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MULTIPLE REGRESSION MODELING THE CHEMICAL COMPOSITION EFFECTS ON THE TENSILE STRENGTH OF Ni-BASED SUPERALLOYS

Abstract. *Based on the previously obtained results of the Data Mining - based Classification and Regression Trees (C&RT) technique application to industrial Ni-based superalloys, multiple regression models were developed to describe quantitatively the chemical composition effects on the alloys tensile strength. The regression models obtained were verified for adequacy in three ways, contrary to the conventional approach requiring only several inadequacy variance values calculations. Namely, the following verification methods were applied: traditional R2 coefficient calculations; comparisons of computer and experimental frequency distributions of the quality indexes; Monte-Carlo simulated and experimental data based scatter plots comparing. It was emphasized that, according to the general statistic principle, close coincidence of the Monte-Carlo simulated and real frequency distributions of any measured characteristic values means full formal (statistical) identity of the real and simulated objects. Hence, in addition, coincidence of the corresponding scatter plots statistical parameters should be considered as a sign of the physical identity of real and modeled regression dependencies. All the applied verification methods show the excellent results that leads to conclusion about high workability of the obtained models in practical and theoretical applications. An additional general advantage of the models was noted: their physically interpretable structure, that provides the opportunity to determine and analyze the effects of individual chemical elements and their interactions under real industrial conditions. Most of the obtained results and the formulated conclusions, especially related to the chemical elements individual effects are in good accordance with the known experimental and theoretic data for polycrystalline Ni-based superalloys. Meantime, some unexpected features, particularly, for the interactions of Nb, Ti, Cu with each other and grain boundaries were revealed, showing necessity of further in dept investigations.*

Keywords: industrial Ni-based superalloys; tensile strength; chemical composition; multiple regression models; chemical elements interaction

Problem formulation

Chemical composition of superalloys determines their service behavior in many aspects [1, 2]. At first it defines nominal levels of the mechanical properties to meet the service requirements. On the other hand, some features of the composition may cause various types of embrittlement [3]. The basic reason of the embrittlement for the most modern engineering materials of the industrial quality is uncontrolled chemical elements interactions with each other and microstructure components. The risk of the embrittlements radically increases with the composition complexity and cannot be predicted theoretically by now due to the well known unresolved “many body” problem [4]. Moreover, the modern, increasingly used manufacturing technologies, such as single crystal formation, 3-D printing, sintering,

super fast cooling etc. do not provide full unlading the embrittlement problems [3; 5; 6]. Besides, industrial manufacturing environment inevitably complicate the elimination of the embrittlement events for industrial products, even if the problem will be solved for the laboratory conditions. So, conducting investigations is objectively necessary, which aimed to specify basic features of the chemical element common and separate effects on the performance indexes for industrial products, namely under real industrial manufacturing conditions. As it was shown in some researches [7; 8], the industrial data based modern computer aided combined statistical investigations are, probably, by now, the most effective way to approach solving the embrittment problems.

Aim of the article

Proceeding from the above, the aim of the article is to obtain quantitative relations characterizing effects of the chemical elements in the industrial Ni-based superalloys on their tensile properties based on the early obtained results of the Data Mining investigations.

Breif recent relevant publications overview

Quantitative relations of the chemical elements concentrations with mechanical properties characteristics for industrial alloys are obtained now as a rule by means of the traditional statistical investigations. The main reason of such passive investigation approach predominant application is minimizing the currently used manufacturing technology disturbances as well as – the research project expenses, compared with the active one [9]. However, according to the traditional statistical investigation practices, as more as possible independent statistical variables are tried to be included into the analysis or – only some of them, subjectively chosen by a researcher among the existing technological parameters. Practically in all such cases, inadequate results are obtained, especially for complex, multi element alloys [7; 8; 11]. The main reasons of the situation, are incorrect statistical analysis techniques application, when all chemical element concentrations are changed and analyzed simultaneously in an alloy as well as – human factor.

As a typical example of the inadequate results of the traditional statistical regression analysis researches is the boron influence on the strength of ASTM A514 steel [8]. According to the results, boron has no statistically significant effects on the yield stress (YS) and ultimate tensile stress (UTS) of the steel, that was in accordance with the corresponding controversial experimental data [10]. Meanwhile, the correctly conducted research [8; 11] based on the C&RT Data Mining approach results, showed, the statistically and experimentally justified, strong dependence of the boron effect on vanadium concentration, exceeding critical value of which changes the boron effect from strengthening to softening one. The analogous interactions of such chemical elements as Al and N in ASTM A516 steel were also revealed and analyzed [11]. Evidently, the traditional statistical treatment of the corresponding raw industrial data without taking into account the elements interactions leads to the averaged zero summarizing effect.

So, the statistical regression analysis researches [7; 8; 11] conducted based on the results of the C&RT Data Mining technique application, show the high effectiveness of the approaches combination in specifying the chemical elements effects on the mechanical properties of multi element industrial engineering alloys. Just the same approaches combination is applied in current work to obtain quantitative regression models for the chemical element effects on the tensile strength for Ni-based industrial superalloys.

Materials and Methods

Researches were conducted based on the results of early performed C&RT Data Mining investigations [12], with the use the same experimental data. Employing the early obtained "dendrograms" for YS and UTS of the considered superalloys [12], multiple regression modeling approach was applied with the use of the "Statistica-10" computer software[13]. The adequacy of the obtained models were verified in three ways. The first one was to calculate the conventional R^2 – coefficient within the frame of the regression analysis conducted. The second and third ways includes Monte-Carlo simulations [14] to calculate: YS and UTS frequency distributions (2-nd way) and the pair scatter plots (3-rd way) for the index dependences on each statistically valuable chemical element with final comparing all the corresponding simulation and experimental results. It should be noted that combination of the later verification ways, according to basic principles of the mathematical statistics, provides, contrary the conventional one (R^2 – coefficient calculations), the exhaustive mathematical description of any measured physical quantity. Due to that, the corresponding regression models may also be used to analyze the corresponding chemical element interactions relevant to the property characteristics under real industrial manufacturing conditions. That is why, the 3-way verified regression models may be considered as able to predict not only the indexes values under the element required concentrations but also – to determine the features of the various chemical element interactions under industrial manufacturing conditions.

Results and Discussion

The regression models, obtained in the work for YS and UTS of the industrial Ni-based superalloys are as follows:

$$YS = 354 + 2\,Ti + 3.4\,TiB - 0.08\,TiBCu, \qquad (1)$$

$$UTS = 900 + 148Cu - 52Nb - 0.26NiCu - \\ -0.58CuCr + 0.35CuFe + 0.09NiNb + 0.15CuNb - \\ -0.11CuTi + 11 \cdot 10^{-4} NiCuCr - 2 \cdot 10^{-3} CuCrFe, \quad (2)$$

where $Ti = C_{Ti} \cdot 100; B = C_B \cdot 1000; Cu = C_{Cu} \cdot 100;$
$Nb = C_{Nb} \cdot 100;\ Cr = C_{Cr} \cdot 10; Ni = C_{Ni} \cdot 10;$
$Fe = C_{Fe} \cdot 10,$

where $C_{Ti};\ C_B;\ C_{Cu}; C_{Nb}; C_{Cr};\ C_{Ni};\ C_{Fe}$ – concentration of the corresponding chemical element in an alloy in wt %.

Calculated values of the R^2 coefficient for the above regression models are $R^2 \approx 0.98$ and $R^2 \approx 0.99$, respectively, that corresponds to high adequacy of each model (1) and (2) according to the conventional estimation technique [13]. Comparing the simulated and experimental data based frequency distributions for the investigated alloys YS is shown on Fig. 1.

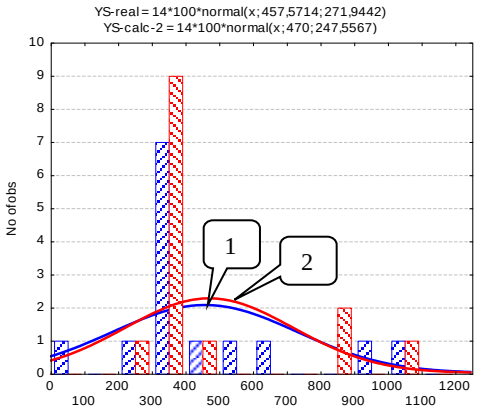

Figure 1 – Experimental (1) and computer simulated (2) frequency distributions for YS of Ni-based superalloys of various chemical compositions

Practically full coincidence of the computer and real experiments results is seen that means the obtained model provides exhausted formal description of the quantity from point of view of mathematics and agrees to the above conclusion concerning the regression models adequacy. Practically the same situation is observed and the conclusions should be made for the experimental and simulated frequency distributions for UTS of the researched superalloys (see Fig. 2).

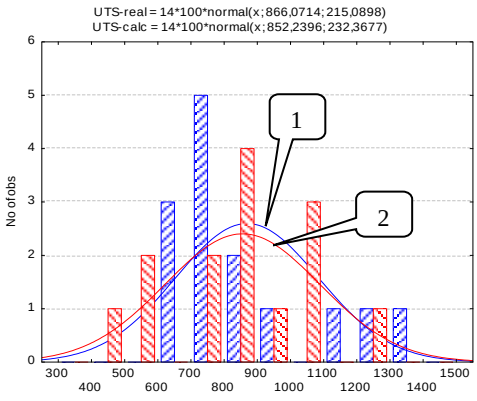

Figure 2 – Experimental (1) and computer simulated (2) frequency distributions for UTS of Ni-based superalloys of various chemical compositions

An additional testing the adequacy, from practical and physical points of view, was performed by comparing the pair scatter plots and their corresponding characteristics for typically considered regression dependences of the performance indexes on the relevant chemical element concentrations. As it known, such scatter plots are obtained under the conditions of simultaneous variations of all chemical elements concentrations and reflect therefore the elements common effects on the investigated characteristics. As it seen from the plots obtained for YS (see Fig. 3), the lines of the computer simulated average YS levels concentration dependences for all chemical elements are practically coincide with the experimental lines or layout within the corresponding 95 % confidence limits.

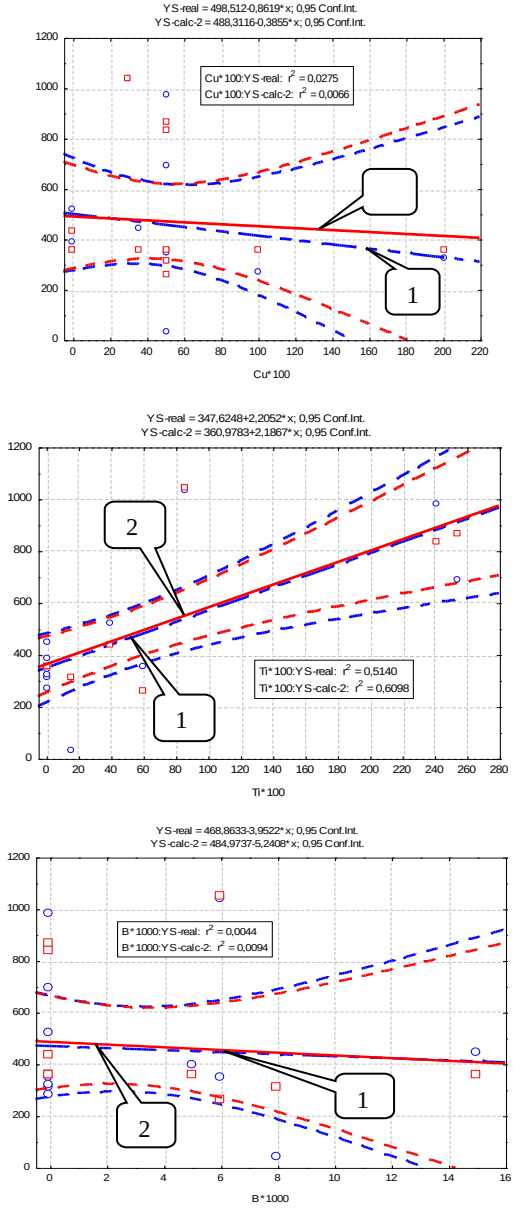

Figure 3 – Experimental data based (1) and computer simulated (2) scatter plots together with the traditional pair regression dependencies for the various chemical elements effect under their joint action on YS of Ni-based superalloys

These results may be considered as not only as confirmation of the regression models adequacy but, moreover, as a demonstration of their high workability in the fields of practical forecasting the YS values for a specific alloy as well as revealing the included chemical elements interactions.

As to the simulated UTS concentration dependencies (see Fig. 4), the conclusions analogous to the above ones may be deduced from the most of the scatter plots. An exclusion is the plot showing the effect of Nb on UTS where the regression line passes the 95 % low confidence limit at certain Nb concentration exceeding.

It is well known that all data points lying within the confidence limits have to be considered as randomly changed ones in respect to the average levels and vise versa – the data liying out the confidence interval are influenced by nonrandom acting factors. So, the following general conclusion may be formulated: Nb has statistically valuable effect on UTS of superalloys, which is in the significant dependence on the other revealed chemical element concentrations in the superalloys. It is in accordance with the form of the regression model (2), which shows the Nb direct interaction with Cu and Ni.

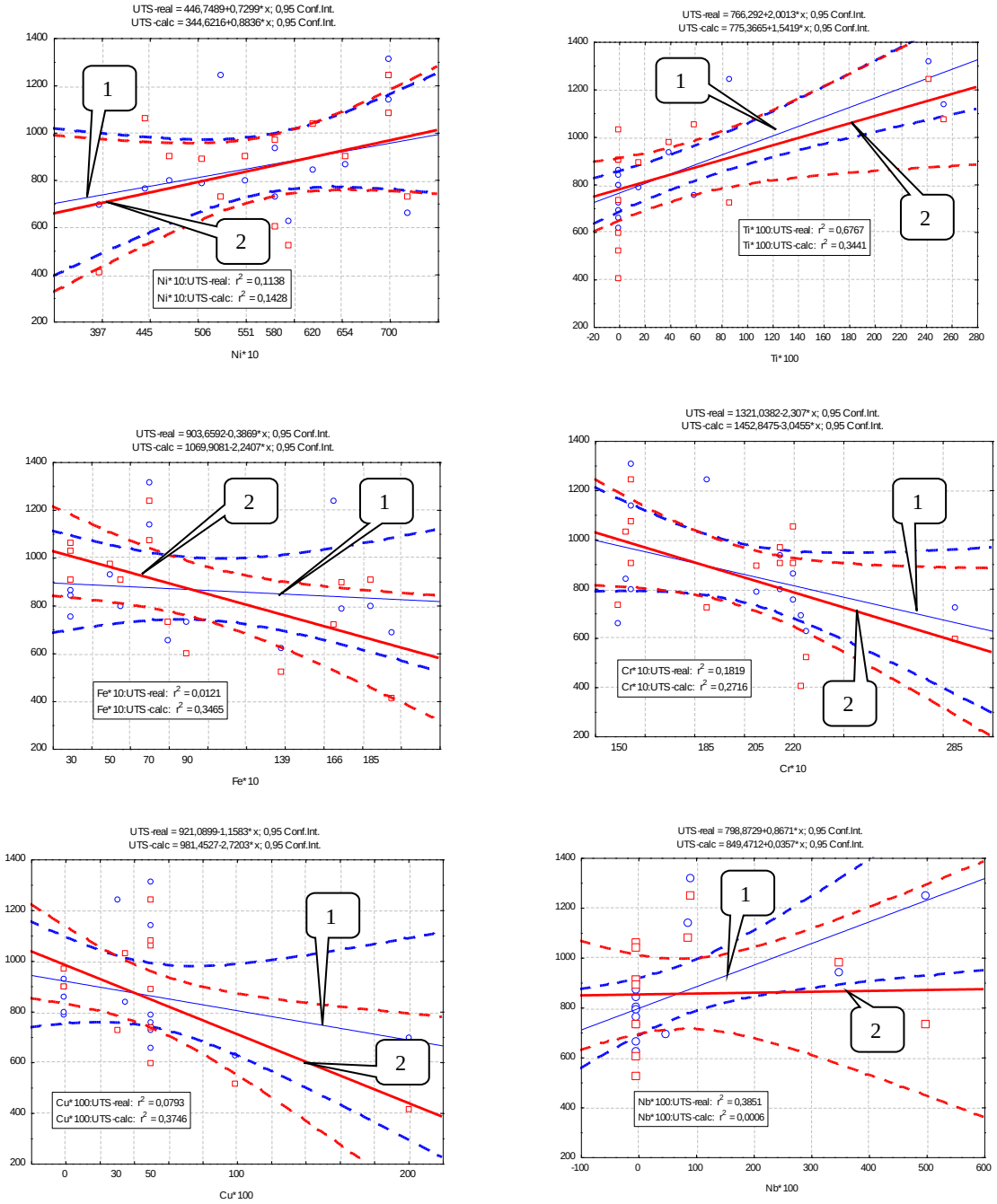

Figure 4 – Experimental data based (1) and computer simulated (2) scatter plots with the traditional pair regression dependencies for the various chemical elements effect under their joint action on UTS of Ni-based superalloys

Taking into account the basic feature of the Nb behavior in austenitic policrystals as the grain boundary segregating chemical element, its interaction with Cu, also forming the segregations, may be explained. In turn, the revealed by the model (2) interactions Cu, Ti and Nb may be qualitatively explained by complex common action (synergetic effects) of the elements and the grain boundaries. Surely the phenomena described require additional thorough investigations.

It is important to emphasize that despite the low determination coefficient R^2 values for the most obtained, experimental data based and the simulated pair scatter plots shown in Fig. 3 and 4, the investigated chemical elements in reality (see eqs. (1) and (2)) provide statistically valuable, considerable effects on the strength of researched superalloys, that cannot be revealed by the traditional regression analysis. Besides, considerable individual effects of some chemical elements such as Ti, shown by the traditional regression analysis (see Fig. 4), according to the developed models, are results of Ti interactions with the other elements in superalloys.

Finally, some common features should be noted for the regression models obtained, that provide their advantages against the early developed ones:

– Usage of only statistically grounded independent variables objectively chosen by the Data Mining technique application;

– Physically interpretable model structures due to the use of only sole independent variables together with their pair and triple multiplicands excluding high degree, having no physical meaning, terms in the models;

– High models adequacy and workability, evaluated, respectively, by the traditional regression analysis and Monte-Carlo techniques application;

– Universal, informal character of the models that provides quantitative, high precision forecasting the controlled characteristic values together with revealing possible synergetic effects, basics of the responsible physical mechanisms of the elements joint action and further in dept investigation directions.

Conclusion

1. Mathematic models were developed for the chemical composition effects on the tensile strength of Ni-based superalloys by applying the computer aided multiple regression analysis technique based on the preliminary Data Mining computer technology employing results.

2. High models adequacy and workability were shown by applying the traditional regression analysis and Monte-Carlo techniques, respectively.

3. Physically interpretable model structures were emphasized, that provide an opportunity to reveal: possible synergetic effects, basics of the responsible physical mechanisms of the elements joint action and further in dept investigation directions.

4. Ability was shown for the developed multiple regression models to predict real effects of the chemical composition as a whole on the properties of industrial multi-element metallic materials, despite of un-revealing the most traditional pair regression dependencies.

5. Complex interactions of Nb, Ti, Cu with each other and grain boundaries in FCC polycrystalline Ni-based superalloys was shown, that requires further in dept investigations.

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МОДЕЛЮВАННЯ ВПЛИВУ ХІМІЧНОГО СКЛАДУ СУПЕРСПЛАВІВ НА БАЗІ НІКЕЛЮ НА ПОКАЗНИКИ ЇХНЬОЇ МІЦНОСТІ ПРИ РОЗТЯГНЕННІ МЕТОДАМИ МНОЖИННОЇ РЕГРЕСІЇ

Анотація. *Базуючись на раніше отриманих результатах застосування однієї з технологій Data Mining-методики Дерев Класіфікації та Регресії (C&RT) до промислових суперсплавів на базі Ni, розроблено множинні регресійні моделі задля кількісної характеристики впливу хімічного складу на міцність таких сплавів при розтягненні. Адекватність отриманих моделей було перевірено трьома способами, на відміну від відомого підходу, що вимагає розрахунків тільки декількох значень дисперсії неадекватності. А саме застосовано такі методи перевірки: традиційні розрахунки коефіцієнта R2; порівняння комп'ютерних та експериментальних частотних розподілів значень контрольних показників якості; порівняння симульованих методами Монте-Карло та експериментальних діаграм розсіювання контрольних показників. Підкреслено, що згідно з загальними принципами математичної статистики, тісний збіг Монте-Карло симульованих та реальних частотних розподілень значень будь-якої характеристики, що вимірюється, відповідає повній формальній (статистичній) ідентичності реального та модельного об'єктів. Звідси додатково випливає, що збіг статистичних параметрів відповідних діаграм розсіювання слід розглядати як ознаку фізичної ідентичності реальних та модельованих регресійних залежностей. Всі застосовані згадані вище методи перевірки показали високі результати, що приводить до висновку про високу працездатність отриманих моделей задля практичного та теоретичного застосування. Відзначено додаткову загальну перевагу вказаних моделей: їх придатну до фізичної інтерпретації математичну побудову, що надає можливість визначати й аналізувати впливи окремих хімічних елементів та їх взаємодії на контрольні показники за реальних промислових умов. Більшість отриманих в роботі результатів і сформульованих висновків добре узгоджуються з відомими експериментальними та теоретичними даними. Водночас виявлено деякі неочікувані особливості, зокрема взаємодії Nb, Ti, Cu між собою та межами зерен, що свідчить про необхідність подальших поглиблених досліджень.*

Ключові слова: промислові суперсплави на базі Ni; показники міцності при розтягненні; хімічний склад; множинні регресійні моделі; взаємодія хімічних елементів

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