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REVEALING SIGNIFICANT CHEMICAL COMPOSITION EFFECTS ON THE SUPER ALLOYS PERFORMANCE BY DATA MINING TECHNIQUES APPLICATION

Abstract. *Based on the early developed integrated investigation approach combining mutually consistent computer aided: statistical exploratory techniques, multiple regression models development, Monte-Carlo simulations and multipurpose manufacturing technology parameters optimization, computer statistical investigations of chemical composition effects on some basic performance characteristics of modern industrial superalloys (SAs) were conducted. According to the developed approach, the Data Mining-based C&RT statistical technology was used in the current work as the first stage of the further analysis. An important feature of the developed approach to the "passive experimentation" in general and the applied technique in particular was emphasized as both providing minimal investigation expanses, as compared to the "active" one and so having no alternative in free market economic conditions. As the stage primary results, the dendrograms were constructed providing the following statistically grounded visual information for each SAs controlled performance index: – a full list of statistically significant chemical elements; allowable variants of the elements combinations; limits of the chemical element concentration intervals spillover of which provides changes in the chemical elements combinations; variation tendencies for the control indexes within the revealed concentration intervals. Interactions of the most of the chemical elements comprised by SAs in their effects on the investigated performance indexes were shown. High effectiveness of the obtained dendrograms application to reveal individual and mutual chemical element effects on the multi element alloys performance together with uniqueness of such an information for industrial alloys were emphasized. Some prospect possibilities were noted for the obtained dendrograms application: - as a first stage of a multi-parameter process analysis in industrial conditions, – a ground stage of the multiple regression models further development and final multipurpose technological processes optimization conducting.*

Keywords: industrial superalloys; chemical compositions; computer statistical investigations; performance indexes; Data Mining techniques; dendrograms

Problem formulation

Super alloys (SAs) belong to the basic group of modern materials aimed to be used under mechanical loading at temperatures above – 540 0C [1-3]. Based on the service conditions, the corresponding technical requirements are formulated – as high as possible values for the characteriristics of: tensile strength, plasticity, corrosion resistance, melting temperature, as well as – low coefficient of thermal expantion etc. [2; 3]. Nowadays there are several types of the SAs produced in industry, [3 – 5] but no one has universal application due to restrictions of SAs performance. One of the main direction to achieve the required aspects of the SAs performance is improving their chemical compositions. Basic data concerned with a separate chemical element effects on the SAs performance are well known for decades [5 – 7], but it is not so relating the various element combinations. Problems arising under specification of a complex system performance caused by a common action of the system components (synergetic effects) are fundamental features of the modern physics and mathematics (many body problem) [8 – 10]. In cases concerned with metal alloys, the problems result in unpredictable (uncontrolled) changes of the alloys microstructures and performance which mostly are undesirable: nonuniform spacial distributions of the chemical elements and structure components, various types of embrittlement etc. Such a problem becomes more actual with increasing the element concentrations in an alloy.

Aim of the article

Proceeding from the above, the aim of the article is to determine basic dependences of the joint and separate effects of the chemical elements in SAs on their main performance indexes.

Recent relevant publications overview

Chemical elements` influence on the SAs performance is studied in numerous works [11 – 13]. However the researches having been conducted considered only the separate and related additive effects of the elements. In other words, possible interactions of the chemical elements in forming service properties of the SAs have not been considered yet. Recently big attention is paid to novel manufacturing processes application, such as – additive manufacturing and synthesis of nanoparticles [4; 14]. However, as the interatomic interactions ultimately determine the performance of a crystalline solid, the chemical elements synergetic effects in alloy crystals have to conserve their importance independently of the alloy manufacturing technologies applied. Taking into account the known fundamental restrictions of modern analytical and experimental procedures for the chemical elements interaction investigations, statistical approaches are considered to be among the promising ones [15; 16]. This notion is confirmed by results of the Data Mining techniques application to solve some quality and reliability problems existing for the industrial multi element structural steels [17 – 19]. Based on results of the works, a combined general approach was developed [20], which provides: – revealing valuably affecting independent variables; creating corresponding highly adequate multiple regression models; conducting Monte Carlo simulations of the variable separate and joint effects on each controlled characteristic; specifying a multidimensional objective function and, finally, conducting multipurpose optimization to obtain, guaranteed with necessary confidence probability, value of the objective function. Besides, the approach gives an opportunity to reveal, in a real industrial manufacturing environment, possible effects unpredictable under the laboratory investigation conditions as well as to discover further investigation fields. By now, the above approach, comprising, particularly, C&RT Data Mining technique, was successfully applied to the embrittlement prevention in B-containing ASTM A514 steel [21]. The obtained results were implemented in industry. So, in view of the above, the developed combined Data Mining based statistical approach was applied to conduct systematic investigations of the chemical composition effects on the basic performance indexes of the industrial SAs. The results obtained in the course of the first stage of the approach application are presented below.

Materials and Methods

Researches were conducted using the well known experimental data on basic performance indexes for various industrial, operational ready SAs [22]. On the first stage of the investigation, the available data were treated using computer aided C&RT Data Mining technique [17; 18; 21]. In result of the statistical computer technology application, the “dendrograms” were constructed. Each of the “dendrogram” provides the following statistically grounded (objective) visual information for each controlled performance index: – a full list of statistically significant independent variables (chemical elements); allowable variants of the variable interactions (chemical elements combinations); limits of the independent variable (chemical element concentrations) intervals spillover of which provides changes of the statistically significant interaction character (chemical elements combinations); variation tendency for the control index within each of the intervals.

Results and Discussion

Some results obtained in the course of the current investigations are shown in the form of dendrograms on Figures 1 – 5. As it seen from the dendrogram shown in Fig. 1, a level of Ultimate Tensile Stress (UTS) for industrial SAs has statistically significant dependence (with the confidence probability no less than 98%) on concentrations of the following chemical elements: Ti, Cr, Nb, Ni, Cu, Fe. At that, direct, the most valuable effect on UTS has Ti, increasing concentration of which within the interval: 0…2,55%, leads to grow UTS from ~ 650 to ~ 1300 MPa (see nodes 1 – 2). Besides, under the condition Ti ≤ 0,73%, statistically significant effect on UTS is the one of Cu (see nodes 3,4), which decreases UTS when its concentration grows. Meantime, if the Ti concentration exceeds ~ 0,73% (node 2), UTS depends on concentration of Nb (see nodes 5,6), reaching its maxima which lay within the range: UTS ≈ (1275 ± 3·49.5) MPa under the highest Nb content: > 0.092% (node 6). Thus, the obtained results show that any of the considered chemical elements in the investigated SAs with the high Ti and Nb concentrations can not influence further the SAs maximum tensile stress. Besides, under the lower Ti concentrations (≤ 0,73%, node 1), combined with any Cu content (nodes 3,4), the following chemical elements can affect the UTS: Ti (nodes 7,8), Ni (nodes 9 – 12; 17; 18), Cr (nodes 13; 14) and Fe (nodes 15; 16). At that, the highest UTS values reached in a such group of SAs do not exceed average ~948 MPa level (see node 8), which is obtained under the conditions: 0,20% < Ti ≤ 0,73%, Cu < 0,43%.

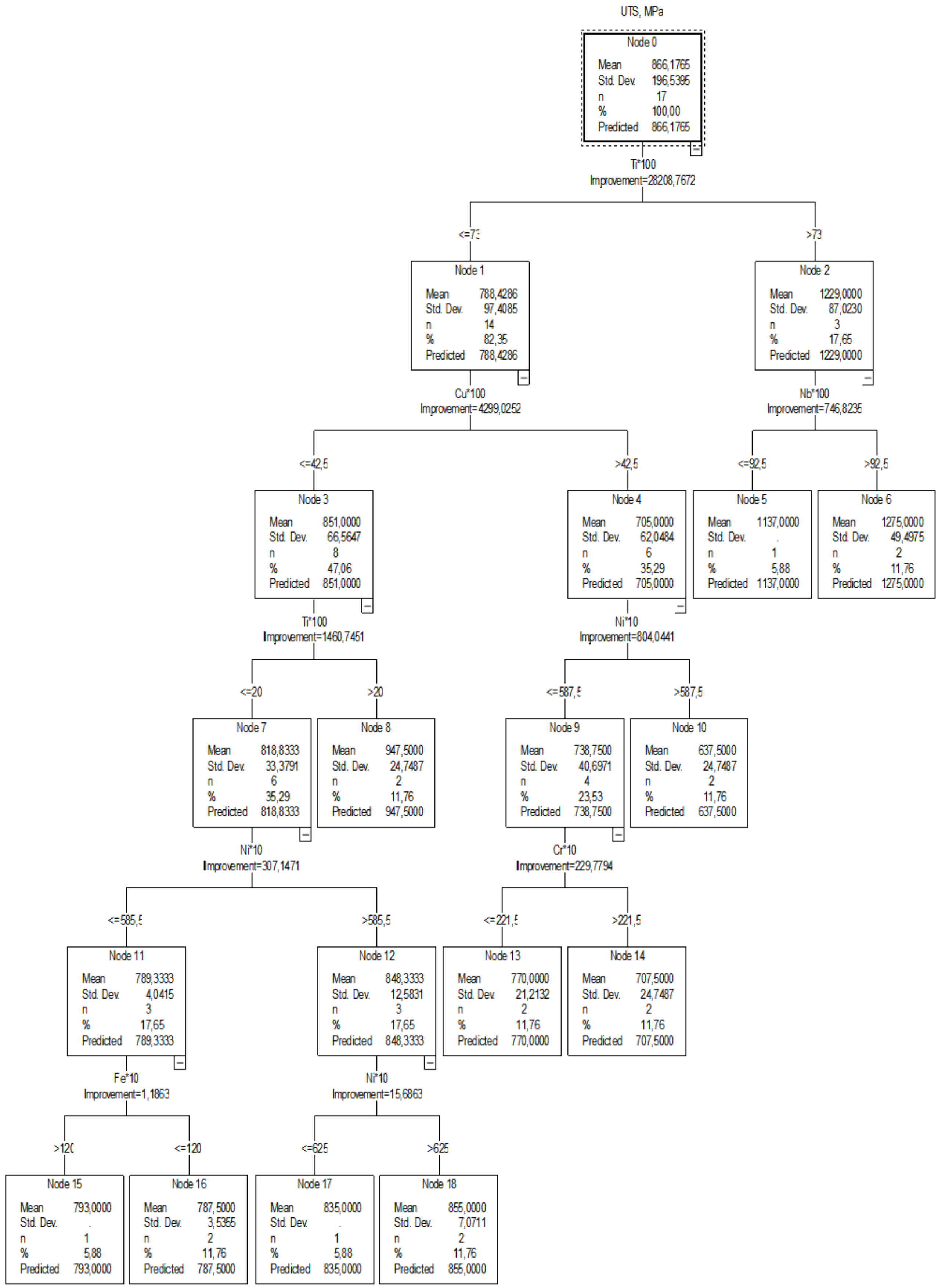

Figure 1 – Computer dendrogram showing the chemical composition effects on ultimate tensile stress (UTS, MPa) of modern industrial super alloys

Overall obtained results may be attributed to the well known strengthening effect of carbide forming elements: Ti, Nb, Cr together with interatomic interaction of Cu and Ti in FCC Ni-based solid solution, probably providing formation of incoherent Ti_xCu_y intermetallic compounds with less strengthening effect than highly fine-dispersed TiC particles.

Dendrogram defining the chemical composition dependence of Yield Stress (YS) for SAs is shown on Fig. 2. It may be seen that most of the above revealed chemical elements, namely: Ti and Cu, affect the YS with practically the same relationships, as it was shown for UTS (see Fig. 1). An additional chemical element, significantly affecting YS, is B (see nodes 7, 8), which radically decreases YS of SAs with grow of its concentration.

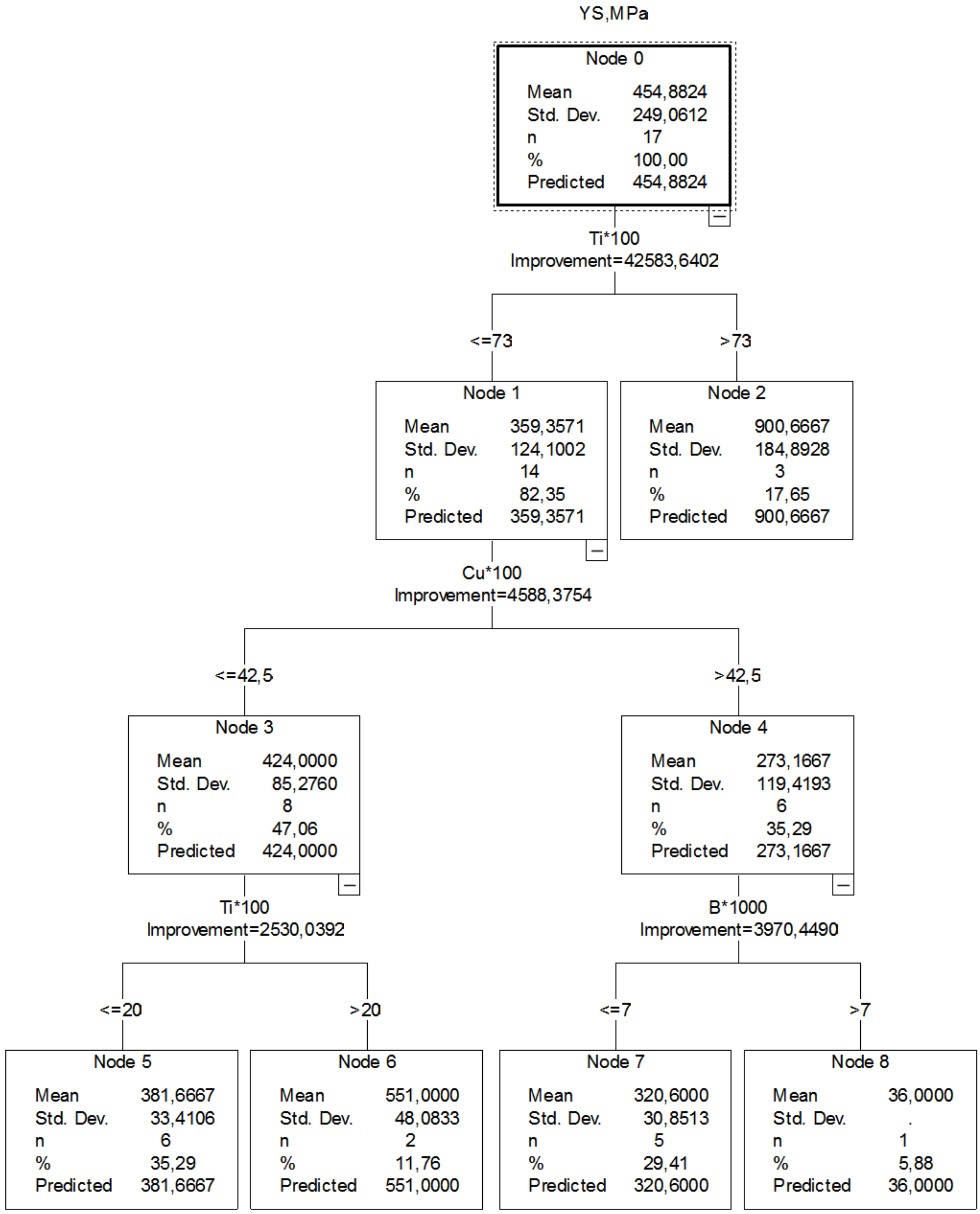

Figure 2 – Computer dendrogram showing the chemical composition effects on yield stress (YS, MPa) of modern industrial super alloys

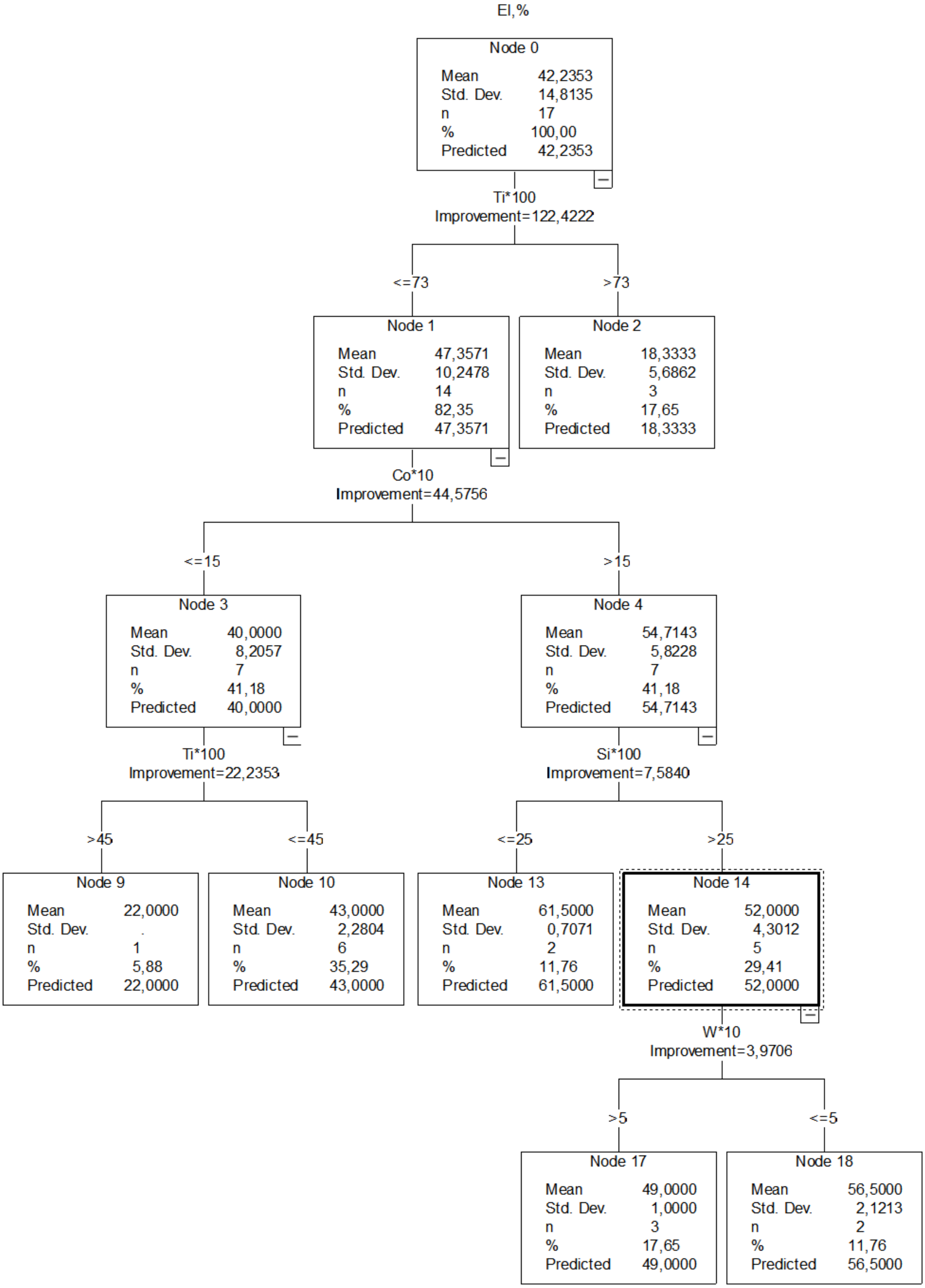

Figure 3 – Computer dendrogram showing the chemical composition effects on relative elongation (El, %) of modern industrial super alloys

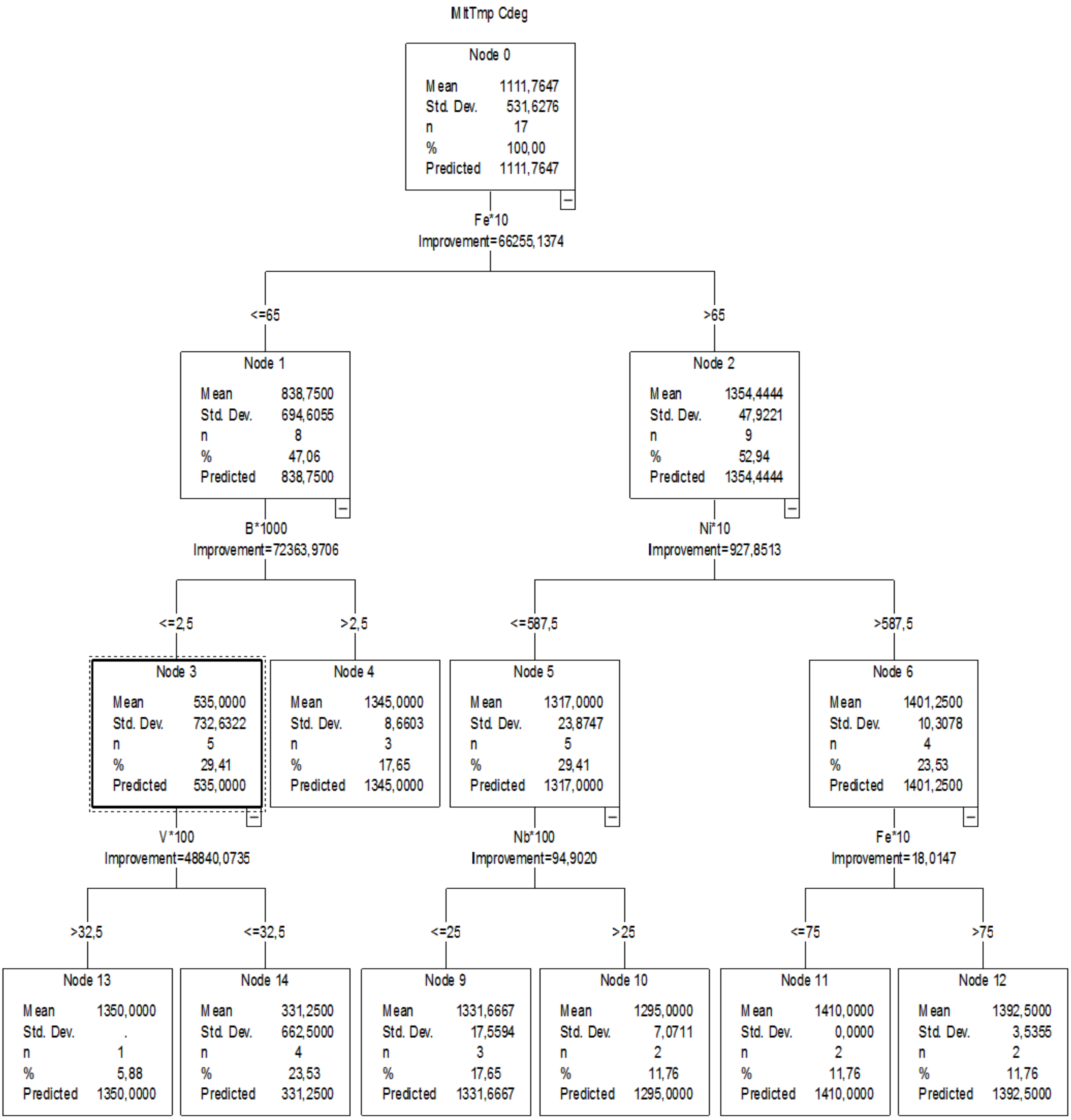

Figure 4 – Computer dendrogram showing the chemical composition effects on melting temperature (MltTmp, C deg.) of modern industrial super alloys

The results obtained are in accordance with the explanation given above in respect to Ti and Cu. They are also confirmed by the well known data [21] about forming Boron grain boundary segregations in metallic alloys, which lead to "weakening" the boundaries, properties of which are responsible for the initial stage of the plastic deformation in polycrystals.

The investigation results concerned with the chemical composition influence on the SAs plasticity are shown as a corresponding dendrogram for Relative Elongation (El) in Fig. 3. As it seen, the most valuably (directly) affecting on El chemical element is Ti (see nodes 1; 2), which demonstrates the alternative regularities comparing with the strength characteristics: UTS and YS (see Fig. 1 and 2). The chemical elements additionally affecting El are: Co, Si and W. Each of them influences on SAs elongation according to the known, expected regularities: Co increases, but Si and

W – decreases the plasticity. As it follows from the dendrogram (see node 13), the maximum El average level (El = 61,5%) is reached under the following conditions: Ti < 0,73%, Co > 1,5%, Si < 0,25%. Meantime, the minimum plasticity (average El on the level 18%) have the SAs with Ti concentration exceeding 0,73%.

Taking into account the important roles of the melting temperature and the thermal expansion coefficient in the SAs performance providing, the chemical composition dependencies of the characteristics were considered. The corresponding dendrograms are shown in Fig. 4 and Fig. 5. As it seen from Fig. 4, the chemical elements which are statistically significant in affecting the SAs melting temperature (MltTmp) are as follows: Fe, B, Ni, V, Nb. Namely, Fe is the most valuable element, increasing MltTmp from 839 ^{0}C, at Fe concentrations < 6.5 %, up to ~1354 C, at Fe > 6.5 % (see nodes 1,2). As it follows from pair comparing the nodes 3,4 and 13,14, the elements radically affecting the SAs melting temperatures including their destabilizing are B and V. Namely, boron increases average MltTmp values from 535^{0}C up to 1317^{0}C under the growing its concentration from the values: < 0.0025% up to: > 0.0025% (see nodes 3, 4). However, under the low B concentrations (see nodes 3), MltTmp is extremely unstable – standard deviation of the characteristic is about 733^{0}C. Analogous situation with MltTmp is observed under the influence of V: increasing V concentration from the values < 0.33% to a level > 0.33%, leads to grow average MltTmp from 331^{0}C to 1350^{0}C. The results obtained are in accordance with the data [21] early revealed for boron contained ASTM A514 steel and may be explained by uncontrolled changes of B and V concentration distributions between grain boundaries and corresponding nitride compounds formed by these elements under their low general content in an alloy. Absolute maximum of SAs melting point, which is one of the required characteristics, on the stable level about 1410^{0}C (see node 11), is reached under the following concentration conditions: 6.5% < Fe < 7.5%; Ni > 58.8%.

Low thermal expansion is one of the desirable properties of an SA, that is why controlling the chemical composition dependence of the corresponding coefficient is very important to improve SAs performance. The necessary dendrogram is shown on Fig. 5. According to the dendroram, among all the affecting chemical elements, the most valuable ones: Fe, B and Ni are the same as to the SAs melting point (see nodes 11 – 18, Fig. 4). However Ni, contrary to Fe and B as well as the case of melting point, decreases ThExpn from $13.8 \cdot 10^{-6}$ deg^{-1} to $12.8 \cdot 10^{-6}$ deg^{-1} with growing its content from < 64.8% to > 64.8%. More considerable ThExpn decreasing, as it seen from the nodes 21,22 and 25,26, may be reached by decreasing concentrations of Al and V. So, minimal thermal expansion coefficient for the considered SAs is provided under the following concentration conditions: Fe < 6.5%; B < 0.0025%; Al < 0.35%; V < 0.33% together with the rest chemical elements concentrations allowed by the existing standards.

Conclusions

1. Systematic investigations of chemical composition effects on some basic performance characteristics of modern SAs were conducted using computer C&RT Data Mining statistical technology.

2. Computer dendrograms were constructed providing statistically grounded (objective) visual information for each controlled performance index: – a full list of statistically significant chemical elements; allowable variants of the elements combinations (interactions); limits of the chemical element concentration intervals spillover of which provides changes of the statistically significant chemical elements combination; variation tendency for the control index within each of the revealed intervals.

3. Ability is emphasized for the dendrograms to be applied for preliminary, semi-quantitative analysis of individual and mutual independent variables effects on the controlled performance characteristics as well as to the multipurpose optimization of the variable values.

4. Valuable individual combined strengthening and embrittlement effects of carbide forming elements (Ti, Nb, W, Fe) were shown to be conserved under the various concentration conditions in SAs, in accordance with the general notions.

5. Dependences are shown to exist for individual performance effects of the most chemical elements in modern SAs on concentrations of the other comprised elements.

6. Statistically significant interactions of Ti with Cu and Co are revealed which provide respective decreasing strength and growth plasticity of SAs in the course of Ti substitution.

7. Extremaly destabilizing effect of B and V on the SAs melting temperature was revealed and attributed to the elements competition in the chemical compounds formation together with boron tendency to segregate on grain boundaries.

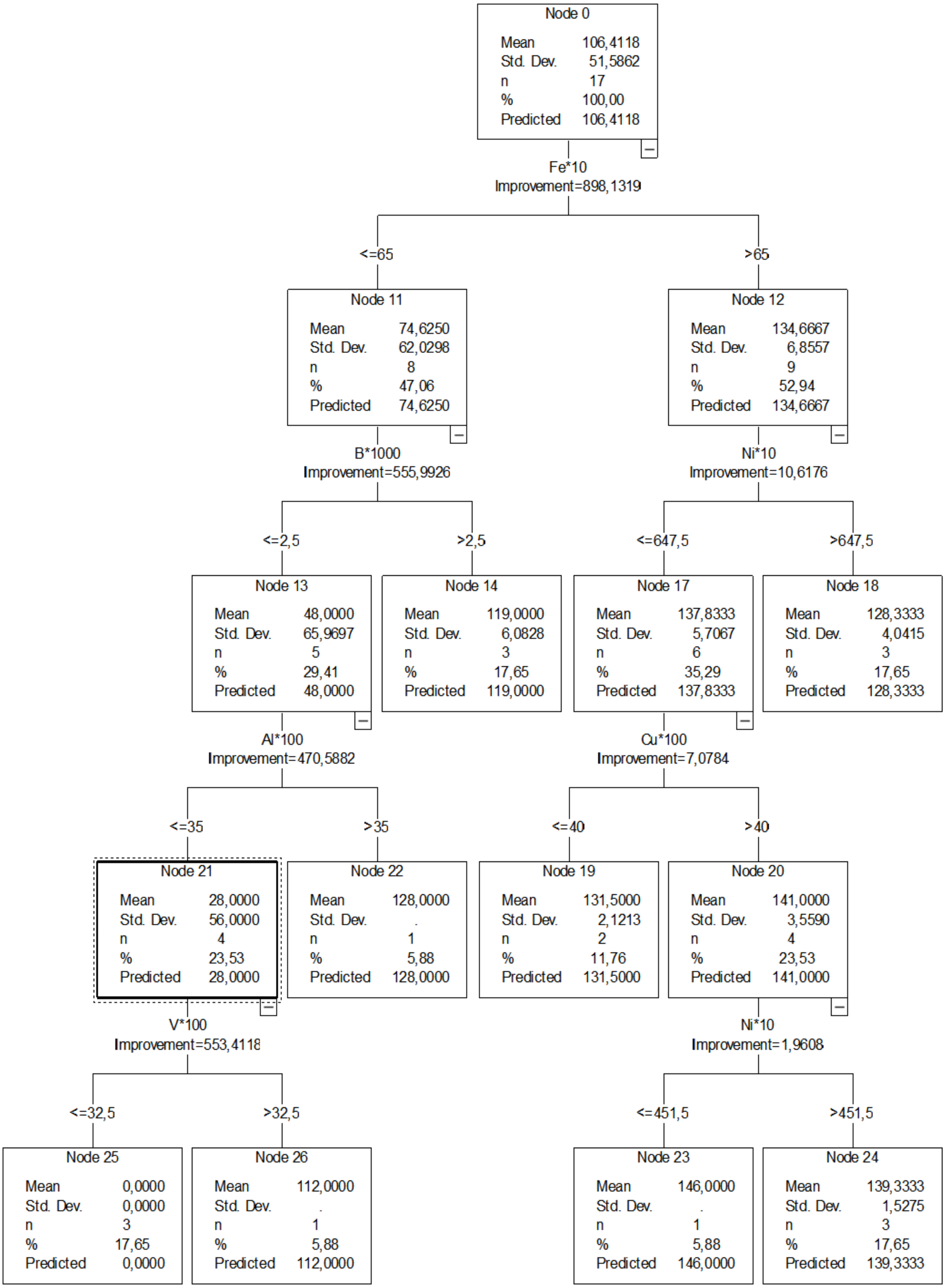

Figure 5 – Computer dendrogram showing the chemical composition effects on thermal expansion coefficient (ThExpn×10^{7}, deg^{-1}) of modern industrial super alloys

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ВИЯВЛЕННЯ СТАТИСТИЧНО СУТТЄВИХ ЕФЕКТІВ ВПЛИВУ ХІМІЧНОГО СКЛАДУ НА ЕКСПЛУАТАЦІЙНІ ХАРАКТЕРИСТИКИ СУПЕРСПЛАВІВ ШЛЯХОМ ЗАСТОСУВАННЯ МЕТОДІВ DATA MINING

Анотація. *На основі раніше розробленого інтегрованого підходу до дослідження, що поєднує взаємно узгоджені комп'ютерні методики, проведено: статистичні дослідницькі методи, розроблення множинних регресійних моделей, моделювання Монте-Карло та оптимізація параметрів багатоцільової технології виробництва, комп'ютерні статистичні дослідження впливу хімічного складу на деякі основні експлуатаційні характеристики сучасних промислових суперсплавів. Відповідно до розробленого підходу в пропонованій роботі як перший етап подальшого аналізу* *було використано статистичну технологію C&RT на основі технології Data Mining. Підкреслено важливу особливість розробленого підходу до «пасивного експериментування» загалом і застосовуваної методики зокрема, оскільки вони забезпечують мінімальні витрати на дослідження порівняно з «активним», а тому не мають альтернативи в умовах вільного ринку. Як первинний результат етапу побудовано дендрограми, які надавали наступну статистично обґрунтовану візуальну інформацію для кожного контрольованого показника продуктивності суперсплавів: повний перелік статистично важливих хімічних елементів; допустимі варіанти поєднання елементів; границі інтервалів концентрації хімічних елементів, поширення яких забезпечує зміну комбінацій хімічних елементів; тенденції зміни контрольних показників у межах виявлених концентраційних інтервалів. Показано взаємодію більшості хімічних елементів, що входять до складу суперсплавів, за їх впливом на досліджувані показники ефективності. Підкреслено високу ефективність застосування отриманих дендрограм для виявлення впливу окремих та взаємних хімічних елементів на експлуатаційні характеристики багатоелементних сплавів, а також унікальність такої інформації для промислових сплавів. Відзначено деякі перспективні можливості застосування отриманих дендрограм: як перший етап багатопараметричного аналізу технологічних процесів у промислових умовах; базовий етап подальшої розробки множинних регресійних моделей та проведення остаточної оптимізації багатоцільових технологічних процесів.*

Ключові слова: промислові суперсплави; хімічні склади; комп'ютерні статистичні дослідження; показники продуктивності; методи аналізу даних; дендрограми

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