experimental result obtained from a similar microalloyed steel reported in [13], [14] was **490 ± 15**MPa. This indicates that the theoretical resistance based on their composition is 12.84% higher than that experimentally obtained.

Table 3. Random hybrid results with proof from 5% to 100%

STRUCTURE	BEST	WORST	BEST AVERAGE	σ AVERAGE
Hybrid 5%	560.5685	**540.5428**	559.5534767	1.332514519
Hybrid 10%	560.7272	544.0187	560.56363	1.355543374
Hybrid 20%	560.7178	547.6995	560.6444533	0.730190119
Hybrid 30%	**560.7346**	559.7758	560.6943067	0.248209605
Hybrid 40%	560.733	554.9217	560.7091967	0.16541446
Hybrid 50%	560.7333	559.1024	560.7089333	0.054319031
Hybrid 60%	560.727	560.569	560.7116867	0.030341118
Hybrid 70%	**560.7346**	560.5694	560.7120367	0.031377934
Hybrid 80%	560.7247	560.5698	**560.71228**	0.036617864
Hybrid 90%	560.7212	560.57	560.7114067	0.031654708
Hybrid 100%	**562.1482**	560.5701	560.7122467	0.039025684

Table 4. Best composition obtained with ILS

Element	%
Fe:	97.4223
C:	0.08
Cr:	0.1
Cu:	0.6
Mn:	1.1999
Mo:	0.03
Ni:	0.0999
V:	0.1499
N:	0.001
Nb:	0.001
Ti:	0.001
P:	0.013
S:	0.002
Si:	0.3

Future Work

Future work involves finding a way to experimentally calculate the strength of steel with the composition obtained theoretically (Table 4). Work can be done on the application of the neighborhood hybrid structure in some other metaheuristics, such as genetic, under a Grid environment. Additional work could involve improving the objective function of the problem to maximize the mechanical strength of a microalloyed steel including a larger number of explicit variables such as grain size, the amount of precipitates, and the chemical composition of steel.

6. Conclusions

Neighborhood hybrid structure proved to be the most qualified in ILS to apply to the problem of maximizing the strength of microalloyed steels. The resistance obtained with ILS, turned out to be better than that obtained experimentally in the laboratory.

7. References

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