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Methodology of high-speed steels design using the artificial intelligence tools

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Methodology of research

ABSTRACT

Purpose: The main goal of the research carried out was developing the design methodology for the new high-speed steels with the required properties, including hardness and fracture toughness, as the main properties guaranteeing the high durability and quality of tools made from them. It was decided that hardness and fracture toughness K_{Ic} are the criteria used during the high-speed steels design.
Design/methodology/approach: In case of hardness, the statistical and neural network models were developed making computation possible of the high-speed steel hardness based solely on the steel chemical composition and its heat treatment parameters, i.e., austenitizing- and tempering temperatures. In this case results of own work on the effect of alloy elements on the secondary hardness effect were used, as well as data contained in catalogues and pertinent standards regarding the high-speed steels. In the second case - high-speed steels fracture toughness, the neural network model was developed, making it possible to compute the K_{Ic} factor based on the steel chemical composition and its heat treatment parameters. The developed material models were used for designing the chemical compositions if the new high-speed steel, demonstrating the desired properties, i.e., hardness and fracture toughness. Methodology was developed to this end, employing the evolutionary algorithms, multicriteria optimisation of the high-speed steels chemical composition.
Findings: Results of the research carried out confirmed the assumption that using the data from catalogues and from standards is possible, which - would supplement the set of data indispensable to develop the assumed model - improving in this way its adequacy and versatility.
Practical implications: Solutions presented in the work, based on using the adequate material models may feature an interesting alternative in designing of the new materials with the required properties. The practical aspect has to be noted, resulting form the developed models, which may successfully replace the above mentioned technological investigations, consisting in one time selection of the chemical composition and heat treatment parameters and experimental verification of the newly developed materials to check of its properties meet the requirements.
Originality/value: The presented approach to new materials design, being the new materials design philosophy, assumes the maximum possible limitation of carrying out the indispensable experiments, to take advantage of the existing experimental knowledge resources in the form of databases and most effective computer science tools, including neural networks and evolutionary algorithms. It should be indicated that the materials science knowledge, pertaining oftentimes to the multi-aspect classic problems and described, or - rather - saved in the existing, broadly speaking, databases, features the invaluable source of information which may be used for discovery of the unknown so far relationships describing the material structure - properties relations.
Keywords: Tool Materials, Computational Material Science, Artificial Intelligence Methods, Materials Design

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1. Introduction

Determining of dependencies among the structure, technological process, and functional properties, as well as materials selection and technological properties forming their structure and properties for employment in complex manufacturing systems, feature the core interest of materials engineering. Selection of the suitable material with the appropriate technological process is of the key importance, ensuring the longest product life at the lowest costs.

Materials Science and materials engineering belong to those disciplines of science, on which, in a great measure, the further development of civilisation will depend [49, 74, 84, 155, 179]. Its role will be to cope with the demand for the contemporary engineering materials meeting the current economy requirements, including tendency to improve competitiveness in manufacturing of materials and products.

The quick knowledge progress pace in many manufacturing engineering branches challenges the tool manufacturers and designers more and more. It is evident that reliability, durability, quality, and other properties of tools, ensuring comfort of their use, depend mostly on the deliberate, well studied materials selection, using the multicriteria optimisation. Economic- and ecological issues get more and more important amid many criteria, apart from the design-, engineering-, and service requirements. Hardness and ductility are the decisive properties in case of materials used for cutting tools. The task of the suitable material selection by the tool designer features the neverending compromise between selection of the material with high hardness, yet with small ductility, or vice versa - selection of the material with good ductility, yet with the relatively lower hardness. High-speed steels are the materials with the best ductility and fracture toughness from all tool materials in use nowadays, which, as it seems, will remain irreplaceable in many applications for a long time.

The continuous intensive development of the tool materials and tool industry, e.g., in countries like Italy, Austria, Germany, Sweden, France, or Slovenia, is connected with changes in the tool- and advanced tool materials market. This is connected with the peculiar character of the contemporary manufacturing, which is compelled by the cheap competition from the Eastern markets, compared to the situation from several-, or a dozen or so years ago. It is still expected, concerning the tool materials, to provide their best feasible service- and use properties, and especially the tools' durability (service time), which extorts the need to carry out investigations of the new materials. Regrettably, the classic approach requires huge financial expenditures and a lot of time, and is connected with the need to carry out the complex fundamental research upon the newly designed tool materials, their manufacturing technologies, technologies improving their properties, and the applied research, consisting in the complex technological tests, making assessment possible of the service properties of tools.

The requirements posed by the multi-aspect engineering design of tools, and also many world literature sources suggest the need of the complex approach to the materials selection problem, along with the technological processes for the contemporary tools, characteristic of the high quality, reliability, and being environment friendly [5, 30, 74, 84, 137].

High-speed steels used to be the object of interest for dozens of years to the scientific society from which the author comes from. Research on these materials carried out first in the Institute of Physical Metallurgy, and later in the Institute of Engineering Materials and Biomaterials (IEMB) were focused on the effect of, among others. heat- and thermo-mechanical treatment of the high-speed steels properties [1, 2, 73, 75], phase transformations [43, 65, 67], and also on substitution possibilities of some alloy elements [45, 57, 64, 66, 68, 69]. Many projects carried out in co-operation with several European centres pertain to the development of the PVD method and its application for coating the conventional steels and the sintered high-speed steels with the single- and multi-layer coatings [32, 33, 34, 35, 37, 44], and currently with the gradient ones also [38, 42, 61, 71, 117, 135]. Research is also ongoing in the Institute on the sintered high-speed steels [38, 42, 61, 71, 117, 139]. Many PhD and DSc dissertations, as well as monographies [4, 29, 39, 62, 63, 77, 93, 114, 134, 216], were the effect of this research, being an essential scientific contribution to the development of the research, not limited to domestic only, on the high-speed steels.

Simultaneously, the Computational Materials Science features the essential area of the scientific interest of IEMB, being created since a dozen years or so by this Team in Poland. The main achievements within the area of application of the computer science tools, including artificial intelligence, were published, among others, in works [46, 50, 51, 52, 53, 54, 55, 58, 59, 60, 129, 198, 199, 200, 201, 207, 208, 209, 210].

The subject matter of investigations performed within this work features the natural development direction of the IEMB's research area of interest.

1.1. High-speed steels and their importance

Machining is one of the most important processes of products forming and fabricating in the contemporary, modern, industrial manufacturing, especially in the mass production. Requirements of the competitive production, merging the high quality and efficiency with the possibly low unit costs, call for use of the highly efficient tool materials [80].

As regards materials used for profile cutting tools, their most important properties are hardness and resistance to failures in service, e.g., cracking or breaking, which are expressed by their material impact toughness or fracture toughness. Especially the high ductility of the material makes the tool predisposed for work in the impact loads conditions, and also in conditions resulting in fatigue failure. Ensuring these expected service properties is achieved for the material with the particular chemical composition during its heat treatment [31, 126, 166].

Three main groups may be indicated among the currently used main tool materials:

- high-speed steels,
- cemented carbides,
- ceramic materials and super-hard materials including alumina based composites, sialons, cubic boron nitride and synthetic diamond.

Chemical composition and structure of the contemporary high-speed steels result from decades of experimental research. It is assumed that the first high-speed steel was the one developed in 1900 by F.W. Taylor and M. White, containing 1.85% C, 0.15% Si, 0.3% Mn, 3.8% Cr, and 8.0% W. Work on development of the high-speed steels led to introducing into the steel an addition of vanadium, and next tungsten in concentration of ca. 18%, as well as cobalt. The next modification of the high-speed steels chemical composition concerned partial replacement of tungsten with molybdenum. Further experimental research led to the simultaneous concentration increase of vanadium and carbon, and next to reducing the tungsten concentration, increasing vanadium concentration, which resulted in development of the new 12-0-4 high-speed steel type with vanadium concentration 3-5% and carbon about 1.6%. Investigations carried out at that time revealed that the MC type carbides, originated to a big extent by vanadium, have higher abrasion wear resistance than the M_6C type carbides. All that made it possible to develop steels with the high concentration of carbon and vanadium, called the super high-speed steels. [184]

Attempts to substitute molybdenum for tungsten were made in 1940-1952 in USA and the 6-5-2 steel developed there is one of the most commonly used high-speed steels nowadays [186].

Therefore, evolution of the high-speed steels composition since their origin until the end of World War II, was accomplished with the scientific empiricism method and required carrying out many experiments, which ended up with failures many a time or were even misleading.

The main alloying elements in the high-speed steels currently are chromium, tungsten, vanadium, and also molybdenum and cobalt. Silicon, niobium, and titanium are introduced as alloy additions sometimes apart from the main elements mentioned above. Methodical investigations of the relationship among the chemical composition, manufacturing- and heat treatment processes, and the high-speed steels properties were initiated only in sixties last century. They revealed that the high-speed steels properties depend significantly on the proportion between the carbon concentration and the summary concentration of the alloy elements [13, 127]. This has led to formulation of the equivalent carbon coefficient (Fig. 1) [13, 127]:

$$C_E = \frac{\%W + 1.9\%Mo + 6.3\%V}{30} \quad (1)$$

where: W, Mo, V - respective mass concentrations of these elements in steel in %

Research results [13, 127] made it possible to realise that it is most advantageous , from the point of view of service properties, that the steels with additions of tungsten, molybdenum, and vanadium should contain the carbon concentration higher by 0.1-0.2% than the equivalent carbon coefficient value C_E (Fig. 1). Increasing the carbon concentration more than 0.2% above the equivalent carbon coefficient C_E value resulted in development of the new high-speed steels group, achieving high hardness and better resistance to tempering while maintaining the unchanged ductility, compared to the conventional grades [13, 14].

At the turn of seventies and eighties of the last century, due to difficulties with acquiring of some alloying elements, many research projects were commenced focused on limiting concentrations in the high-speed steels of very expensive or scarce, at that time, elements like tungsten, vanadium, molybdenum, and cobalt by replacing them with others - cheaper and easily available elements, including silicon, aluminium, titanium or niobium [40, 43, 65, 77, 83, 91, 127, 185, 195, 213].

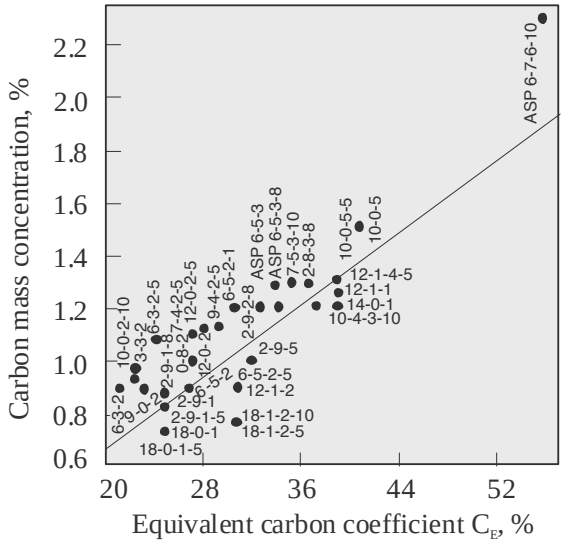


Fig. 1. Mass concentrations of carbon and alloying elements in various grades of high-speed steels [39]

As it is, it was found out in case of silicon that it can substitute tungsten and molybdenum [9, 10, 11, 12, 43, 57, 65, 69, 70, 75, 77, 91, 167, 168, 169, 170, 195, 213], which fructified with development of the new high-speed steel grades with the increased silicon concentration [68, 76, 77].

Research [12, 17, 20, 41, 63, 64, 66, 67, 68, 69, 70, 99, 100, 102, 115, 122, 127, 160, 185, 216] revealed that using niobium is purposeful for partial substitution for vanadium.

However, investigation results for the high-speed steels with addition of titanium [45, 62, 63, 64, 66, 67, 83, 88, 176, 184], indicate that it can partially be a substitute for vanadium. Moreover, works [21, 22, 24, 119, 120, 121, 122, 180, 181, 182, 183] made it possible to develop the non-ledeburitic high-speed steels demonstrating lack of carbides segregation, with other properties comparable with the conventional high-speed steels.

The development process of the high-speed steels presented here, in the area of improvement of their chemical compositions and fabrication processes, was very lengthy and complex.

Conventional manufacturing of the high-speed steels consists of processes of melting, casting, plastic forming, and heat treatment. The crucible process was the first high-speed steels fabrication method used mostly for casting of small ingots. It was replaced by the induction- and arc electrical furnaces used very successfully until today. Emergence of the electroslag- and vacuum remelting, as well as arc remelting, featured the important progress in the high-speed steels metallurgy in sixties, which ensured improvement of the metallurgical purity of the high-speed steels and possibility to control crystallization of the fabricated products. Alloying elements are added as ferro-alloys, like: iron-tungsten, iron-molybdenum, iron-vanadium, being the main ones

taking into account their mass fractions and prices, and their fraction depends on carbon concentration [108]. Using the ESR (*electroslag refining*) and VAR (*vacuum arc remelting*) processes, as well as more popular electron beam or plasma arc melting better cooling rate control is achieved and local crystallisation connected with it. CESM (*continuous electroslag melting*),called also the continuous electroslag melting, is a variation of the ESR [107, 108]. In this case, the electrode getting melted is replaced by the steel ingot fed continuously to the tundish along with the alloying elements. Another method ensuring reduction of the inhomogeneity of the chemical composition and segregation of primary carbides is the vacuum-arc refining in the VAD (*vacuum arc deposition*) process. High-speed steels fabricated with this method have lower concentration of harmful impurities, especially oxygen and sulphur, and demonstrate more homogeneous primary austenite grain size after hardening compared to steels smelted in a conventional way. Continuous casting method was not employed in case of the high-speed steels fabrication because of difficulties with obtaining structure free from segregation, connected with casting rates [108].

Fabrication of cast steels calls for using hot working for breaking the cell structure of the cast high-speed steel with the eutectic carbides lattice, preceded with the homogenizing treatment operation. Therefore, technological factors exerted the significant influence on development of the conventional high-speed steels, first of all by employing swaging machines for reforging the high-speed steels [95, 96, 97]. They make it possible to achieve the advantageous structure by nearly complete liquidation of the primary carbides segregation, occurring during rolling.

Beginning from seventies of the last century development of the high-speed steels and tools made from them took place in the area of their fabrication technology, including powder metallurgy methods for their fabrication, thermo-chemical treatment and PVD processes for coating tools from these steels with hard surface layers for improvement of their service properties, and also development of the heat treatment technologies less harmful to the environment than the traditional one, making use of the salt furnaces. Employment of the thermo-chemical treatment, including gas nitriding, ionitriding, vacuum nitriding, and gas sulfonitriding, improves significantly properties of tools made from the high-speed steels [1, 3, 81, 82, 124, 125, 177]. Fabrication method for the sintered high-speed steels, known as the ASEA-Stora process, was developed in Sweden in 1970 [103]. Many research-, as well as research and development projects in the last decade of the XX century were focused just on the sintered high-speed steels which do not demonstrate the troublesome segregation of the primary carbides with the density close to the one corresponding the conventional steels and with service properties of tools, especially those with the big cross sections, better than of those made from the conventional steels [42, 47, 48, 94, 104, 105, 117, 133, 140, 141, 142, 143, 152, 187, 188, 189, 190, 191, 194, 205, 206, 211, 212].

A crucial development, for the improvement of the tools service properties, was introduction of the PVD method - the low temperature physical deposition from the gaseous phase of the surface coatings made-up of the titanium carbides and nitrides, and also of the multilayer coatings. The coated tools demonstrate service life even many times longer than tools made in a conventional way. Coatings put down in the PVD process may be either single (composed of one material, metal or phase) and complex (composed of more than one material; however these materials occupy different positions in the coating). In addition, within the complex coatings group, one may distinguish the multicomponent coatings, multilayer-, multiphase-, composite- and gradient ones [15].

Research projects on implementation of this contemporary technology, including also the complex coatings (multicomponent-, multilayer-, composite-, and gradient ones) for improvement of the tools service properties are carried out intensively in the last dozen or so years and widely published [4, 15, 32, 33, 34, 35, 36, 37, 38, 44, 56, 61, 71, 90, 93, 135, 171, 207].

Other trends of development and improvement of the high-speed steels heat treatment, also taking into consideration its ecological aspect [28], pertain to employment of sub-zero quenching mostly for improvement of tool life [25, 87, 130, 151], vacuum heat treatment [131, 132, 205], plasma spraying being a combination of the PVD method and powder metallurgy [148], as well as alloying of the high-speed steels surface [8, 106]. Work [7] presents interesting results of the research of phase transformations kinetics effect during continuous heating and isothermal annealing on the tempered steels properties when the so called preliminary tempering is used, which makes modification of the heat treatment technologies used to date.

Structure and properties of high-speed steels are formed both during their fabrication and during their heat treatment. Properties of high-speed steels depend to a great extent on their primary structure developed during crystallization. Transformations sequence during crystallization and phase composition of carbides developed as their outcome depend mostly on the type and concentration of the carbide forming elements in steel, and also on their cooling method [12, 39, 43, 77, 89, 92, 128, 185]. Heat treatment of high-speed steels consists in hardening and tempering, in the beginning usually in slat baths. But now, due to ecological reasons heat treatment of high-speed steels is purposeful in vacuum furnaces, chamber furnaces with controlled atmospheres, furnaces with fluidized bed or with induction heating [39]. Two- or sometimes three stage heating up of tools to the austenitizing temperature is used during hardening with holding in salt baths with the temperatures of 550, 850, and eventually 1150°C. Ensuring the high hardenability and making precipitation hardening possible during tempering requires partial dissolution of the primary carbides in the solid solution and saturation of austenite with carbon and alloy additions. This is achieved by employing the high austenitizing temperature, usually about 50-70°C lower than the solidus temperature, and the short austenitizing time, usually 80-150 sec [13, 39, 126].

The extent of austenite saturation with the alloying elements depends also on carbides size and their distribution in the spheroidizing annealed steel structure. Some carbides pass into the solid solution at the properly selected austenitizing temperature and their remaining, undissolved, part inhibits the excessive primary austenite grains growth. The austenitizing temperature which is tool low does not ensure the necessary saturation of the austenite with carbon and alloying elements coming from the carbides dissolved in the solid solution and lowers hardness of steel after tempering. On the other hand,

however, the excessively high austenitizing temperature and the too long heating time during hardening result in the increase of the retained austenite fraction in steel, and therefore, in reduction of its hardness immediately after hardening. This is accompanied by the simultaneous steel fracture toughness increase and the primary austenite grain size growth [39], Transformations occurring in the high-speed steel during cooling from the austenitizing temperature may be determined using the time-temperature-transformation TTT curves during continuous cooling CTPc or using the λTPc phase transformations curves [126, 144, 145, 146].

Tempering brings about an essential effect on structure and properties of high-speed steels. During tempering in the 400-450°C temperature range precipitation of cementite in martensite occurs, depending on steel grade [39, 77]. This causes improvement of mechanical properties; however, the steel fracture toughness deteriorates [156, 158]. Tempering at the temperature of 500-580°C because of the partial dissolution of cementite in the tempered martensite, causes reduction of strength and fracture toughness K_{Ic} being a measure of crack resistance [166] (Fig. 2).

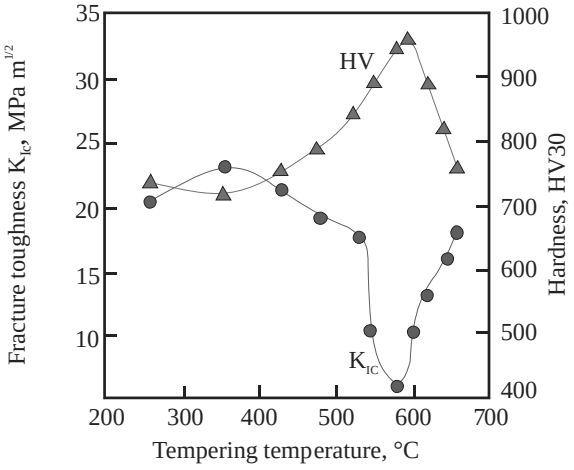


Fig. 2. Effect of tempering temperature on fracture toughness K_{Ic} and hardness of the 6-5-2 type steel [166]

At the same time fine alloying carbides precipitation occurs, influencing the secondary hardness effect. In steels containing more than 1% V the M_4C_3 carbides of the MC type are responsible for the secondary hardness effect, demonstrating the specific particular crystallographic relationships in respect to the tempered martensite matrix. Apart from the M_4C_3 type carbides, in steels with low V concentration (ca. 1%) in the tempering temperature range corresponding to the secondary hardness, the M_2C type carbides may also precipitate, and at even lower concentrations of this element the $M_{23}C_6$ and M_6C type carbides precipitate. [2, 13, 39, 72, 73]

During tempering, the big fraction of the retained austenite enhances significantly the secondary hardness effect due to the retained austenite transformation into martensite. Presence of martensite is indispensable for the retained austenite conditioning process during holding at the tempering temperature, at which preparation of this phase for the martensitic transformation takes place, occurring during cooling from the tempering temperature [72, 73]. During holding at the tempering temperature the diffusion equalizing of carbon takes place in the retained austenite neighbouring with the martensite impoverished in carbon because of the alloying carbides precipitation in martensite. A higher temperature of the martensitic transformation start of the retained austenite impoverished in carbon makes the martensitic transformation of this phase possible during cooling from the tempering temperature [39, 72, 73, 172]. Martensitic transformation of the retained austenite takes place in part after tempering already at the temperature by 50-100°C lower than the temperature ensuring the maximum secondary hardness [39]. However, nearly the entire retained austenite is transformed into martensite during cooling after tempering at the temperature lower by 20-30°C than the maximum secondary hardness temperature [39]. Tempering is performed usually two or three times. Structure composed nearly in whole from the high tempered martensite and carbides is obtained only after the second-, and in case of the cobalt steels, even after the third tempering.

Wrapping up, structure of the high-speed steels after tempering is composed of matrix, MC and M_6C (sometimes also M_2C) primary carbides, dispersive MC, M_2C and M_4C_3 secondary carbides, and of the retained austenite in particular cases. The MC and M_6C type coarse grained carbides (of the several micrometers order of magnitude size) crystallize directly from the liquid state or as precipitations nucleated along with the γ iron as a result of the eutectic reaction and, therefore, are called the primary carbides. Just these carbides demonstrate the highest hardness of all the structural components. Simultaneously they have the decisive effect on the tool wear resistance. The M_2C type carbides may precipitate also in certain crystallization conditions or when the steel contains the Mo and V alloying elements. The matrix is the tempered martensite. The fine (dispersive) carbides of the MC, M_2C and M_4C_3 types (of the several dozen nanometers order of magnitude size) precipitate during tempering. They influence the secondary hardness effect occurring in the high-speed steels and, therefore, are also called the secondary carbides. Analysing the sequence of development of phases in the structure, they originate at the endmost stage of forming the final structure of the high-speed steels. The variety of the alloy additions occurring in the high-speed steels (C, W, Mo, V, Si, Cr, Nb, Ti, Co) makes them the extraordinarily complex multi-phase system. The diversity of transformations, physical relationships, decides that their structural investigations call for using the most subtle investigation methods employed in the materials engineering.

One could judge that the dynamic development of the new ceramic-, ceramic-carbide materials, cemented carbides, and also using the coating technologies for these materials to reduce of their wear and extend the tool service time will result in the gradual abandoning of using the high-speed steels [191]. However, small ductility demonstrated by the sintered- and ceramic tool materials causes that they do not feature competition for the high-speed steels, and these both material groups should be considered as complementary (Fig. 3).

However, the high-speed steels still remain the dominating material in cases where a high ductility is a property especially required from the materials for cutting tools and also their good machinability in the softened state.

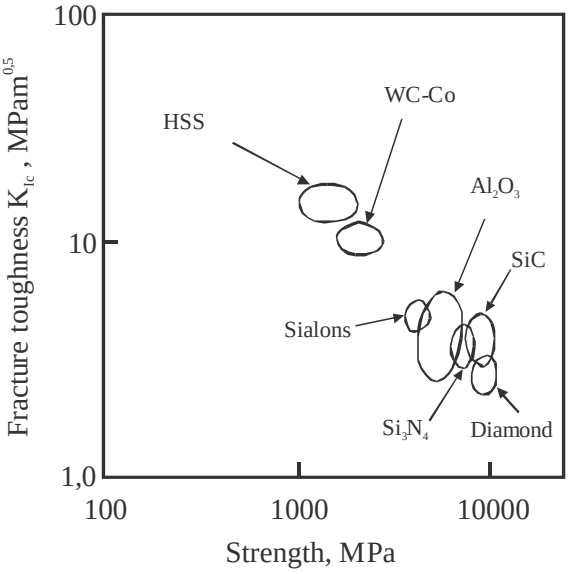


Fig. 3. Fracture toughness plotted against strength for a range of tool materials (the strength for high-speed steel and the WC-Co cemented carbide is the yield strength, for the other materials the compressive strength has been plotted) [149]

Resistance of the tool to failures, is - apart from its durability - the most important property from the tool user's point of view. Hardness alone cannot be the property deciding the material quality in case of the high-steels with their secondary hardness effect, as the high-speed steels with the same hardness, yet different microstructure, may have different fracture toughness [85, 116, 165, 166]. This fact was the root of many research projects focused on determining the relationships between the steel microstructure and its fracture toughness [132, 157, 162, 163, 165, 166, 196, 197]. Results of works [161, 164], show that the primary carbides may play an important role, while not only their volume fraction in the structure is important, but also their size and distribution in the matrix, expressed by, e.g., the average distance among them. The significance of the carbides size for the steel fracture toughness seems to be questionable, as there is an opinion that carbides with the conventional average size, distributed evenly in the matrix guarantee the best properties. The mechanism of crack propagation in steels confirmed by investigations [128, 157, 160] indicates that such segregation of carbides does not create a crack propagation barrier and material failure progresses many times solely on the carbide - matrix phase boundary. Therefore, one may believe that big carbides with dimensions exceeding the crack propagation front (plastic deformation zone) may be advantageous for improvement of the steel fracture toughness. They feature, when the cracks encounters them, a certain barrier slowing down the cracking process. The next phase, to which effect on fracture toughness is attributed, is the retained austenite. Earlier investigations of the high-speed steels were focused, among others, on determining their treatment parameters ensuring the minimum fraction of the retained austenite in steel structure, as the undesirable phase. However, investigations results [116, 163, 165, 196] show that austenite as a phase with much better plastic properties than martensite may improve the steel fracture toughness. A separate problem remains the issue of its distribution in structure and of the stabilisation method on the steel plastic properties [118]. Investigations of the effect of the primary austenite grain size depending on the austenitizing temperature are closely connected with this issue [157].

In the area of the high-speed steels secondary hardness investigations, pertaining the effect of the alloy elements and their heat-treatment parameters, the problem seems to be explored quite well and its thorough analysis was presented in works [29, 39, 62, 63, 114, 134, 216].

Only a few literature sources mention attempts to develop the alternative fracture toughness calculation methods for steel and other metal materials [98, 101, 136, 132, 178]. They are based on investigation results of the fracture toughness K_{Ic} or impact toughness. In cases of hardness modelling of the high-speed steels the literature sources indicate that they refer to the particular sintered steels types only [40, 135]. However, in own works [92, 103], research was carried out on development of the high-speed steels hardness model for the possibly broad range of grades of these steels [41, 45]. Genetic programming methods [98], artificial neural networks [101, 132], statistic methods [128, 174] and finite element method [193, 202, 203, 204] are used as computer modelling tools.

1.2. Computational Material Science and its role in design of new materials

Progress in the area of materials engineering is connected inseparably with employment and development of mathematical modelling, numerical methods, computational intelligence methods, and artificial intelligence. Computer modelling and simulation make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application. Therefore, modelling becomes the indispensable tool in materials science and materials engineering ensuring the chemical and physical description of materials in a broad scale both of length and time. This is connected with the need to investigate behaviour of materials in various scales, from atomic, through the mezo- to macro scales, employing knowledge of physics and chemistry principles pertaining to the solid matter state and properties. In this way, the contemporary materials science, and especially materials design, whose essence is computer simulation for evaluation of materials properties in the virtual environment, makes adjustment possible of their chemical composition and structure to the set of properties required for the new materials and products, before fabrication of these materials [5, 74, 154, 155].

One should differentiate two aspects of materials design. The first one, referring to selection of the material for the particular product from those developed and known to date [5, 27, 30, 84, 137, 138], and the second one connected with development of new materials for applications undefined so far, or materials meeting the service requirements better [59, 74, 147, 159, 171,

179]. Just in this second aspect it is especially important that the new materials solutions are reached not with the trial and error method, but with the mathematical or physical modelling, and the optimum solution is obtained with computer assistance without the need to carry out the time consuming and costly experiments. Knowledge of phenomena - electrical, magnetic, mechanical, thermal, structural or others, and their further skilful exploration taking into account the theory pertaining to their fundamentals, using the contemporary modelling methods (e.g., artificial intelligence), analytical techniques and advanced investigation methods explaining behaviour of materials, makes design of new materials possible, with properties which meet best their practical application requirements (Fig. 4). Activities mentioned above feature the area of interest of the new engineering specialization - Computational Materials Science (called also Materials Informatics).

Knowledge discovery in databases (KDD) and data exploration (data mining) in the existing interdisciplinary databases are useful when there is no generally accepted theory pertaining to the phenomenon or model describing it [86]. Works from the area of diagnostics of machinery [19, 150] are an example of research carried out in this field at the Faculty of Mechanical Engineering. These techniques may feature often the indispensable tool making integration possible of the scientific information in the form of, e.g., investigation results with the existing theory in discovery of the new materials [109, 111, 112].

It seems that in case of domains like biology, pharmacy, astronomy, diagnostics of machinery or social sciences, use of computer science techniques is relatively advanced. One can judge, however, in case of materials engineering, that applications, especially of the advanced computer science techniques, are in their infancy. One may suspect the reason for that in specific features of the domain like the materials engineering, where pursuit of the experiment result is a time consuming process and requires using many sublime techniques and highly specialised equipment. As a consequence, the resources of the experimental data are not that extensive as in case of other science branches and still remain scattered to a relatively great extent. Currently, one can recognise works of Ashby with his associates [5, 6, 214] as the most systematized in this area. Merging the determined phenomenological relationships with the discrete data contained in materials catalogues yielded a crop as development of the materials classification models in the form of the so called "maps" presenting in a multivariant way materials properties according to a standardized template (Fig. 5). What is important, information like structure-properties for materials belonging to different classes were put together for the first time.

Admitting the unquestionable value of this approach one should; however, mention its certain limitations in the area of prediction both within the space of the developed maps and outside of this space. One may not freely extrapolate properties of materials from one class to another (materials from different classes, e.g., ceramics and steel) without taking into account a number of limitations, e.g., manufacturing technology or other properties, like e.g., density.

The main task of the Computational Materials Science is integration of the materials science knowledge and computer science tools (Fig. 6) to find the new, undiscovered yet relationships and development of materials models based on the knowledge, which was acquired in experimental research over many years.

Research in the area of mathematical modelling, computational intelligence, and artificial intelligence indicate to the big potential connected with using the hybrid models [78]. Merging methods in one model makes analysis possible of a broader problem space, and - which is even more important - benefiting from advantages of every method and achieving the synergetic effect. Assumption that these methods are complementary is the base for development of such solutions.

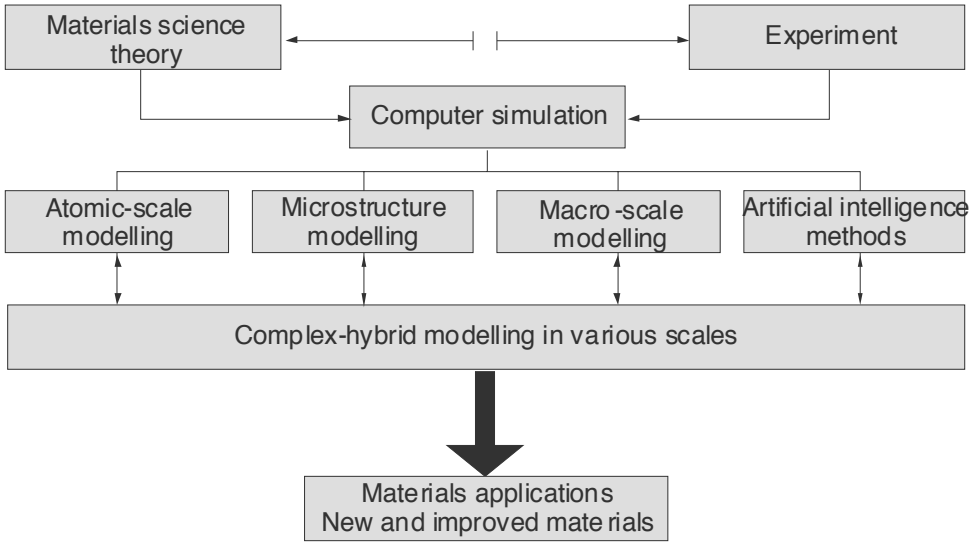


Fig. 4. Relationships among the materials science theory, computer simulation, and experimental activity [31]

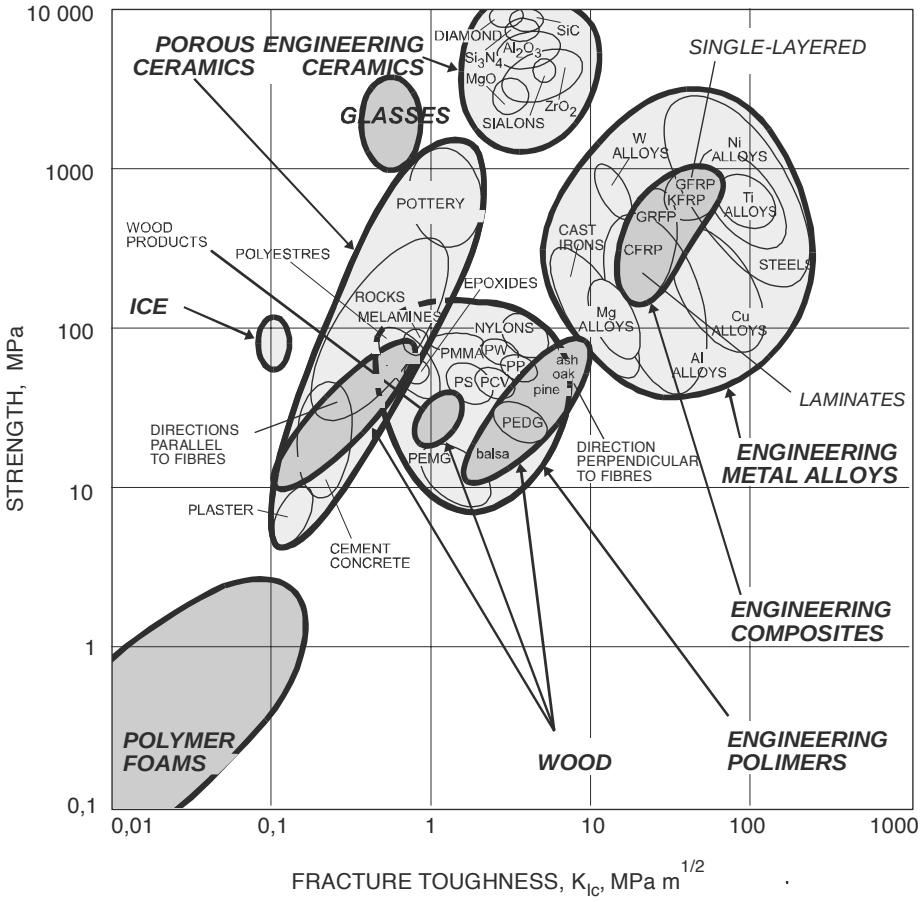


Fig. 5. Example of Ashby map - comparison of strength and fracture toughness (elaborated in [31])

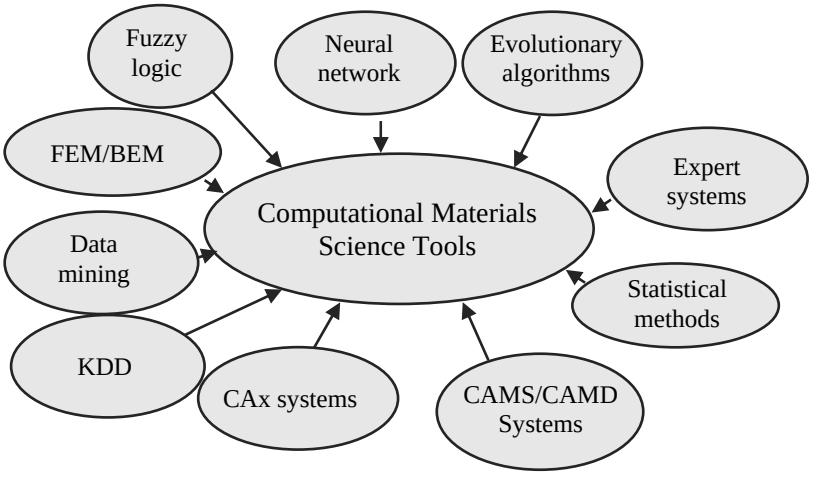


Fig. 6. Computational Materials Science Tools

Solving tasks from two classes is possible using computer tools, including computer simulation:

- Simple (analysis) where forecasting of materials properties is carried out depending on their chemical composition, structure and processing state.
- Reverse (synthesis) where material composition is defined and its processing state, which ensure acquiring properties required by its user or designer.

The new materials design problems feature, in the prevailing number of cases, reverse tasks, where it is necessary many a time to work out a new material demonstrating a set of many mechanical-, service-, economic-, or ecological properties. In this case, carrying out these tasks is possible based on the existing experimental data resources and using the artificial intelligence tools.

In the hybrid strategies systems composed from the artificial neural networks and finite element methods are used. They are characteristic of different integration levels resulting from the realised analysis type and are used for solving tasks of various types. An interesting approach to development of hybrid systems is merging the finite element method and evolutionary algorithms [16].

The artificial neural networks are also often used in conjunction with other computational intelligence methods and statistical methods. Merging the artificial neural networks with one of the optimization methods, based, for example, on genetic algorithms, makes working out possible of many algorithms dedicated to solving their particular problems.

The advantages of hybrid methods employing the computational intelligence elements used since long in many branches of science in Poland seem to be unnoticed in the area of materials engineering.

2. Goal, thesis, and scope of the work

The available research results pertaining to the high-speed steels and new computational tools, especially the artificial intelligence tools, provide the opportunity to extend the research area on these materials, among others, to reduce their manufacturing costs by replacing the time consuming and costly metallurgical processes by analyses and simulations carried out using computer tools. Significant reduction of time needed for analyses is an essential factor, as employment of the new techniques makes it possible to avoid a lot of the labour consuming experimental research and replacing it with computer simulations whose correct results feature, many a time, the main source for further analyses.

Bibliography review and results of the own research carried out to date make it possible to formulate the following dissertation thesis:

Based on results of the experimental research carried out to date using the artificial intelligence tools it is possible to design the new high-speed steels demonstrating the required combination of hardness and fracture toughness using solely computer simulation, with no need to carry out experimental research.

However, **the main goal of the research carried out is development of the design methodology for new materials demonstrating a set of the required properties, based on the existing experimental research results resources using the contemporary artificial intelligence methods.**

For the high-speed steels design, as a task which is the optimization one because of the computational method employed, it was assumed that the criterial properties are hardness and fracture toughness expressed by the fracture toughness K_{Ic}. Moreover, the heat treatment technological parameters are optimised also, i.e., austenitizing-, and tempering temperatures. Achieving the main goal required carrying out the following partial tasks, consisting in:

- development of the high-speed steels hardness model making it possible to compute hardness based on the steel chemical composition and its heat treatment parameters (austenitizing and tempering temperatures).
- development of the model making it possible to determine the high-speed steels fracture toughness, based on the steel chemical composition and its heat treatment parameters (austenitizing and tempering temperatures).

Moreover, the supplementary research was done of the structure and mechanical properties of the selected high-speed steel grades to complement the set of the relevant data collected so far, necessary for the experimental verification of the developed material models. Investigations of the mechanical properties included hardness tests of steel in the hardened state and after tempering and measurements of the fracture toughness K_{Ic}. Microscope examinations included the volume fraction of carbides and their segregation with the light microscopy methods and scanning electron microscopy methods using the image analysis system.

The scope of the research work carried out is shown in Figure 7.

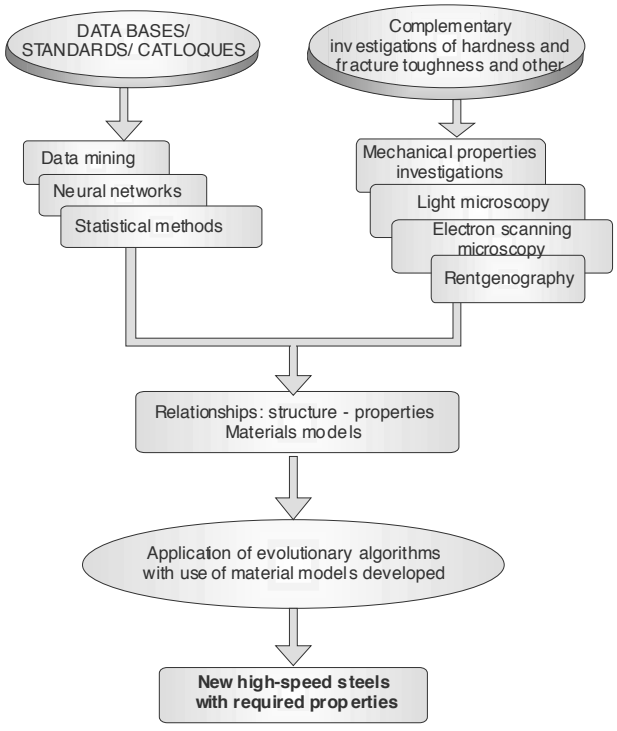


Fig. 7. Scope of the research work carried out

3. Material for investigations and research methodology

The following data feature the base for development of models making it possible to compute the high-speed steels properties based on their chemical composition and austenitizing- and tempering temperatures only:

- investigation results of the newly developed high-speed steels [62, 63, 114, 134, 216],
- data contained in the relevant standard [174],
- data from the high-speed steels manufacturers' catalogues [110],
- results of the own supplementary investigations of the selected high-speed steels grades.

Alloy elements' concentrations for the newly developed steels, collected from standards, and from catalogues of steel manufacturers are presented in Tables 1 - 3 respectively. The austenitizing temperature range for which the data was processed is 1120°C-1280°C, and the tempering temperature range is 480°C-630°C.

For development of models making it possible to compute the high-speed steels hardness based solely on their chemical composition, as well as on their austenitizing- and tempering temperatures, the multiple regression statistical method and the artificial neural networks were used. In case of the steel fracture toughness model the artificial neural networks were used.

The supplementary investigations carried out for verification of the developed models were made for the selected high-speed steels grades with chemical compositions shown in Table 4. Their heat treatment parameters which were determined individually for each steel grade are shown in Tables 5-7. Bars from the high-speed steels were soft annealed before machining in the argon protective atmosphere for 1.5 h at the temperature 10°C higher than A_{c1k} with the subsequent cooling with isothermal holding at the temperature of 740°C. The material was furnace heated to temperature of (A_{c1k}+10°C) with the isothermic stop at 550°C; the bars were furnace cooled to 500°C followed with air cooling next. Heat treatment of the test pieces was carried out in the battery of the salt bath furnaces by heating them up to the austenitizing temperature in two stages for 10 min at the temperatures of 550 and 850°C. Austenitizing of the test pieces was carried out in the salt bath for 100-120 s. Test pieces were hardened gradually with cooling for 5 min in the salt bath with the temperature of 550°C and were air cooled next to the temperature of ca. 80°C. Immediately after hardening the test pieces were tempered twice for 2 h.

Table 1.
Chemical composition of the newly developed high-speed steels used for development of the secondary hardness models [62, 63, 114, 134, 216]

Steel type	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
9-2-2+Si	0.94	4.5	9.0	1.72	1.8	0.0
9-2-2+Si+Ti	0.93	4.5	9.0	1.88	1.7	0.0
9-2-2+Si+Ti (1)	0.93	4.7	8.9	2.0	1.5	0.0
9-2-2+Si+Nb	0.94	4.5	9.0	1.85	1.67	0.0
9-2-2+Si+Nb (1)	0.92	4.5	9.1	1.87	1.3	0.0
9-2-2-5	0.94	4.4	8.8	2.4	1.6	5.2
11-0-2+Si	0.93	4.5	11.2	0.0	1.8	0.0
11-0-2+Si+Ti	0.98	4.6	10.8	0.0	1.6	0.0
11-0-2+Si+Ti (1)	0.93	4.4	10.6	0.0	1.4	0.0
11-0-2+Si+Nb	0.94	4.5	11.4	0.0	1.6	0.0
11-0-2+Si+Nb (1)	0.93	4.5	11.5	0.0	1.3	0.0
11-0-2-5	0.91	4.5	10.9	0.0	1.8	5.2
11-2-2+Si	1.1	4.4	11.3	1.88	1.8	0.0
11-2-2+Si+Ti	1.05	4.5	11.2	1.9	1.7	0.0
11-2-2+Si+Ti (1)	1.04	4.2	11.1	1.8	1.5	0.0
11-2-2+Si+Nb	1.0	4.4	11.2	1.95	1.7	0.0
11-2-2+Si+Nb (1)	1.02	4.5	11.3	1.82	1.4	0.0
11-2-2-5	1.03	4.5	11.3	1.94	1.8	4.9

Table 2.
Chemical compositions of high-speed steels specified in their relevant standard [174] used for development of the secondary hardness models

Steel grade	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
HS18-0-1	0.78	4.15	17.95	0	1.1	0.0
HS0-4-1	0.81	4.15	4.25	1.1	1	0.0
HS1-8-1	0.82	4.15	8.5	2.85	1.2	0.0
HS6-5-2	0.84	4.15	4.95	6.3	1.9	0.0
HS1-4-2	0.9	3.95	4.45	1.8	1.95	0.0
HS6-5-2C	0.9	4.15	4.95	6.3	1.9	0.0
HS6-5-2-5	0.91	4.15	4.95	6.3	1.9	4.75
HS3-3-2	0.99	4.15	2.7	6.3	2.35	0.0
HS2-9-2	1.0	4.15	8.7	1.7	1.95	0.0
HS6-6-2	1.05	4.15	6	6.3	2.45	0.0
HS2-9-1-8	1.1	4.15	9.5	1.55	1.1	8.0
HS6-5-3	1.2	4.15	4.95	6.3	2.95	0.0
HS10-4-3-10	1.28	4.15	3.55	9.5	3.25	10
HS6-5-3-8	1.28	4.15	5.0	6.3	2.95	8.4
HS6-5-3C	1.29	4.15	4.95	6.3	2.95	0.0
HS6-5-4	1.33	4.15	4.6	5.6	3.95	0.0

Table 3.
Chemical compositions of high-speed steels specified in Erasteel manufacturer catalogues used within the project framework for development of the secondary hardness models [110]

Steel type	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
1-5-1-8	0.72	4.0	5.0	1.0	1.0	8.0
18-0-1	0.75	4.1	18	0	1.1	0
2-9-1	0.83	3.8	8.5	1.8	1.2	0
0-4-1	0.84	4.0	4.2	0	1.1	0
1-5-2	0.89	4.0	4.5	1.2	1.9	0
6-5-2	0.9	4.2	5.0	6.4	1.8	0
2-5-1-2	0.91	3.7	5.0	1.8	1.2	2.5
6-5-2-5	0.93	4.2	5.0	6.4	1.8	4.8
3-3-2	0.99	4.1	2.7	2.8	2.4	0
2-9-2	1.02	3.8	8.6	1.8	1.9	0
5-6-2-8	1.05	4.0	6.0	5.0	1.6	7.8
6-6-2	1.05	4.0	6.3	6.3	2.5	0
2-9-1-8	1.08	3.8	9.4	1.5	1.2	8.0
4-8-3	1.2	4.2	8.5	3.5	3.0	0
6-5-3	1.2	4.1	5.0	6.3	3.0	0
10-4-3-10	1.27	4.0	3.6	9.5	3.2	10.0
12-1-4	1.28	4.2	0.8	12	3.8	0
6-5-4	1.3	4.2	4.5	5.6	4.0	0
9-4-3-11	1.41	4.2	3.6	8.8	3.4	11.0

Table 4.
Chemical compositions of high-speed steels used in supplementary investigations

Steel grade	Mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
HS 6-5-2	0.9	4.19	6.13	4.84	1.99	0.02
HS 18-0-1	0.85	4.08	17.57	0.56	1.3	0.07
HS 10-4-3-10	1.26	4.28	9.04	3.31	3.54	9.92

Table 5.
Austenitizing- and tempering temperatures used for HS6-5-2 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1150	500	550	580
1180	500	550	580
1225	500	550	580
Soft annealing temperature 860°C			

Table 6.
Austenitizing- and tempering temperatures used for HS18-0-1 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1180	520	550	580
1220	520	550	580
1255	520	550	580
1280	520	550	580
Soft annealing temperature 860°C			

Table 7.
Austenitizing- and tempering temperatures used for HS10-4-3-10 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1180	540	560	580
1200	540	560	580
1225	540	560	580
1240	540	560	580
Soft annealing temperature 880°C			

Hardness tests with Rockwell method in scale C were carried out on the automatic ZWICK ZHR hardness tester Each time 15 to 25 readings were made and their arithmetic average was assumed as the test result, after screening them for the eventual doubtful readings

Crack resistance in the plane state of strain is expressed by the K_{Ic} coefficient value. It is a measure of the material's resistance to crack propagation in conditions in which the plane state of strain prevails in vicinity of its vertex, while the plastic strain is limited. Crack resistance of metals in the plane state of strain K_{Ic} is determined by loading the test piece with the initiation fatigue crack. Investigation of the K_{Ic} factor was carried out according to standard [173] on the MTS 810.22 testing machine made by MTS SYSTEMS GmbH using the three-point bending method. Dimensions of test pieces for investigation of fracture toughness K_{Ic} is presented in Figure 8. Width ***W***=20 mm and thickness ***B***=10 mm were used for investigations, and the slit length ***a*** is between 0.45 and 0.55 of the width ***W***. Chevron-notch was used in the examined test pieces, guaranteeing the linear shape of the nucleated fatigue notch (Figs. 8 and 9).

Microscope examinations of the carbides' fractions and of their segregation were made with the scanning electron microscope methods on SUPRA 25 ZEISS device. To determine the fraction of carbides analysis of 15 measurement fields was used to evaluate parameters describing their segregation, i.e., their average diameter, sphericity, and the average distance between carbides. Observations of the steel structure were made using the light microscopy methods on the LEICA MEF4A device with the image analysis system.

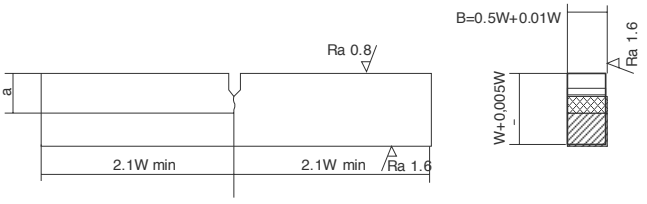


Fig. 8. Bend-test specimen [173]

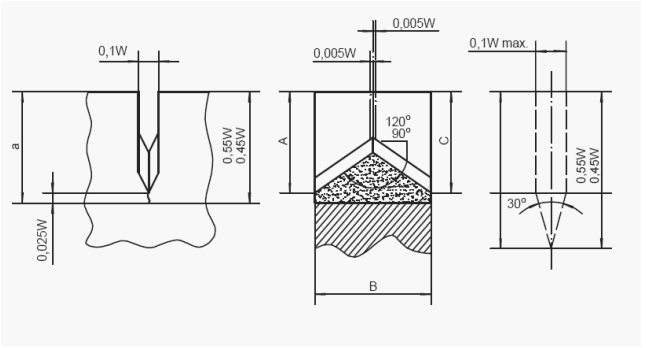


Fig. 9. Fatigue crack initiating notches and maximum allowable notch sizes along with the fatigue crack [173]

4. Complementary high-speed steels properties research results

4.1. Hardness test results

Hardness tests of steel in Rockwell C scale were made on the transverse section of the test pieces subjected previously to the fracture toughness K_{Ic} investigation, making 15-25 readings. Test results for each of the investigated steels are presented in Tables 8-10 and their graphical representation is shown in Figures 10-12. Standard deviation values of the hardness test values did not exceed 0.6 HRC in any case.

Table 8.
Hardness test results for HS6-5-2 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	520	550	580
	Hardness, HRC		
1150	62.06	63.58	60.45
1180	65.25	65.58	63.64
1225	65.57	66.15	63.71

Table 9.
Hardness test results for HS18-0-1 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	500	550	580
	Hardness, HRC		
1180	65.37	65.3	63.3
1220	66.52	66.59	65.36
1255	66.16	66.87	65.92
1280	66.53	67.05	66.44

Table 10.
Hardness test results for HS10-4-3-10 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	540	560	580
	Hardness, HRC		
1180	66.53	66.89	65.94
1200	66.87	67.39	66.17
1225	67.98	68.31	67.56
1240	68.52	68.54	67.49

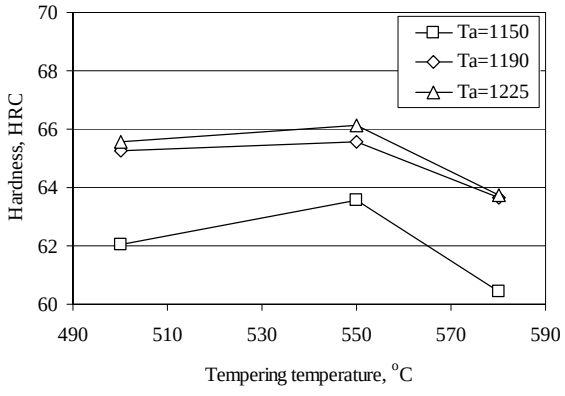


Fig. 10. Hardness test results for HS6-5-2 steel

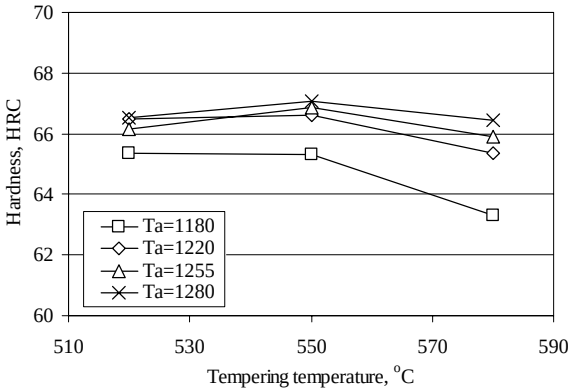


Fig. 11. Hardness test results for HS18-0-1 steel

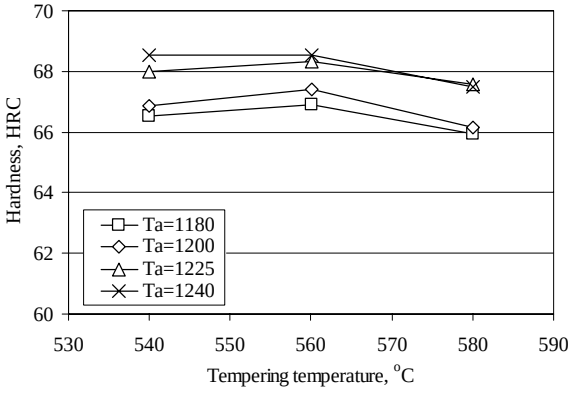


Fig. 12. Hardness test results for HS10-4-3-10 steel

4.2. Investigation results of the fracture toughness K_{Ic}

Crack resistance in the plane state of strain is expressed most often by the K_{Ic} coefficient value. The chevron-notch was used for the test pieces and the tests were made on three specimens for each heat treatment variant. Test results for each of the investigated steels are shown in Tables 11-13. The obtained test results are presented in the graphical format in Figures 13-15. Moreover, comparison of hardness and fracture toughness K_{Ic}. value for the investigated steels are shown in Figures 16-18.

Table 11.
Test results of K_{Ic} coefficient for HS10-4-3-10 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	520	550	580
	Fracture toughness K_{Ic}, MPa·m$^{1/2}$		
1150	20.63	17.53	21.63
1180	15.9	13.6	17.7
1225	15.23	13.67	17.0

Table 12.
Test results of K_{Ic} coefficient for HS18-0-1 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	500	550	580
	Fracture toughness K_{Ic}, MPa·m$^{1/2}$		
1180	14.97	14.97	17.7
1220	13.3	13.3	15.8
1255	14.53	12.03	14.5
1280	14.93	13.97	15.6

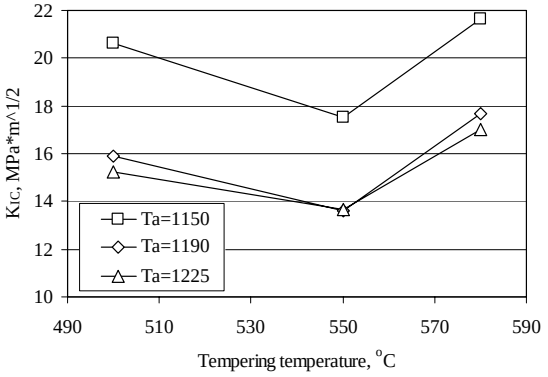


Fig. 13. Test results of fracture toughness K_{Ic} for HS6-5-2 steel

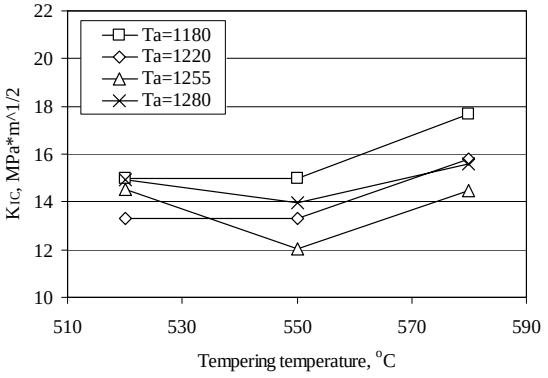


Fig 14. Test results of fracture toughness K_{Ic} for HS18-0-1 steel

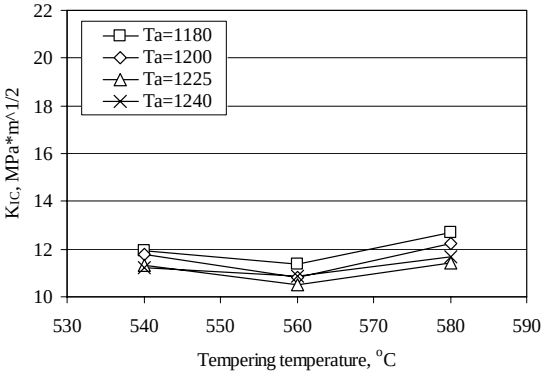


Fig. 15. Test results of fracture toughness K_{Ic} for HS10-4-3-10 steel

Table 13.
Test results of K_{Ic} coefficient for HS10-4-3-10 steel

Austenitizing temperture, °C	Tempering temperature, °C		
	540	560	580
	Fracture toughness K_{Ic}, MPa·m$^{1/2}$		
1180	11.95	11.35	12.7
1200	11.8	10.8	12.23
1225	11.3	10.53	11.4
1240	11.2	10.87	11.67

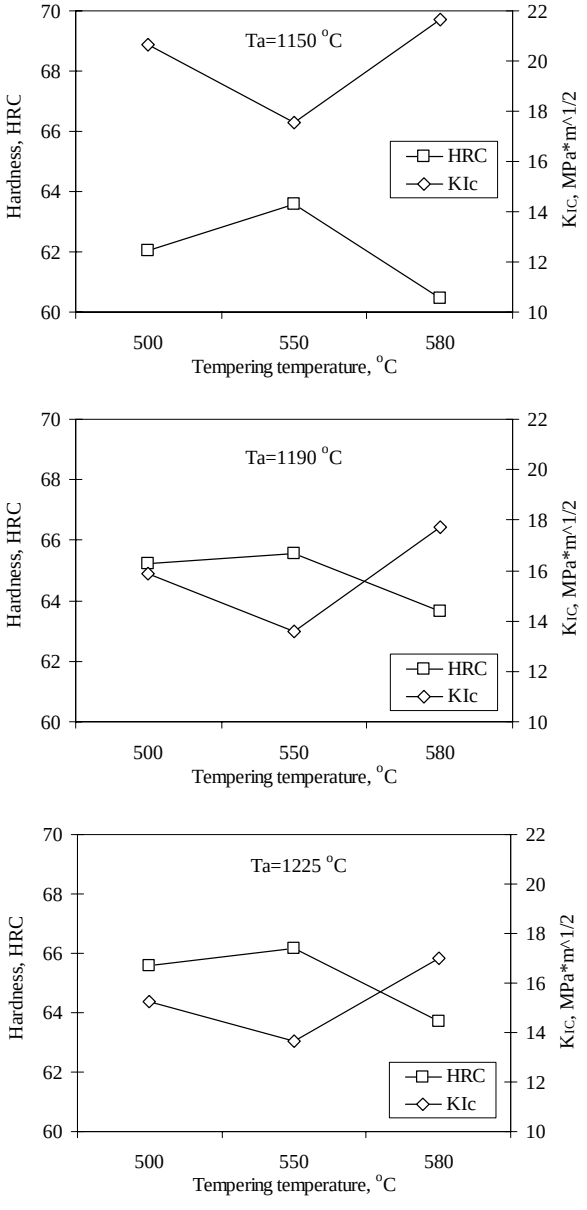
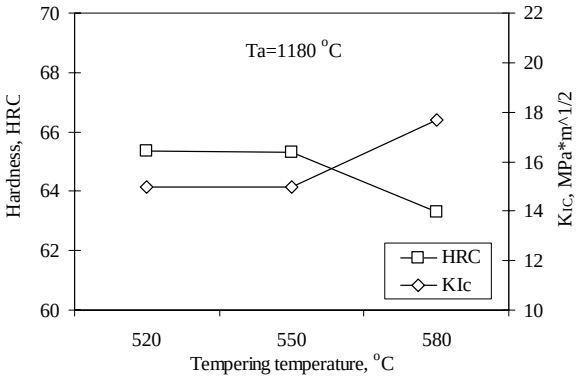
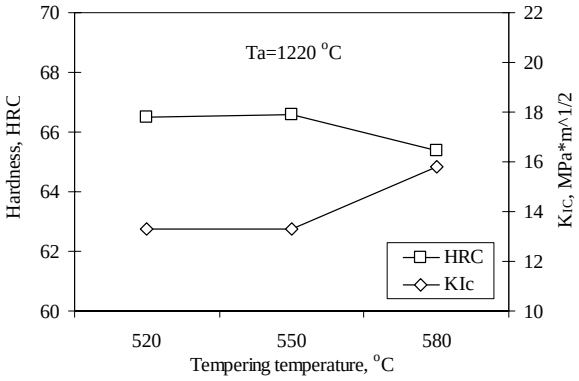
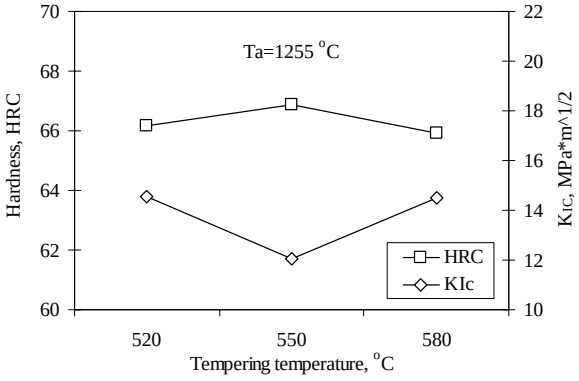


Fig. 16. Comparison of hardness and fracture toughness K_{Ic} test results for HS6-5-2 steel







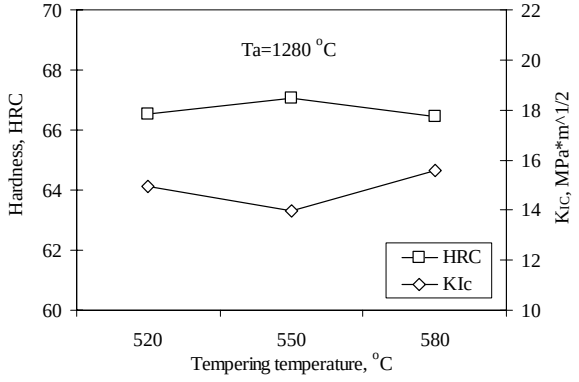
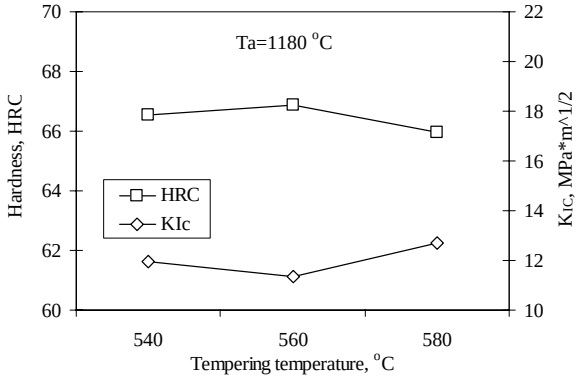
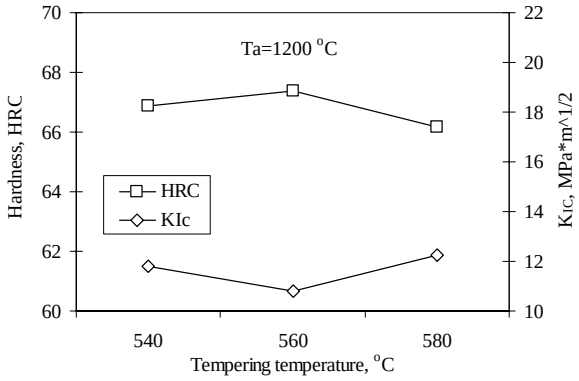
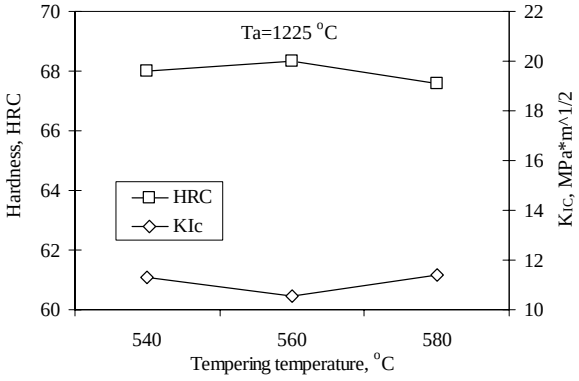


Fig. 17. Comparison of hardness and fracture toughness K_{Ic} test results for HS18-0-1 steel







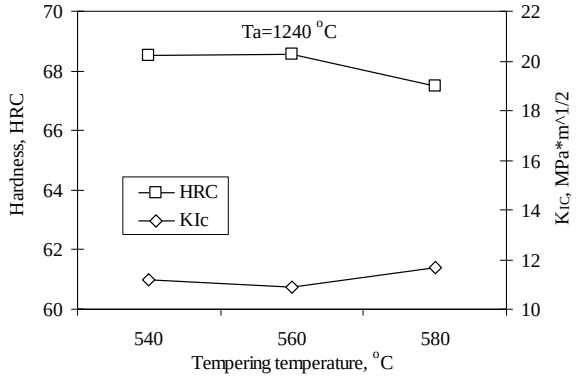


Fig. 18. Comparison of hardness and fracture toughness K_{Ic} test results for HS10-4-3-10 steel

4.3. Structure examinations

The goal of the structure examinations carried out was determining the volume fraction of eutectic carbides and their average size. The un-etched steel structure images were used acquired on the scanning microscope, made using the backscattered electrons (BSE). Assessment of carbides fractions for each steel and for each heat treatment variant was made based on analysis of 15 images. Leica QWin computer image analysis system was used for that.

Statement of results of carbides fraction for each steel are presented in table 14 and in Figures 19-21. Exemplary structures obtained on the scanning microscope are presented in Figs. 22-24, and on the light microscope in Figures 25-27.

Table 14.
Test results of carbides fractions for each steel

Austenitising temperature°C	Tempering temperature, °C	Carbides fraction, %	Standard deviation, %	Mean carbides diameter, μm
HS6-5-2 steel				
1150	500	15.4	0.59	1.17
	550	12.9	0.52	1.38
	580	15.9	0.76	1.06
1180	500	10.4	0.55	1.33
	550	10.2	0.32	1.39
	580	9.7	0.22	1.42
1225	500	10.8	0.41	0.97
	550	9.3	0.77	0.92
	580	11.7	0.20	1.34
HS18-0-1 steel				
1180	520	19.5	0.81	1.52
	550	16.5	0.34	1.16
	580	17.4	0.44	1.42
1220	520	16.9	0.64	1.49
	550	15.5	0.43	1.37
	580	14.6	0.67	1.33
1255	520	13.1	0.36	1.33
	550	13.5	0.64	1.59
	580	13.2	0.51	1.62
1280	520	10.7	0.28	1.92
	550	11.9	0.64	2.08
	580	11.4	0.49	1.95
HS10-4-3-10 steel				
1180	540	10.6	0.55	1.37
	560	9.7	0.47	1.28
	580	12.0	0.65	1.34
1200	540	13.3	0.69	0.97
	560	10.3	0.59	1.34
	580	11.4	0.66	1.29
1225	540	9.9	0.68	1.32
	560	9.3	0.68	0.98
	580	10.0	0.68	1.25
1240	540	9.7	0.83	0.91
	560	9.5	0.93	0.99
	580	10.4	0.79	0.76

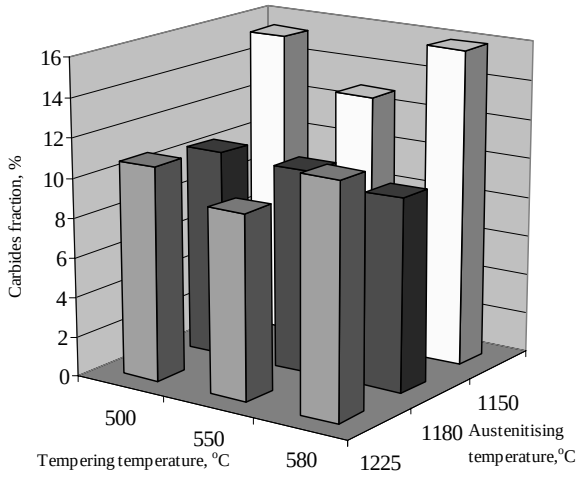


Fig. 19. Volume fraction of primary carbides in HS6-5-2 steel

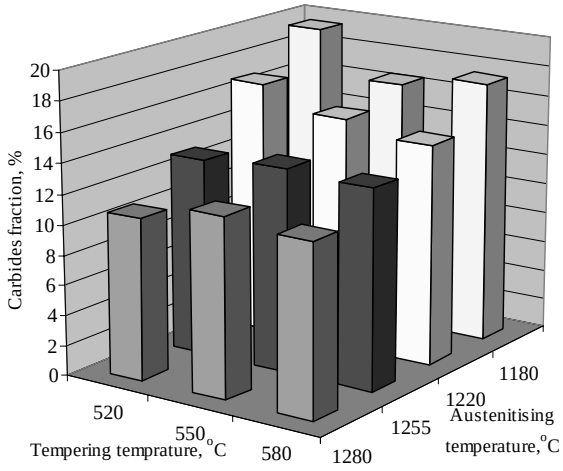


Fig. 20. Volume fraction of primary carbides in HS18-0-1 steel

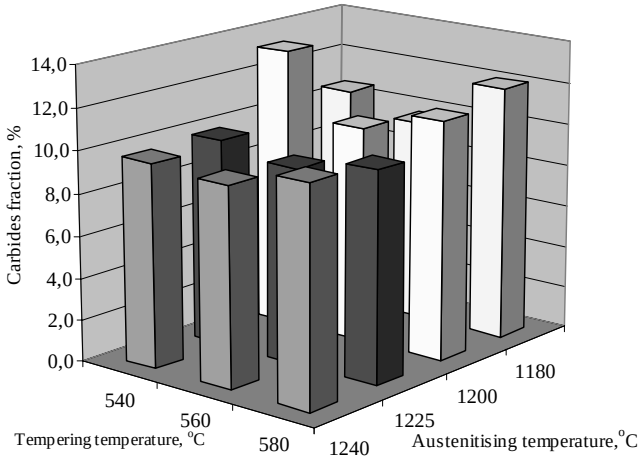


Fig. 21. Volume fraction of primary carbides in HS10-4-3-10 steel

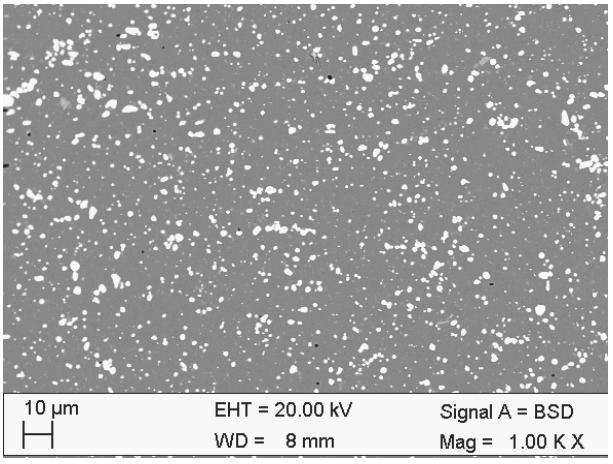


Fig. 22. Unetched structure of HS6-5-2 steel, Ta=1150°C, Tt=500°C

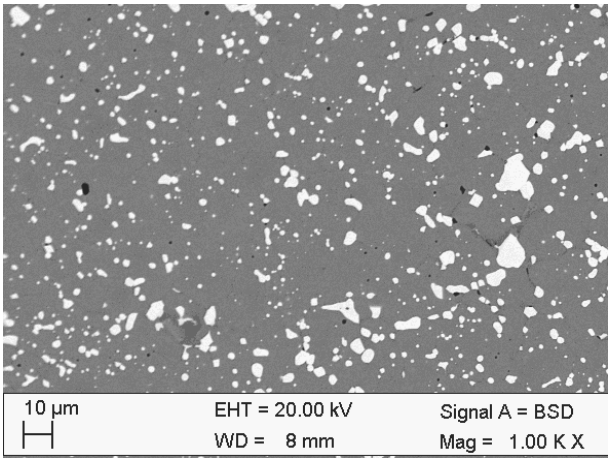


Fig. 23. Unetched structure of HS18-0-1 steel, Ta=1255°C, Tt=550°C

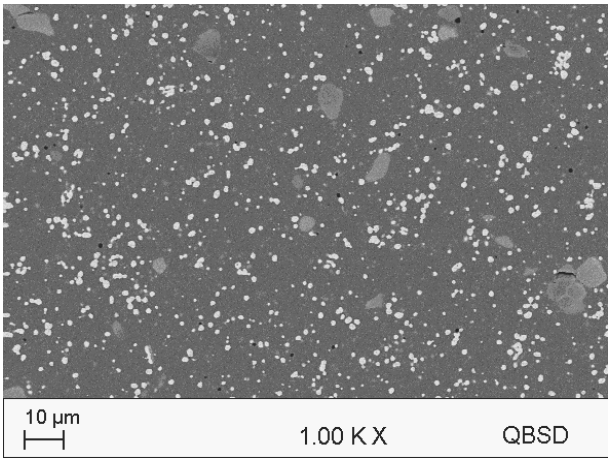


Fig. 24. Unetched structure of HS10-4-3-10 steel, Ta=1225°C, Tt=560°C

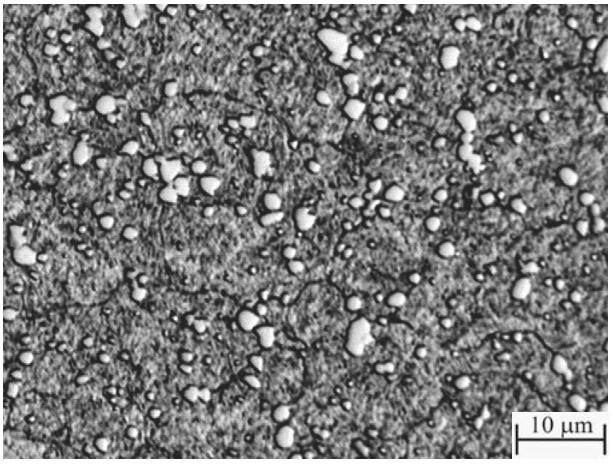


Fig. 25. Etched structure of HS6-5-2 steel, Ta=1150°C, Tt=500°C

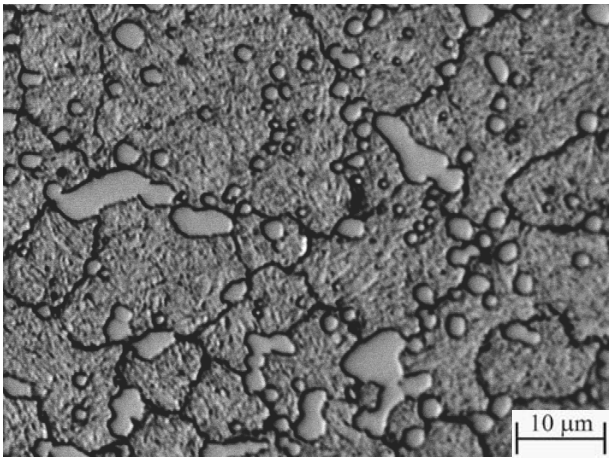


Fig. 26. Etched structure of HS18-0-1 steel, Ta=1255°C, Tt=580°C

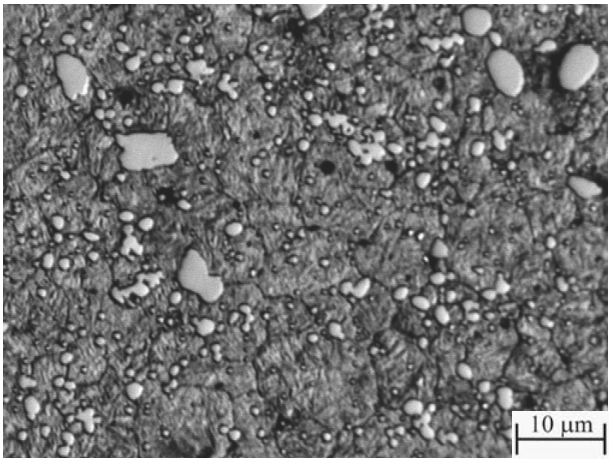


Fig. 27. Etched structure of HS10-4-3-10 steel, Ta=1180°C, Tt=580°C

5. Modelling of the high-speed steels properties

The main goal of the research carried out is development the design methodology of the new high-speed steels with the required service properties. It was decided that hardness and crack propagation resistance expressed by the fracture toughness K_{Ic} will be the criteria used during the high-speed steels design. Therefore, the following models were developed first:

- high-speed steels hardness,
- steel fracture toughness K_{Ic}

The first model developed makes computation possible of the high-speed steel hardness based solely on the steel chemical composition and its heat treatment parameters, i.e., austenitizing- and tempering temperatures. Its development was based on works [62, 63, 114, 134, 216] focused on the influence of the alloy elements on the secondary hardness effect, and also on data contained in catalogues and relevant standards referring to the high-speed steels [110, 174]. Results of earlier works [199] confirm that it is possible to use the catalogue and standard data to develop the assumed model which improves its adequacy and versatility.

The second model developed makes determining possible of the fracture toughness K_{Ic} of the high-speed based on the steel chemical composition and its heat treatment parameters, with no need to carry out numerous complex and time consuming metallurgical examinations. In this case results of the own investigations of the selected high-speed steel grades were used, presented in Table 4.

5.1. High-speed steels hardness models and their verification

For development of hardness models results were used of investigations carried out on the newly developed high-speed steels, relevant standards, and manufacturers' catalogues. Detailed data pertaining to alloy elements' concentrations for the newly developed steels, collected from standards, and from catalogues of steel manufacturers are presented in Tables 1 - 3 respectively. The austenitizing temperature range for which the experimental data was processed is 1120°C-1280°C, and the tempering temperature range is 480°C-630°C.

Results of the supplementary investigations were not used for development of models and were used only for the final experimental verification of the developed models.

As tools for development of models making computation of the high-speed steels hardness possible based solely on their chemical composition, as well as on their austenitizing- and tempering temperatures the following were used:

- statistical method of multiple regression,
- artificial neural networks.

The main assumption made first was that steel hardness depends on concentrations of the main alloy elements occurring in these steels: carbon, chromium, tungsten, molybdenum, vanadium, and cobalt, as well as on their austenitizing- and tempering temperatures.

In the multiple regression method the general form of the equation - model was used:

$$HRC = \sum_{i=1}^{k} a_i f_i(X) \tag{2}$$

where: a_i – coefficients of the regression equation, HRC - steel hardness, f_i - functions of the equation variables, X - vector of the equation variables, (X = [% C, % Cr, ..., Ta, Tt]).

Several dozen forms of equation (2) were analysed during research, and coefficients ai were determined using the classic regression method (least squares).

In the second high-speed steels hardness calculation method the artificial neural networks were used of the multilayer perceptron type, employing various learning methods. Use of a constant number of input neurons was decided (8) as a consequence of the main assumption that hardness depends on C, Cr, W, V, Co, and Co, as well as on the austenitizing- and tempering temperatures. The analysed networks had 1 output corresponding to the steel hardness. The numbers of hidden layers and neurons were modified in the investigations.

The adequacy of the developed models was checked by analysing the error between the calculated hardness and its corresponding hardness tested experimentally.

The average error for the tested data file was assumed as the criterion:

$$R = \sum_{i=1}^{N} \left(HRC_{ci} - HRC_{mi} \right) \tag{3}$$

where: N – test file size, HRC_{ci} – calculated hardness (i–th), HRC_{mi} – measured hardness (i–th).

The assumption was made that the model that would make it possible to obtain the calculation error ca. 1 HRC will be a valid one.

Statistical model

Based on the prepared experimental data set several dozen phenomenological mathematical models were analysed for computation of steel hardness based on the alloy elements concentrations and heat treatment of the high-speed steels.

Results of these mathematical models analysis indicate that hardness calculations for the various forms of the mathematical equation tend to the computation error value of 0.7 HRC. Therefore, model (4) demonstrating the computation error of 0.71 was assumed to be the best one and used in the next analyses, among others, computations of tempering curves for the selected steel grades, shown in Figures 28-34.

$$\begin{aligned} HRC = {} & a_1 C + a_2 Cr + a_3 W + a_4 Mo + a_5 V + a_6 Co + \\ & a_7 Ta + a_8 Tt + a_9 Ta^2 + a_{10} Tt^2 + a_{11}(Tt \cdot Ta)^{1/2} + \\ & a_{12} Ta/Tt \end{aligned} \tag{4}$$

where:

a_1 =	5.1	a_5 =	-0.81	a_9 =	0.37
a_2 =	-0.13	a_6 =	0.17	a_{10} =	-4.86
a_3 =	-0.06	a_7 =	-21.4	a_{11} =	58.23
a_4 =	0.11	a_8 =	-1.63	a_{12} =	-23.46

It should be noted that in case of the austenitizing- and tempering temperatures their readings were normalised by dividing them by 100. Therefore, using the developed mathematical models, the real temperature should be presented in this way as a variable in the model. So, e.g., if the real austenitizing temperature is 1200°C, then its value after normalising should be entered to the model, i.e., 12.

Neural network model

Next, the artificial neural networks were used for the secondary hardness modelling. Results of the experimental research, containing information about the chemical compositions and the steel hardness test results, shown in Tables 1-3, feature the base for the neural networks design. A set of 2714 reference standards was available, which may be considered as the sufficient number to develop the fully adequate neural networks model.

It was assumed, referring to the developed neural networks structure, that the network has 8 inputs, corresponding to concentration values of the six main alloy elements occurring in this steel group and to the austenitizing- and tempering temperatures, and one output, corresponding to hardness. The StatSoft STATISTICA Neural Networks v. 4.0 program was used for development, training, and testing of the neural networks.

Neural networks as the numerical modelling tool are more versatile tool, and capable to reproduce complex functions, than the statistical regression method used earlier. Adaptation of the neural networks to let them carry out the particular task does not require either specifying the algorithm and coding it to get the computer program, nor to formulate it in the particular mathematical model form. This process replaces training by employing a series of typical excitations and corresponding to them desired reactions.

In cases, when the physical nature of the phenomenon is not fully known, the main feature of the neural networks becomes especially desirable, i.e., capability to generalize their knowledge for the new data which was not presented during the training. Neural networks do not require collecting and continuous access to the entire domain knowledge, are tolerant to discontinuities, random noise, or gaps in the training set. This makes their use possible where problems occur with data processing and analysis, its classification or prediction.

In the artificial neuron mathematical model the input neuron signals are summed up with the relevant weight and subjected to the non-linear activation function (e.g., unit step function), which leads to obtaining the output signal y_i described by the formula [153]:

$$y_i = f\left(\sum_{i=1}^{N} W_{ij} x_j\right) \tag{5}$$

where: x_j (j=1,2,...,N) – input signals, W_{ij} - weight coefficients (weights), f() – activation function.

Neural networks are adaptable, which makes adjusting them possible to carry out the particular task by selection of structure and method, as well as the training parameters. The adaptive selection of weights occurs during the training process, between the processing elements, making network operation possible, consisting in reproduction of the input data into the output data with the possibly small error. Weight adjustment taking place in the consecutive cycles may be expressed with the relationship [153]:

$$W_{ij}(n+1) = W_{ij}(n) + \Delta W_{ij}(n) \tag{6}$$

where: n - training cycle number, $W_{ij}(n)$ – previous weight, $W_{ij}(n+1)$ – new weight connecting i-th neuron with the j-th one.

Network efficiency error, called the mean-square error, is described by the equation [153]:

$$Q(n) = \sum_{m=1}^{N_L} \varepsilon_i^{(L)^2}(n) = \sum_{i=1}^{N_L} (d_i^{(L)}(n) - y_i^{(L)}(n))^2 \tag{7}$$

where: $\varepsilon_i^{(L)}$ – error at the output of the i-th neuron of the last network layer (L), $d_i^{(L)}$ – reference signal, $y_i^{(L)}$ – signal at the neuron output.

Network training is carried out to minimise the error function. Methods that are used especially often include the gradient ones. Information about the steepest function value growth are included in the gradient vector which consists of the particular network weights partial derivatives of the error function vectors are modified according to equation [153]:

$$W(n+1) = W(n) + \mu p(W(n)) \tag{8}$$

where: $p(W(n))$ – direction of the error function minimisation, μ – learning coefficient.

Training method based on the error backpropagation algorithm was used as one of the methods employed for training the unidirectional multilayer networks. The error signal for this method is calculated starting from the output layer, through the hidden layers, in the direction of the input layer. The sum of the squared errors at the network output is calculated to determine the error function minimum, according to equation (7). The starting weights values are usually set randomly, and the Cauchy's method (steepest descent method) is used for their modification. The weights change rate modified by the algorithm depends on the learning coefficient. A low learning coefficient value leads to a very weak convergence, ensuring, however, the more stable and precise training process flow. If the error surface is not complicated, then increasing the learning coefficient makes reaching the acceptable error level possible faster, without the risk of overlooking its minimum. Introducing an additional element called momentum makes increasing the network learning rate possible, ensuring at the same time the weights modification process stability. The new direction of the error function minimum search using momentum, is expressed by the weighted sum of the current gradient and of the previously determined direction. The momentum factor makes it often also possible to leave the local error function minimum resulting in a weights change leading to the transient function value growth.

The next algorithm used for the neural networks training is the conjugate gradients algorithm. The error gradient, calculated during one training epoch, is a sum of error gradients for each case. In this method, search for the error function minimum proceeds along the selected directions on the error surface. For the function of a single variable this process is carried out in two stages. In the first stage, three points are searched for, out of which the middle one represents the error function value lower than the other two. The second stage boils down to reducing the search area and lasts until the minimum position is spotted with the satisfactory accuracy. Finding the minimum point makes the algorithm move to the next search of the linear error function minimum, carried out in the next epoch along the straight line making with the previous direction a conjugate one. The next step of the conjugate gradients algorithm does not deteriorate the result obtained before thanks to the conjugate directions determining method, ensuring preservation of the minimum values obtained before. Assumption that the error function is approximately quadratic in the local minima neighbourhood is the base for determining the conjugate directions. Updating of weights is

carried out once during one training epoch. The base for modification of weights features the gradient value averaged in respect to all cases presented in one epoch. Training the neural network using the conjugate gradients algorithm does not require defining the learning coefficient nor momentum value. Values occurring in this method, whose roles may be compared to the moment of inertia and learning coefficient are not constant but keep changing in the mathematically optimal way [153].

Several hundred neural networks were generated using the Statistica Neural Network program with the various numbers of neurons in the hidden layers. Some of them were eliminated at the initial design stage due to the excessive error or the excessive number of neurons in the hidden layers. Training error graph for every network was studied after completing the training process or in its course. Based on that the networks were checked if the overtraining did not take place and the overtrained ones were eliminated from the subsequent analysis. The average absolute error, quotient of standard deviations, and correlation coefficient were assumed as the network quality coefficients. Finally one network was selected, from the entire set of the developed networks -the multilayer perceptron with the 8-7-1 structure (i.e., 8 inputs, 7 neurons in the hidden layer, and 1 output), with the average calculation error of 0.59 HRC. Quality coefficients of the developed network are shown in Table 15.

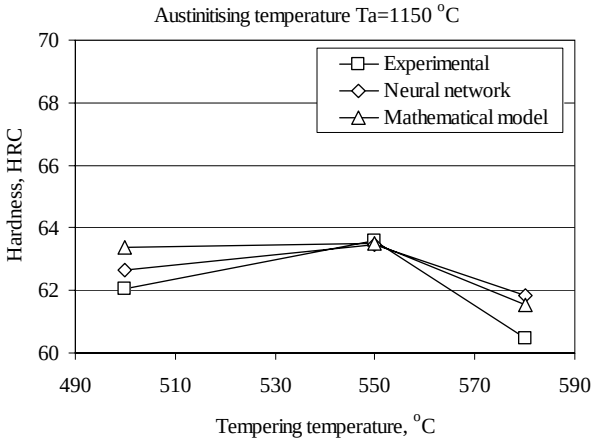
The developed models were subjected to additional verification based on the supplementary investigation results described in Chapter 4.1. Hardness calculations were made using the developed models for steels with chemical compositions presented in Table 4. The calculation errors were estimated next according to equation (3), which for the statistical model and neural network are 0.99 HRC and 1.01 HRC respectively. Therefore, one can state that the developed models meet fully the calculation accuracy assumptions.

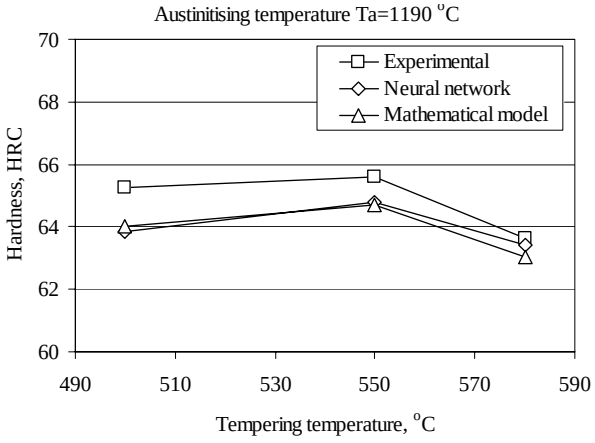
Comparison of the verification calculations results are presented in Figures 28-30. In Figures 31-33 comparison of the calculated and experimental tempering curves are shown for three steels, from all included in the data set used to develop the models.

Table 15.
Quality coefficients of the neural network developed for the steel hardness calculation

Network structure	Training method/number of training epochs	Data set		
		Training	Validating	Testing
MLP 8-7-1	BP/50 CG/462	Average absolute error, HRC		
		0.53	0.57	0.59
		Quotient of standard deviations		
		0.23	0.25	0.27
		Correlation coefficient		
		0.97	0.97	0.96

BP – error back-propagation learning method
CG – conjugate gradients learning method





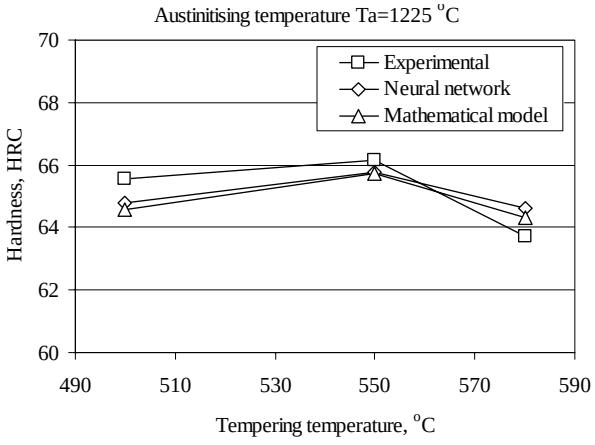
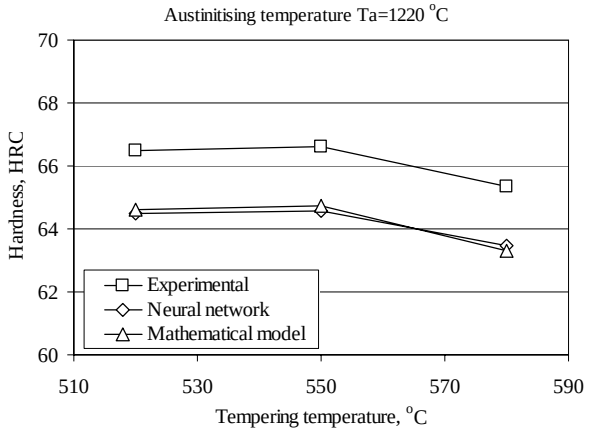
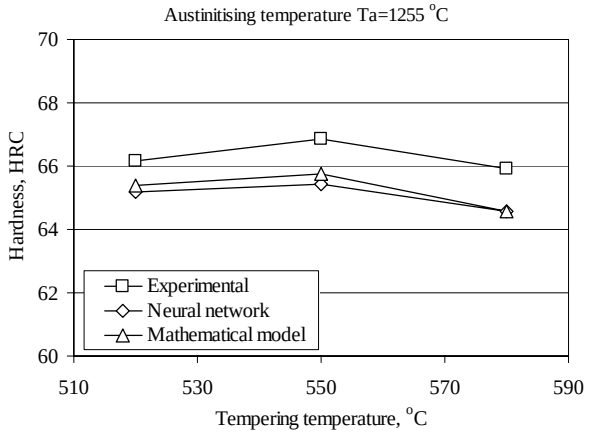


Fig. 28. Comparison of the verification calculations results using the developed neural network and the mathematical model for HS6-5-2 steel





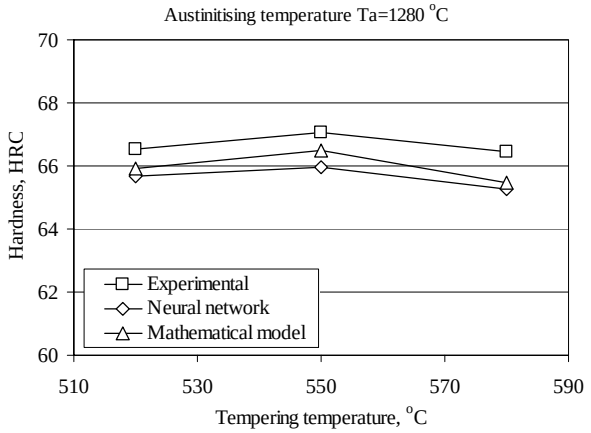
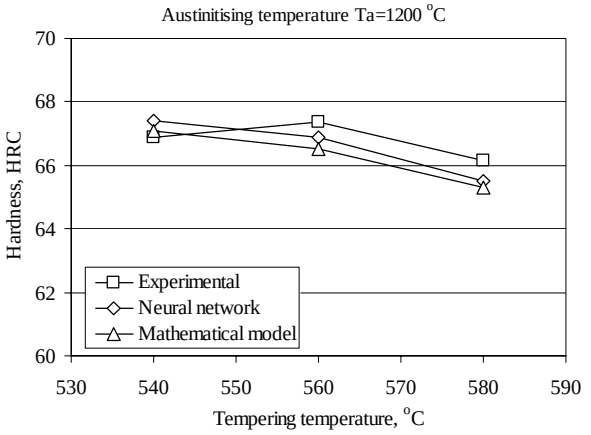
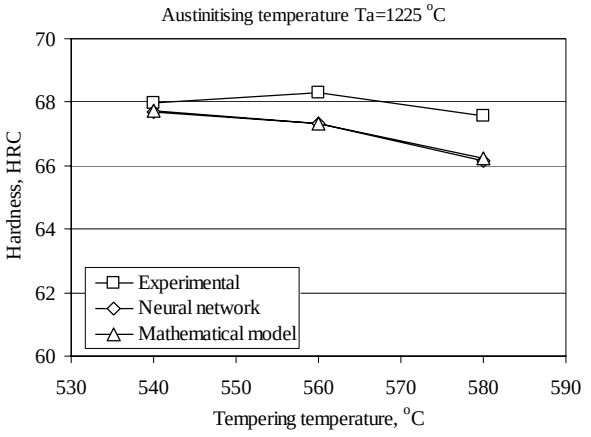


Fig. 29. Comparison of the verification calculations results using the developed neural network and the mathematical model for HS18-0-1 steel





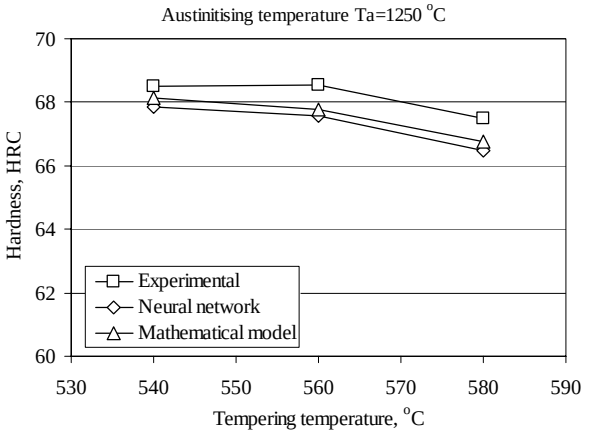
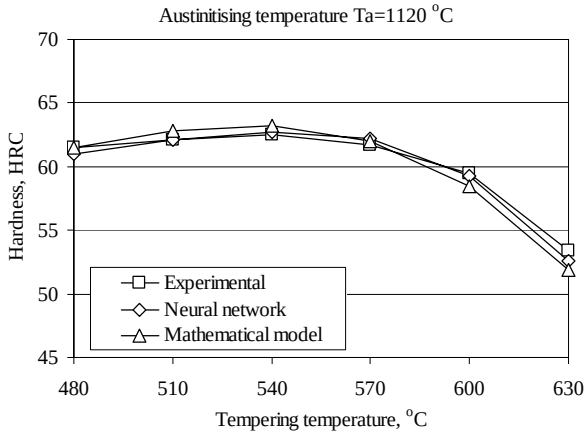
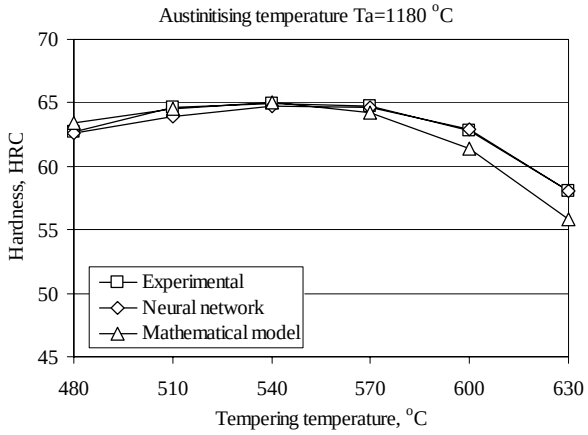


Fig. 30. Comparison of the verification calculations results using the developed neural network and the mathematical model for HS10-4-3-10 steel





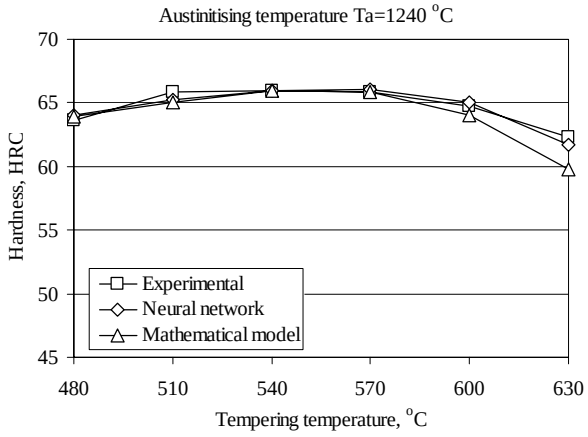
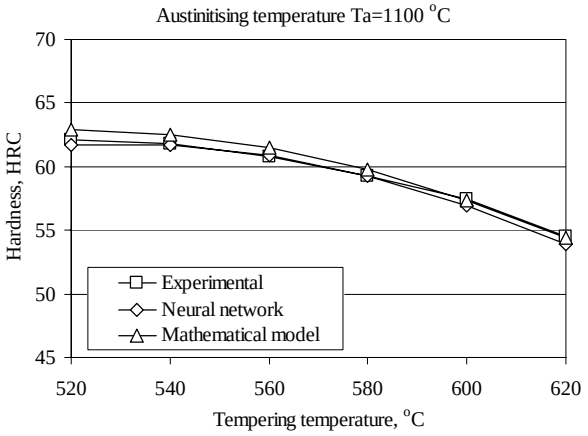
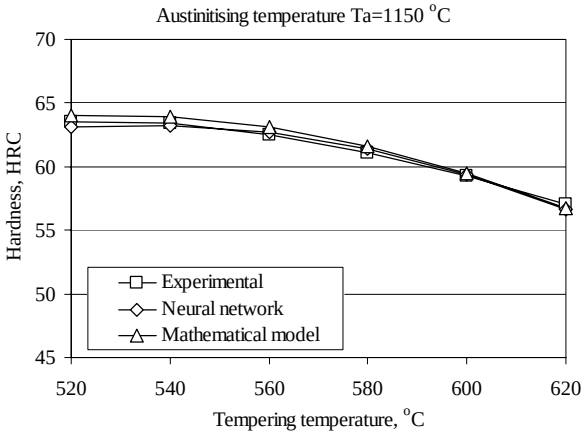


Fig. 31. Comparison of experimental results and hardness calculations using the developed neural network and the mathematical model for 9-2-2+Si type steel





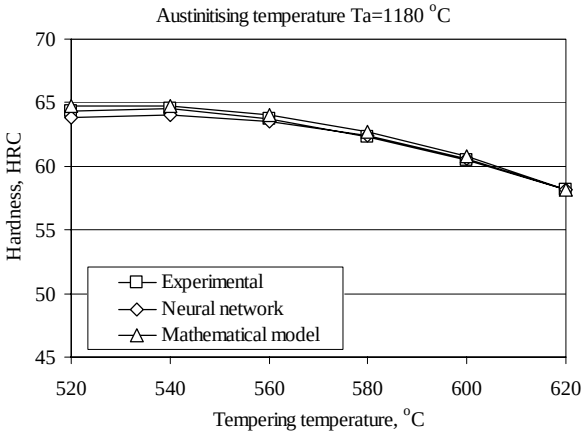


Fig. 32. Comparison of experimental results and hardness calculations using the developed neural network and the mathematical model for 3-3-2 steel type

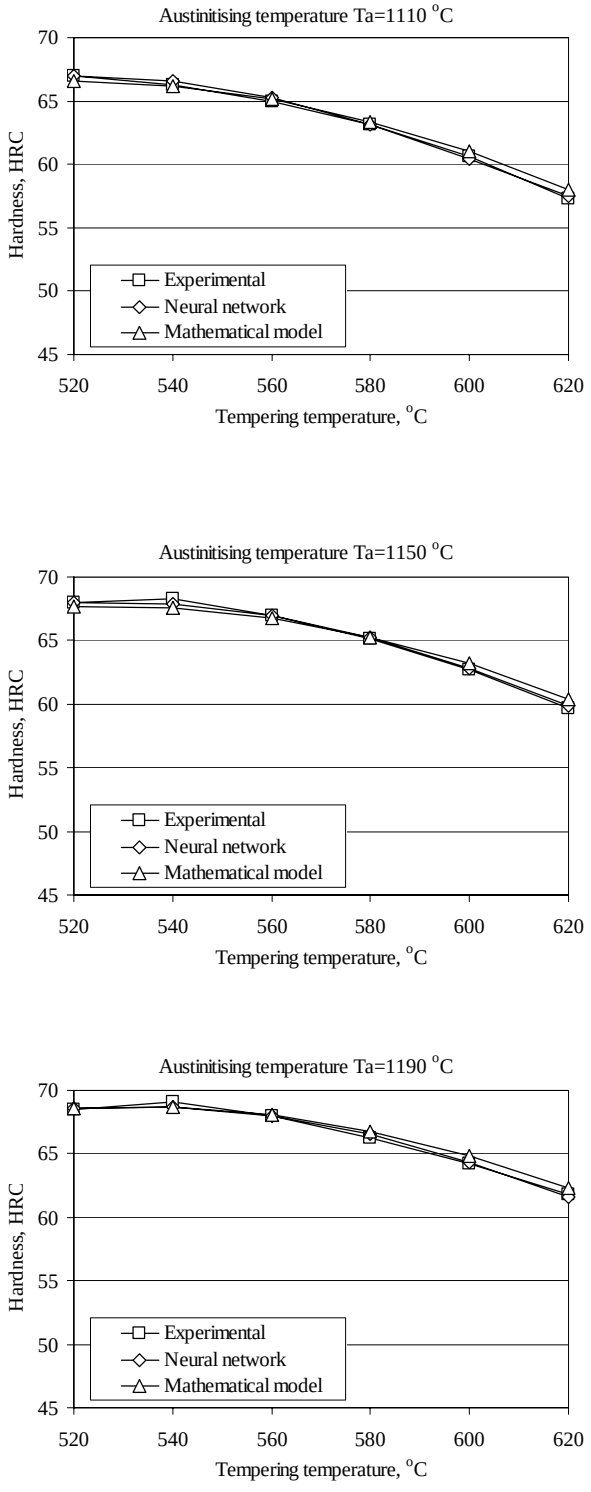


Fig. 33. Comparison of experimental results and hardness calculations using the developed neural network and the mathematical model for 2-9-1-8 steel type

5.2. High-speed steels fracture toughness model

Only one model described in [132] from the few ones presented in literature, making it possible to evaluate fracture toughness of various materials, mentioned in Chapter1.2, may be used for the high-speed steels. It makes calculation possible of the fracture toughness K_{Ic} for the high-speed steels based on hardness and parameters describing the microstructure (fraction of eutectic carbides, fraction of the retained austenite, and the average distance between the carbides d_p) according to the relationship:

$$K_{IC} = 1.363\left(\frac{HRC}{HRC-53}\right)\cdot\left[\sqrt{E\cdot d_p}\cdot(f_{carb})^{-16}\cdot(1+f_{aust})\right] \tag{9}$$

where: f_{aust} – fraction of the retained austenite, f_{carb}– fraction of carbides, E – Young's modulus of steel, d_p - average distance between the carbides, HRC – steel hardness in Rockwell scale C.

The average distance between carbides d_p may be calculated according to relationship [132]:

$$d_p = D_p(1-f_{carb})\cdot\sqrt{2/(3\cdot f_{carb})} \tag{10}$$

where: D_p - mean diameter of the carbides.

Research on fracture toughness modelling was commenced with verification of model (9). Test calculations were made to this end for the selected steel grades for various heat treatment states. Structure investigation results were used for that, described in Chapter 4.3, and in addition, results of the X-ray examinations of the retained austenite fraction made with the Averbach-Cohen method were used.

Results of the verification investigation indicated the deficient relevancy of this model, as the relative assessment error of the K_{Ic} coefficient was up to 50% of its experimental value. One should mention that model (9) was developed based on the investigation results of the M2 high-speed steel (HS6-5-2) subjected to heat treatment in vacuum in the limited tempering temperature range (500 and 540°C only). The microstructure examination results presented suggest that the retained austenite fraction in this steel is from 1.1% to 25.7% depending on the heat treatment variant. In case of the conventional high-speed steels subjected to heat treatment in salt baths the retained austenite fraction after tempering twice is negligible or is at the detection threshold of the X-ray methods [39]. This, as it seems, may be the cause of the big errors in the K_{Ic} coefficient value. Moreover, using this model for the fracture toughness assessment is connected with the need to carry out a number of complex and time consuming metallographic examinations, which was the direct reason to give up further work in which it would be employed for the fracture tougnhess K_{Ic}.

Therefore, the further works were focused on development the model making it possible to determine the high-speed steel fracture toughness solely based on the steel chemical composition and heat treatment parameters, based on the investigation results described in Chapter 3.

The artificial neural networks were used as a modelling tool. It was assumed, referring to the developed neural networks structure, as in case of hardness modelling, that the network has 8 inputs, corresponding to concentration values of the six main alloy elements occurring in this steel group and to the austenitizing- and tempering temperatures, and one output, corresponding to the value of the fracture toughness K_{Ic}.

The StatSoft STATISTICA Neural Networks v. 4.0 program was used for development, training, and testing of the neural networks. After entering the training data to the program, the neural network design process was started.

Several dozen neural networks were generated using the program, with the various numbers of neurons in the hidden layer. About half of them were eliminated immediately due to the excessive error or the excessive number of neurons in the hidden layers. Training error graph for every network was studied after completing the training process or in its course. Based on that the networks were checked if the overtraining did not take place and the overtrained ones were eliminated from the subsequent analysis. The average absolute error, quotient of standard deviations, and correlation coefficient were assumed as the network quality coefficients. Finally one network was selected, from the entire set of the developed networks -the multilayer perceptron with the 8-6-1 structure (i.e., 8 inputs, 6 neurons in the hidden layer, and 1 output), with the average calculation error of 0.39 MPa·m$^{1/2}$. Quality coefficients of the developed network are shown in Table 16. Comparison of the calculated K_{Ic} coefficient values with the experimental data is shown in Figures 34-44.

Table 16.
Quality coefficients of the neural network developed for the fracture toughness K_{Ic} calculation

Network structure	Training method/ number of training epochs	Data set	
		learning	validating
MLP 8-6-1	BP/50 CG/56	Average absolute error, MPa·m$^{1/2}$	
		0.39	0.39
		Quotient of standard deviations	
		0.15	0.22
		Correlation coefficient	
		0.99	0.98

BP – error back-propagation learning method
CG – conjugate gradients learning method

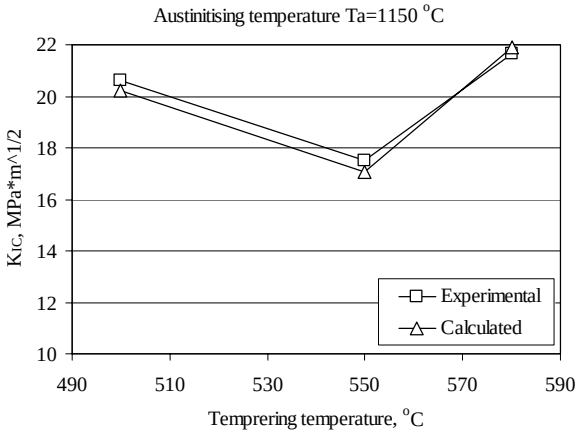


Fig. 34. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS6-5-2 steel (Ta=1150°C)

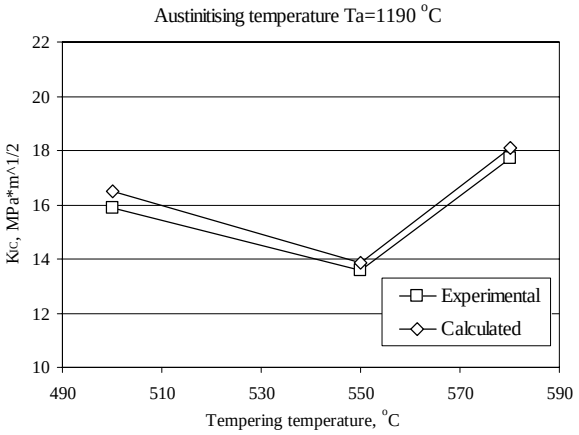


Fig. 35. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS6-5-2 steel (Ta=1190°C)

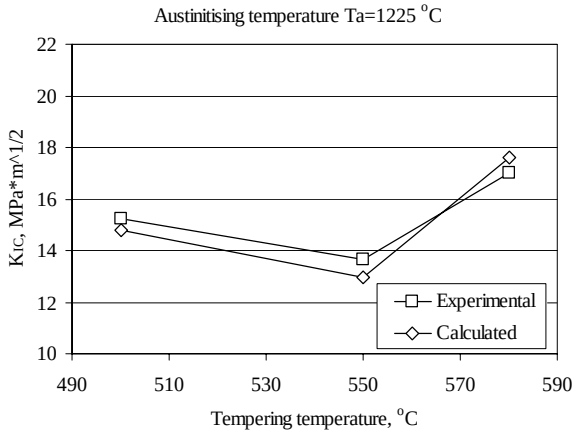


Fig. 36. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS6-5-2 steel (Ta=1225°C)

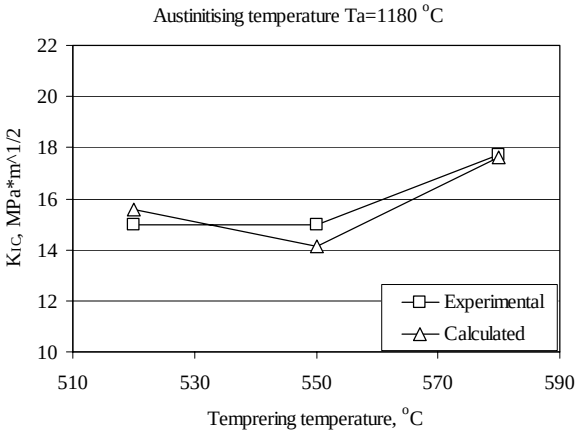


Fig. 37. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS18-0-1 steel (Ta=1180°C)

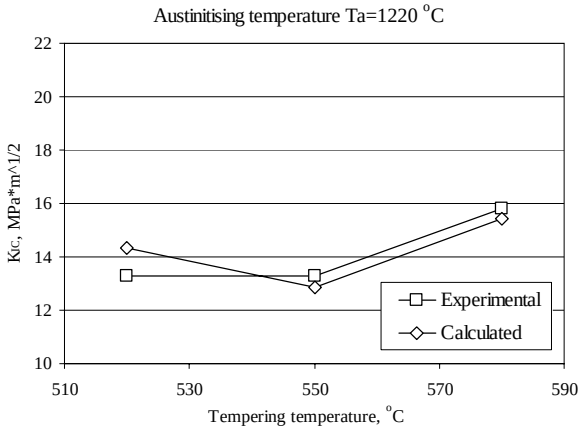


Fig. 38. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS18-0-1 steel (Ta=1220°C)

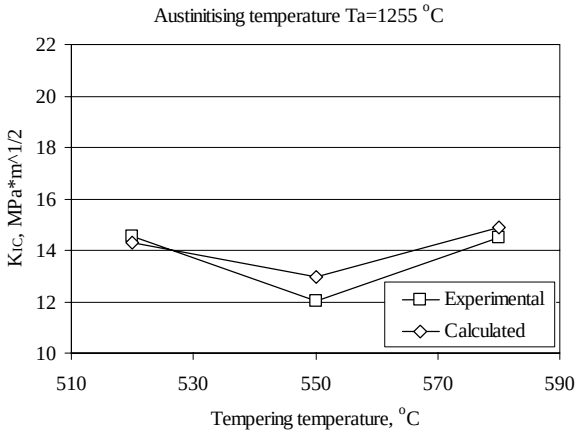


Fig. 39. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS18-0-1 steel (Ta=1255°C)

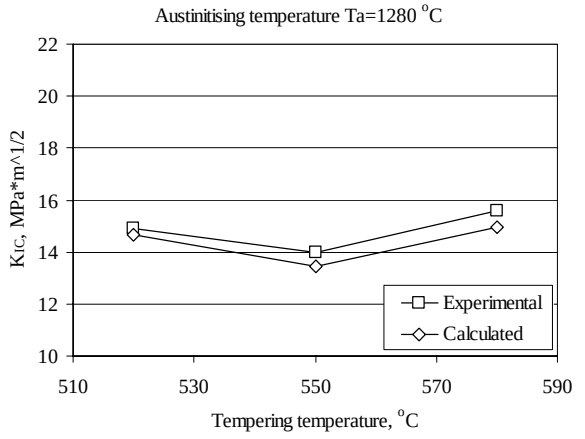


Fig. 40. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS18-0-1 steel (Ta=1280°C)

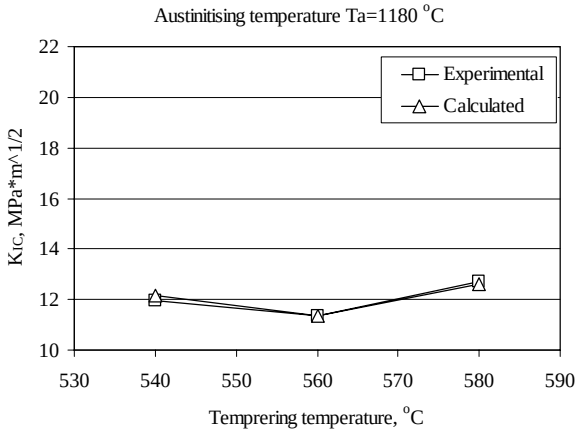


Fig. 41. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS10-4-3-10 (Ta=1180°C)

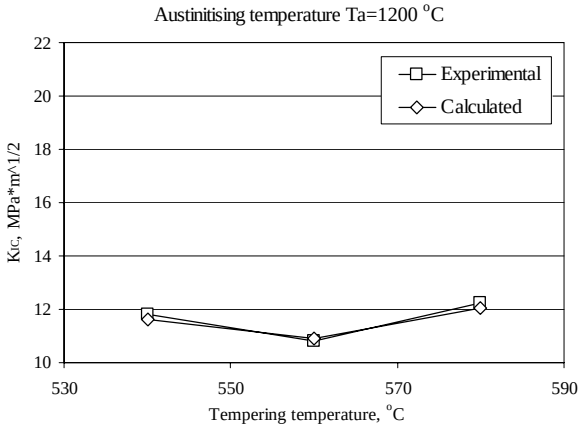


Fig. 42. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS10-4-3-10 (Ta=1200°C)

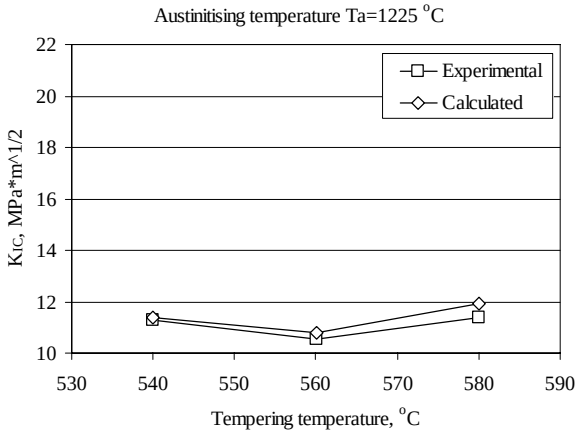


Fig. 43. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS10-4-3-10 (Ta=1225°C)

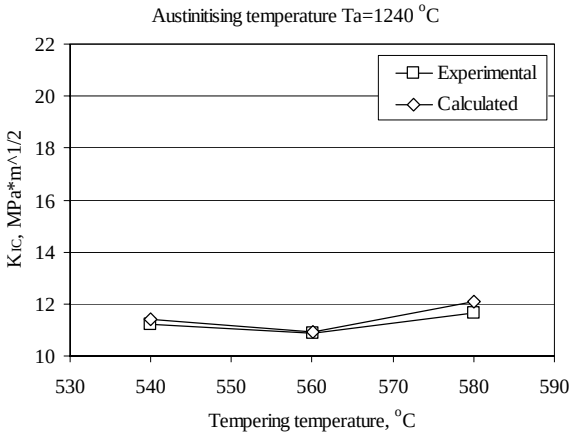


Fig. 44. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS10-4-3-10 steel (Ta=1240°C)

6. Design of chemical composition of high-speed steels with the required hardness and fracture toughness

For the high-speed steels chemical compositions design, which is the optimisation problem, the evolutionary algorithms were used. The object function is the index defining the set of the optimised properties, in this case hardness and fracture toughness. It was assumed that it will be possible to determine weights for each property, which will make it possible to make a decision which of the properties in the optimisation procedure actually carried out is the most important one. The opitimisation result, with the maximum secondary hardness as the goal, are the chemical compositions high-speed steels with the highest hardness, and with the fracture toughness as a goal, the chemical compositions of steels demonstrating the highest fracture toughness K_{Ic}. Moreover, the possibility was assumed to limit the search area for the optimum chemical composition meeting the assumed criteria. Because of the form of the developed material models employed for design of the chemical composition, not only the alloy elements concentrations are optimised, but also the heat treatment parameters, i.e., the austenitizing- and tempering temperatures. The evolutionary optimisation methods are based on natural sciences describing the phenomena of the natural selection and inheritance and boil down to survival of specimens best adapted to the particular environment, while the specimens adapted to a lesser degree are eliminated. These specimens, in turn, that survive - convey their genetic information to their offspring. Crossing of the genetic information obtained from the "parents" leads to a situation in which the subsequent generations are, on the average, better and better adapted to their environment conditions. It is, therefore, the global optimisation process with the exceptional convergence and resistance to disturbances.

Compared to other analytical and stochastic methods the following features of the evolutionary methods may be mentioned:

- they are resistant to local maxima,
- operate on coded data,
- process solution generations, and not the single solutions only,
- use the object function only (adaptation),
- they are indeterministic,
- find the approximate solutions only.

The assumptions made were used in optimisation, pertaining to relationships among the particular concentrations of the alloy elements occurring in the high-speed steel and its hardening- and tempering temperatures - and its properties.

The own computer program was developed to carry out the high-speed steel chemical composition optimisation task, with the maximum hardness and fracture toughness as the goal, in which the genetic algorithm was employed with the hardness- and fracture toughness functions as the neural network models.

Optimisation procedure assumptions

The object function was optimised expressing the high-speed steel hardness and its fracture toughness in the following form

$$Z = a \cdot HRC(x) + b \cdot K_{IC}(x) \tag{11}$$

where: HRC(x) - hardness function (neural network model), $K_{Ic}(x)$ – fracture toughness function (neural network model), x_i, - vector of parameters (mass concentrations of alloying elements, austenitizing- and tempering temperatures), a, b – weight coefficients for both of the object function components, assuming values from the <0;1> range.

The chemical composition optimisation procedure calls for specifying the limits the optimised function parameters, i.e., alloy elements concentrations ranges and the austenitizing- and tempering temperatures. Based on analysis of concentrations of chemical compositions of steels shown in Tables 1-3, optimisation limits used in the genetic algorithm are presented in Table 17; whereas, the additional limitations are listed in Table 18. The roulette method was used in this algorithm for selection. Figure 45 presents the genetic algorithm functioning principle. User interface windows of the developed computer program are shown in Figures 46-48.

Table 17.
Boundary of the optimisation procedure

Parameter	C	Cr	W	Mo	V	Co	Ta	Tt
MIN	0.72	3.7	0	0	1	0	1150	500
MAX	1.41	4.7	18	9.5	4.5	11	1280	630

Table 18.
Optimisation procedure constrains used in calculation

Constrain	Cr+W+Mo+ V+Co	(Cr+W+Mo+ V+Co)/C	Mo+V +Co	W+Mo +V
MIN	9.3	11.1	1.1	5.3
MAX	31	30.9	18.7	19.2

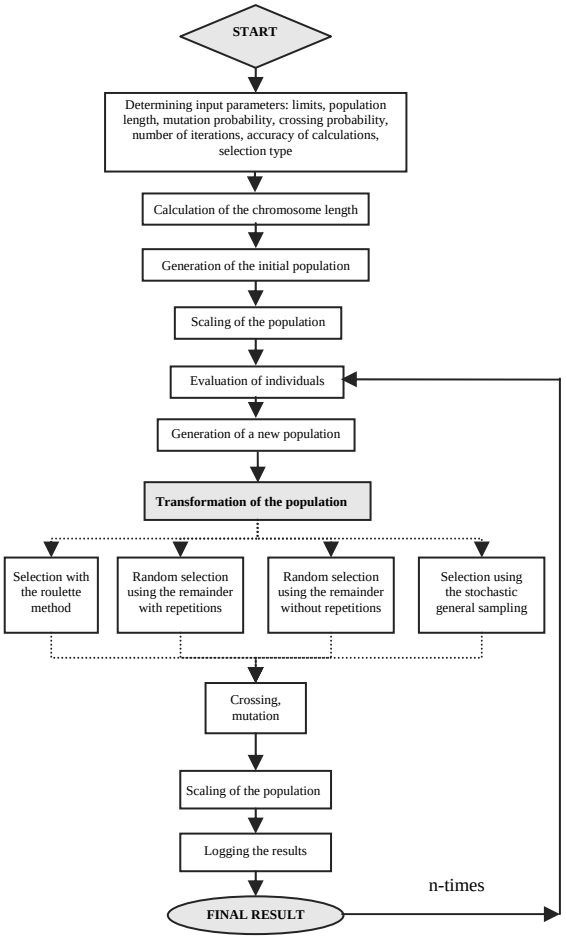


Fig. 45. Functioning schema of the genetic algorithm with four selection methods

Parameters of the algorithm defined by the user in the developed program are:

- **Number of generations** - determines the number of algorithm repetitions;
- **Population size** - number of indivduals
- **Crossing coefficient** - value from the range from 0 to 1 (0 denotes the probability of crossing equal to 0, 1 denotes the probability of 0.2), specifying probability of the selection of the relevant pair of specimens to transform the population (default value of 1);
- **Mutation coefficient** - value from the range from 0 to 1 (0 denotes the probability of mutation equal to 0, and 1 denotes the probability of 0.2), specifying probability of the selection of the particular specimen for mutation operation (default value of 0.5);
- **Number of iterations** - determines the number of algorithm repetitions;
- **Accuracy of calculations** - specifies precision of the environment search
- **Weights a and b** - specifying weights attributed to each object function component

The optimisation algorithm functioning consists in such selection of the alloying elements and hardening- and tempering temperatures so that the chemical composition of the steel is obtained with the possibly highest hardness and fracture toughness, while maintaining proportions for these properties specified by their weights (eq. 11). As an illustration of research carried out using the developed program some selected examples of are presented of the chemical composition optimisation results, obtained for various genetic algorithm parameters and for various limits imposed on the search space of the optimum chemical composition.

The following assumptions were made for the consecutive examples:

1. The entire range of the alloy elements (with the exception of tungsten and molybdenum, for which a higher minimum concentration limit was assumed - 2%, as null concentrations of these elements occur for two steel grades only, which may be considered as non-representative) and the full ranges of the austenitizing- and tempering temperatures. Weights for hardness and fracture toughness equal to 1
2. Limitations as in **example 1.** The austenitizing temperature range was limited to 1190-1240 °C as ensuring the maximum hardness.
3. Limitations as in **example 2.** The tempering temperature range was limited to 520-590 °C.
4. Fracture toughness was considered to be more important. Limitations as in **example 3** Weights for hardness 0.95, and for fracture toughness equal to 1.
5. Hardness was considered to be more important. Limitations as in **example 3** Weights for hardness 1, and for fracture toughness equal to 0.95.
6. Limitations as in **example 3** Cobalt was eliminated from the chemical composition of the steel.

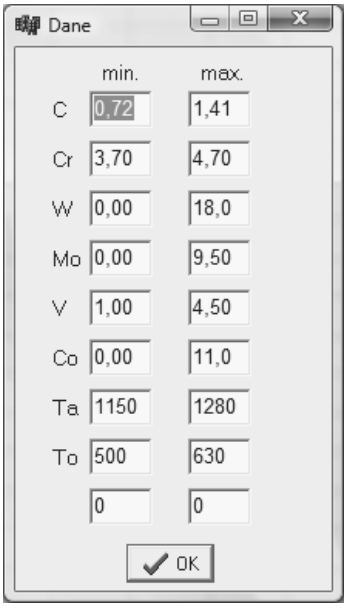
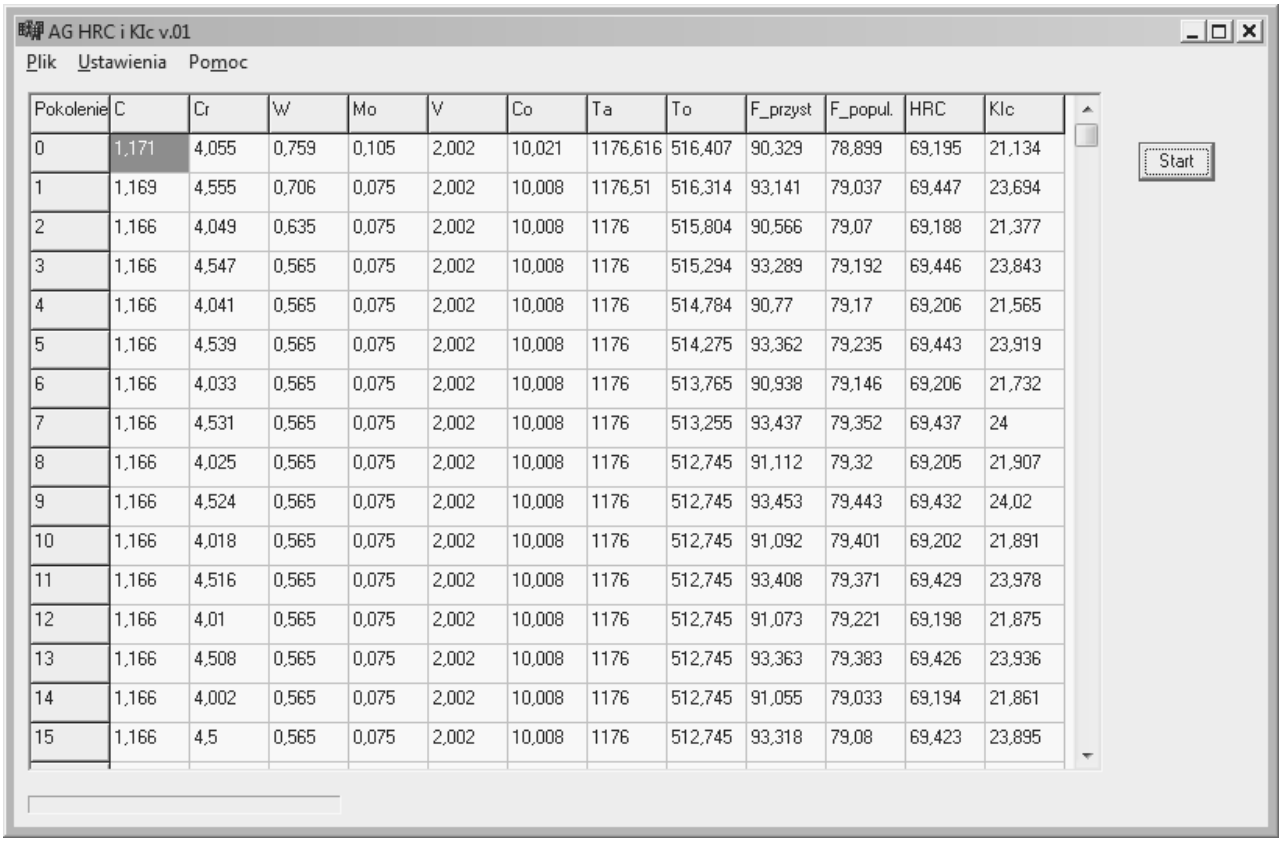


Fig. 46. Optimisation procedure boundaries edition window

Fig. 47. Optimisation algorithm parameters window



Pokolenie	C	Cr	W	Mo	V	Co	Ta	To	F_przyst	F_popul.	HRC	KIc
0	1,171	4,055	0,759	0,105	2,002	10,021	1176,616	516,407	90,329	78,899	69,195	21,134
1	1,169	4,555	0,706	0,075	2,002	10,008	1176,51	516,314	93,141	79,037	69,447	23,694
2	1,166	4,049	0,635	0,075	2,002	10,008	1176	515,804	90,566	79,07	69,188	21,377
3	1,166	4,547	0,565	0,075	2,002	10,008	1176	515,294	93,289	79,192	69,446	23,843
4	1,166	4,041	0,565	0,075	2,002	10,008	1176	514,784	90,77	79,17	69,206	21,565
5	1,166	4,539	0,565	0,075	2,002	10,008	1176	514,275	93,362	79,235	69,443	23,919
6	1,166	4,033	0,565	0,075	2,002	10,008	1176	513,765	90,938	79,146	69,206	21,732
7	1,166	4,531	0,565	0,075	2,002	10,008	1176	513,255	93,437	79,352	69,437	24
8	1,166	4,025	0,565	0,075	2,002	10,008	1176	512,745	91,112	79,32	69,205	21,907
9	1,166	4,524	0,565	0,075	2,002	10,008	1176	512,745	93,453	79,443	69,432	24,02
10	1,166	4,018	0,565	0,075	2,002	10,008	1176	512,745	91,092	79,401	69,202	21,891
11	1,166	4,516	0,565	0,075	2,002	10,008	1176	512,745	93,408	79,371	69,429	23,978
12	1,166	4,01	0,565	0,075	2,002	10,008	1176	512,745	91,073	79,221	69,198	21,875
13	1,166	4,508	0,565	0,075	2,002	10,008	1176	512,745	93,363	79,383	69,426	23,936
14	1,166	4,002	0,565	0,075	2,002	10,008	1176	512,745	91,055	79,033	69,194	21,861
15	1,166	4,5	0,565	0,075	2,002	10,008	1176	512,745	93,318	79,08	69,423	23,895

Fig. 48. Main program window with optimisation results

Example 1

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1150	500
Maximum value	1.41	4.7	18	9.5	4.5	11	1280	630

Calculation results

Individual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	1.22	4.67	10.53	2.12	1.98	1.12	1253	512	84.3	81.5	66.4	17.9
2	1.16	4.65	2.13	4.24	1.06	10.01	1254	589	86.9	80.3	68.5	18.5
3	0.99	4.59	3.51	2.24	1.00	7.72	1264	533	87.5	82.7	68.8	18.6
4	1.18	4.61	2.13	3.35	1.37	3.62	1253	585	86.0	78.2	67.0	19.0
5	1.34	4.68	9.03	3.62	1.00	0.69	1267	501	85.3	79.5	67.1	18.1

Example 2

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1190	500
Maximum value	1.41	4.7	18	9.5	4.5	11	1240	630

Calculation results

Individual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	1.05	4.31	2.00	3.24	2.24	10.53	1219	552	83.5	75.1	68.3	15.2
2	0.85	4.66	4.89	2.35	2.00	6.17	1220	598	86.5	79.3	63.4	23.1
3	0.89	4.61	2.38	4.44	1.00	2.24	1215	591	87.5	82.1	64.5	22.9
4	1.06	4.63	2.82	4.00	1.93	0.00	1190	604	89.3	83.4	61.9	27.4
5	1.20	4.63	9.03	2.00	1.88	4.75	1235	509	85.5	81.2	66.5	19.1

Example 3

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1190	520
Maximum value	1.41	4.7	18	9.5	4.5	11	1240	590

Calculation results

Individual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	0.83	4.41	4.01	2.24	1.98	0.04	1218	572	84.6	78.5	63.6	21.0
2	0.82	4.62	4.01	3.88	1.36	8.50	1197	584	86.1	83.7	65.4	20.7
3	1.22	4.62	4.76	2.00	2.22	2.50	1210	590	85.6	80.2	64.2	21.4
4	1.08	4.64	3.26	3.85	1.60	9.97	1229	545	84.8	79.9	69.8	15.0
5	1.01	4.62	5.01	4.00	1.36	0.17	1191	586	87.2	83.4	64.4	22.8

Example 4

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	0.95
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1190	520
Maximum value	1.41	4.7	18	9.5	4.5	11	1240	590

Calculation results

Individual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	0.86	4.20	3.00	2.71	1.17	10.53	1215	572	82.1	74.3	67.1	18.3
2	0.98	4.40	5.51	2.44	1.12	6.51	1212	520	80.9	74.3	67.2	17.0
3	1.09	4.68	3.95	2.00	2.25	0.04	1205	584	84.7	83.2	64.0	23.9
4	0.83	4.45	4.01	3.35	1.62	1.81	1226	578	81.4	80.3	64.4	20.2
5	1.16	4.61	5.77	2.35	2.22	0.00	1235	577	80.8	75.7	65.9	18.2

Example 5

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	0.95
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1190	520
Maximum value	1.41	4.7	18	9.5	4.5	11	1240	590

Calculation results

Inividual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	0.80	4.65	2.00	2.74	3.13	9.02	1196	577	83.6	79.3	63.9	20.7
2	1.13	4.45	3.51	2.00	1.49	6.73	1233	580	84.3	77.5	66.5	18.8
3	1.16	4.45	5.89	4.15	1.74	10.44	1227	542	82.1	76.1	69.8	13.0
4	1.20	4.59	6.02	3.88	1.44	10.40	1219	558	82.9	77.0	69.7	13.9
5	0.82	4.67	11.54	2.35	1.12	0.69	1193	586	85.3	83.0	63.6	22.9

Example 6

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta ,°C	Tt,,°C
Minimum value	0.72	3.7	2	2	1	0	1190	520
Maximum value	1.41	4.7	18	9.5	4.5	0	1240	590

Calculation results

Individual	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	0.80	4.66	7.27	2.00	1.62	0.00	1235	577	85.5	82.7	64.4	21.1
2	0.95	4.61	7.27	4.00	1.74	0.00	1204	571	83.4	78.6	65.4	18.1
3	1.06	4.38	2.38	2.24	3.00	0.00	1230	572	82.7	77.6	64.2	18.5
4	0.76	4.45	4.95	2.35	2.00	0.00	1199	560	83.9	78.4	63.0	20.9
5	0.82	4.45	3.51	3.00	1.49	0.00	1203	584	87.4	79.7	63.1	24.3

7. Computer simulations using the developed models

The neural network models developed within the framework of the research make computer simulations possible pertaining, among others, to:

- changes of the high-speed steel hardness, depending on the varying tempering temperature (tempering curves) for the arbitrarily specified chemical composition and assumed austenitizing temperature,
- effect of the selected element on steel properties or increase of this property value for the fixed concentrations of the other alloy elements and constant austenitizing- and tempering temperatures,
- analysis of the simultaneous effect of two selected elements on steel properties, for 6 fixed concentrations of the other alloy elements and constant austenitizing- and tempering temperatures.

Simulation investigations were carried out in the concentration ranges of the alloy elements occurring in the investigated steels, specified in Table 19.

Table 19.
Ranges of mass concentrations of the alloying elements occurring in the analysed high-speed steels

	Mass concentration of alloying element, %					
	C	Cr	W	Mo	V	Co
Minimum	0.72	3.7	0	0	1	0
Maximum	1.41	4.7	18	9.5	4.5	11

7.1. Simulation of the high-speed steels tempering curves

Chemical compositions obtained as the optimisation results presented in Chapter 6 were used for simulation calculations carried out to determine the tempering curves. From each of the examples presented there one was selected from 5 chemical compositions, acquiring the highest objective function value. The result was that 6 various high-speed steels chemical compositions were obtained, shown in Table 20, taking into account compositions being the optimal ones for limitations used in every optimisation cycle. Simulation calculations of the tempering curves, which are presented in Figures 49-54, were carried out for the selected chemical compositions using the developed neural network model.

The presented tempering curves calculation results feature an example of the application potential of the developed neural network models, as the computer simulation tools. It is possible to carry out the unrestricted numerical investigations in the chemical compositions space within the limits defined by concentrations of the chemical elements occurring in steel grades covered by investigations. However, it should be mentioned, that - while determining the chemical compositions of steels for which the simulation calculations are to be carried out - one may not omit the important limitations resulting, for instance, from the carbon equivalent (eq. 1) for the high-speed steels or others, e.g., used as supplementary in the optimisation procedure (Table 18). Also, the unambiguous conclusions pertaining the tempering curves flow may be formulated only after carrying out the relevant experimental research. On the other hand, however, calculation results for hardness of the high-speed steels after heat treatment, obtained using the developed neural network, demonstrate their very good consistency with the experimental data, as the results of the verification calculations for the single hardness value for the specific austenitizing- and tempering temperatures differed by only about 1 HRC from it. This may, therefore, justify the statement that the presented exemplary tempering curves obtained with computer simulation are a very good approximation of the real results.

Table 20.
Chemical compositions of high-speed steels used for determining the tempering curves

Chemical composition	Mass concentration of alloying element, %					
	C	Cr	W	Mo	V	Co
I	0.99	4.59	3.51	2.24	1.0	7.72
II	1.06	4.63	2.82	4.00	1.93	0.0
III	1.01	4.62	5.01	4.00	1.36	0.17
IV	1.09	4.68	3.95	2.00	2.25	0.04
V	0.82	4.67	11.54	2.35	1.12	0.69
VI	0.82	4.45	3.51	3.00	1.49	0.0

7.2. Simulation of a single element effect on the high-speed steels hardness

In this example the developed neural network model was used for simulation of the effect of a single selected alloy element on hardness growth, with the fixed concentrations of the other elements. The exemplary analysis was carried out of the effect of the selected elements (tungsten and molybdenum) with and without the alloy addition of cobalt in steels.

It is also possible, apart from the presented examples, to carry out extended simulation analyses of the effect of the chemical composition on the secondary hardness effect within the range of concentrations of the alloy elements occurring in the analysed group of steels.

Examples of the analyses carried out of the effect of the selected alloy element with the fixed concentrations of the other alloy elements given in Table 21 are presented in Figures 55-63.

Table 21.
Fixed concentrations of alloy elements used in calculations

Mass concentration of alloying element, %					
C	Cr	W	Mo	V	Co
1.0	4.2	6.5	4	2	0

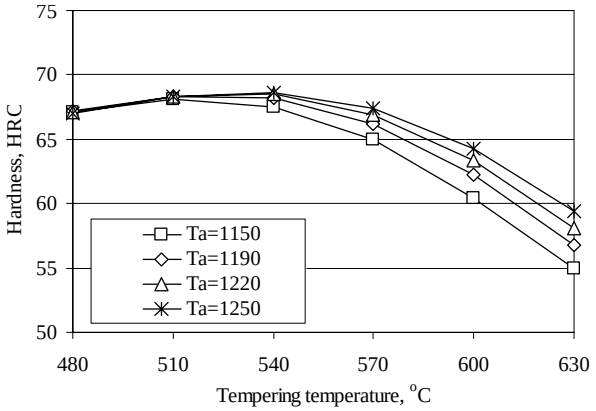


Fig. 49. Tempering curves for chemical composition No I (simulation)

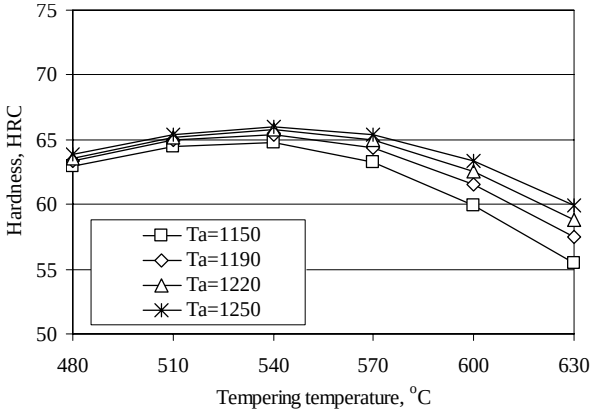


Fig. 50. Tempering curves for chemical composition No II (simulation)

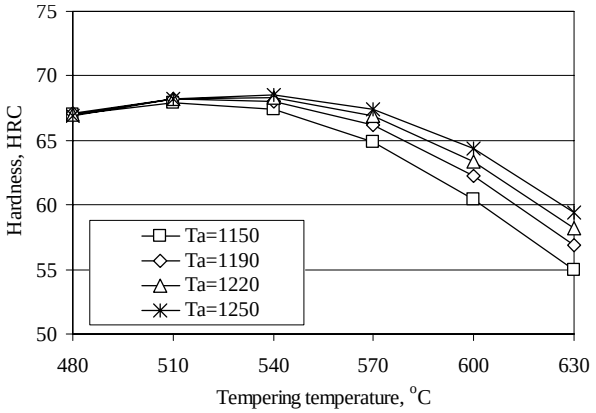


Fig. 51. Tempering curves for chemical composition No III (simulation)

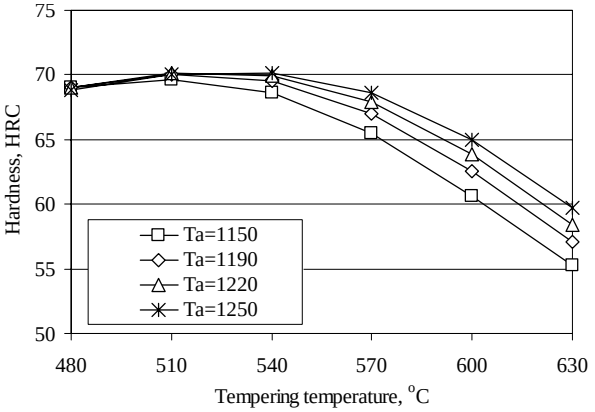


Fig. 52. Tempering curves for chemical composition No IV (simulation)

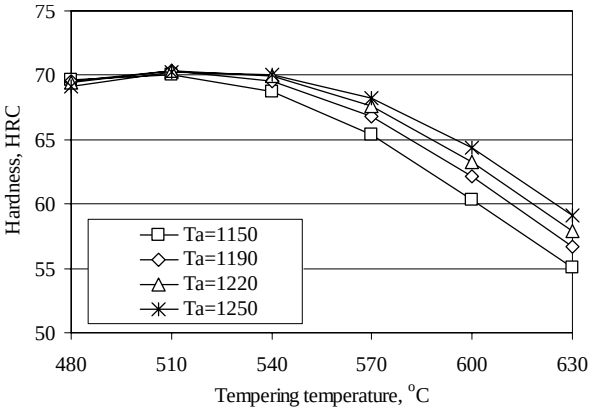


Fig. 53. Tempering curves for chemical composition No V (simulation)

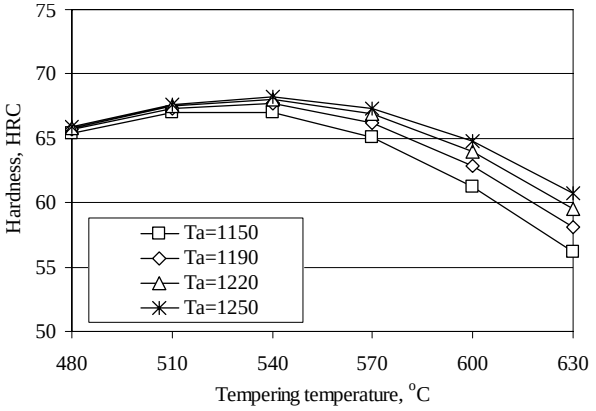


Fig. 54. Tempering curves for chemical composition No VI (simulation)

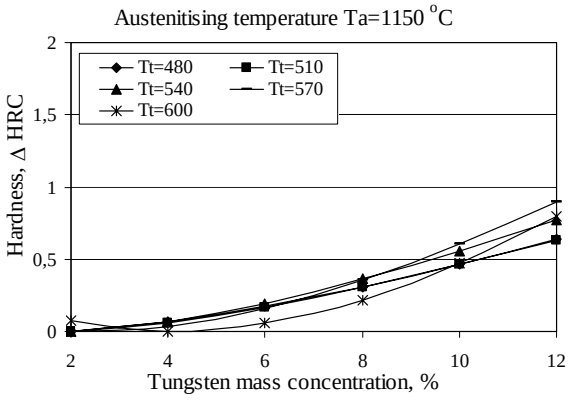


Fig. 55. Effect of tungsten on the high-speed steel hardness growth (Ta=1150°C)

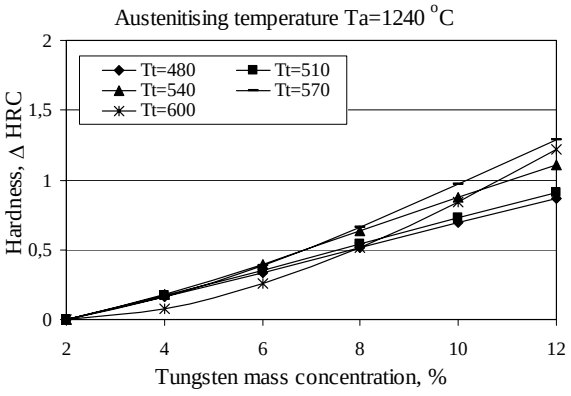


Fig. 56. Effect of tungsten on the high-speed steel hardness growth (Ta=1240°C)

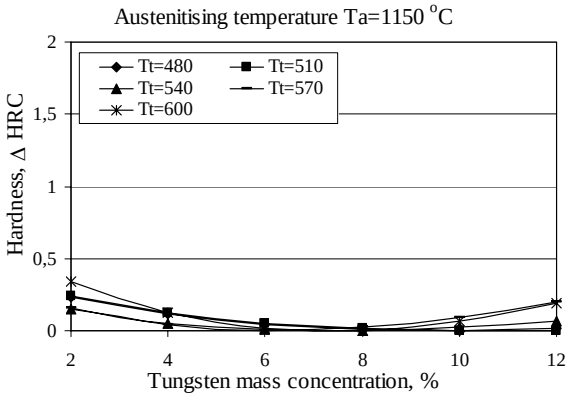


Fig. 57. Effect of tungsten on the high-speed steel hardness growth, Co=5.5% (Ta=1150°C)

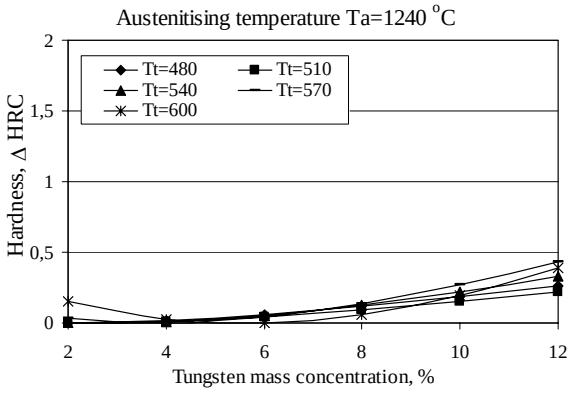


Fig. 58. Effect of tungsten on the high-speed steel hardness growth, Co=5.5% (Ta=1240°C)

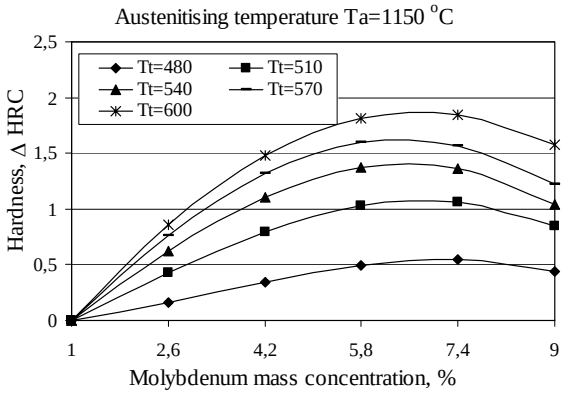


Fig. 59. Effect of molybdenum on the high-speed steel hardness growth (Ta=1150°C)

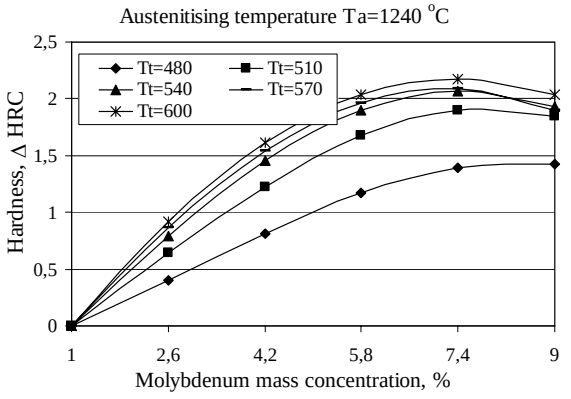


Fig. 60. Effect of molybdenum on the high-speed steel hardness growth (Ta=1240°C)

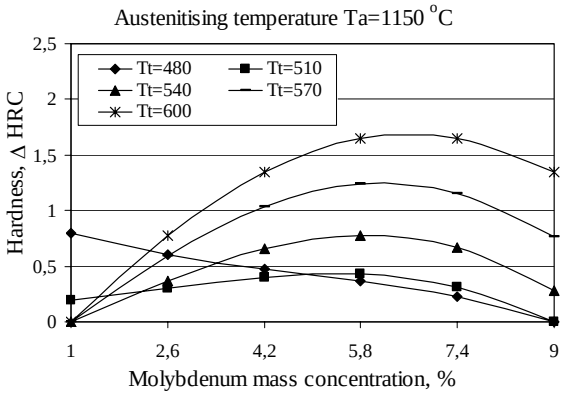


Fig. 61. Effect of molybdenum on the high-speed steel hardness growth, Co=5.5% (Ta=1150°C)

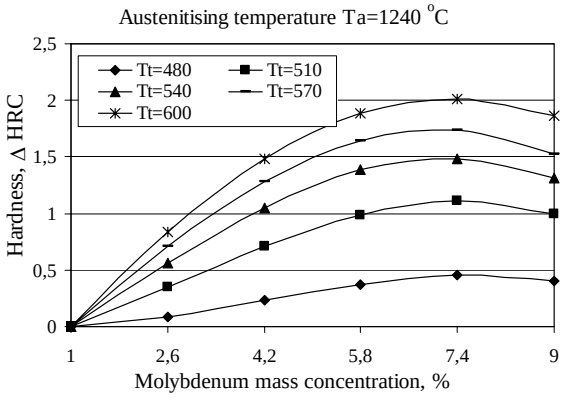


Fig. 62. Effect of molybdenum on the high-speed steel hardness growth, Co=5.5% (Ta=1240°C)

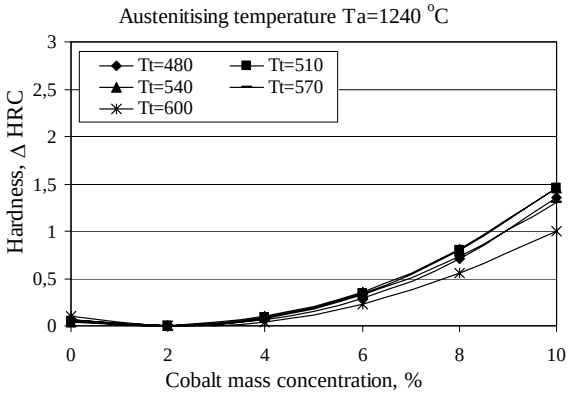


Fig. 63. Effect of cobalt on the high-speed steel hardness growth (Ta=1240°C)

7.3. Simulation of two elements effect on the high-speed steels properties

The second simulation example presents the effect of two selected alloy elements on steel hardness with the fixed concentrations of the other elements and heat treatment parameters, as well as the fracture toughness. In case of fracture toughness, results of the effect of two elements are presented as well as of the heat treatment temperature. Fixed concentration was used and heat treatment parameters presented in Table 22.

Results of the simulation for various combinations of elements are presented in Figures 64-75.

Table 22.
Fixed concentrations of alloy elements used for simulation of the effect of two elements

Mass concentration of alloying element, %						Temperature, °C	
C	Cr	W	Mo	V	Co	Ta	Tt
0.95	4.1	6.5	4.5	1.8	0	1220	550

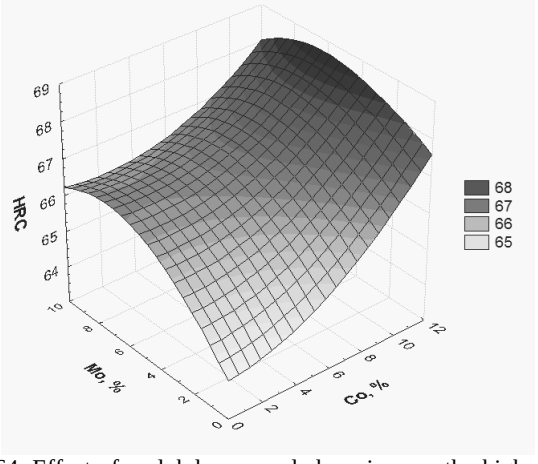


Fig. 64. Effect of molybdenum and chromium on the high-speed steels hardness

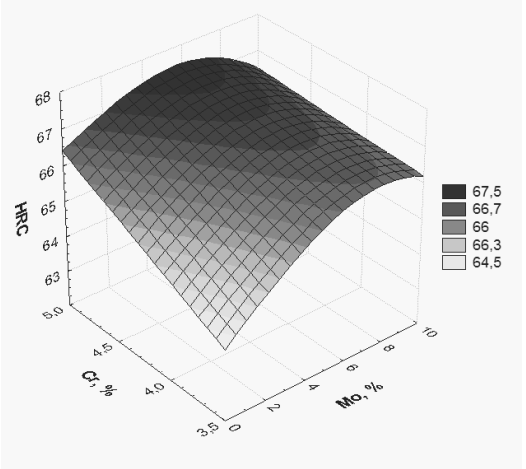


Fig. 65. Effect of molybdenum and chromium on the high-speed steels hardness (Co=5.5%)

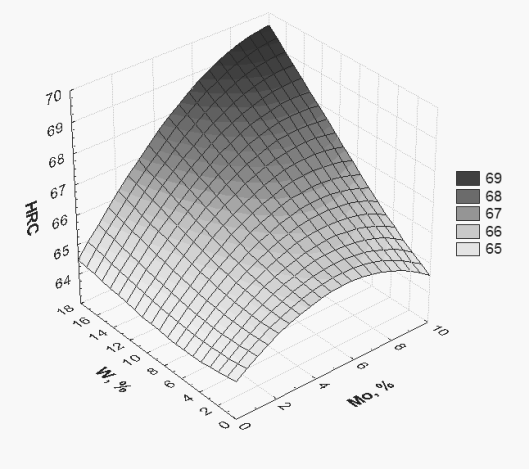


Fig. 66. Effect of tungsten and molybdenum on the high-speed steels hardness

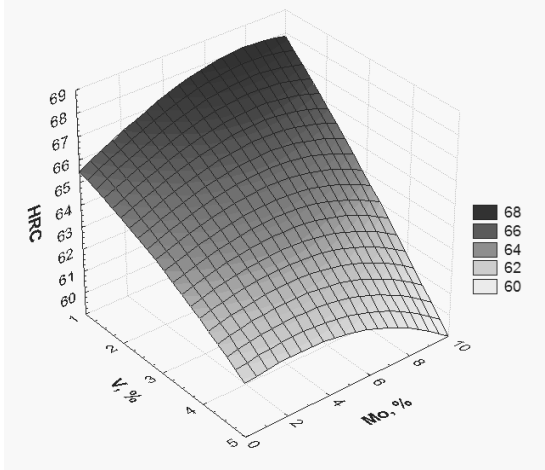


Fig. 69. Effect of vanadium and molybdenum on the high-speed steels hardness (Co=5.5%)

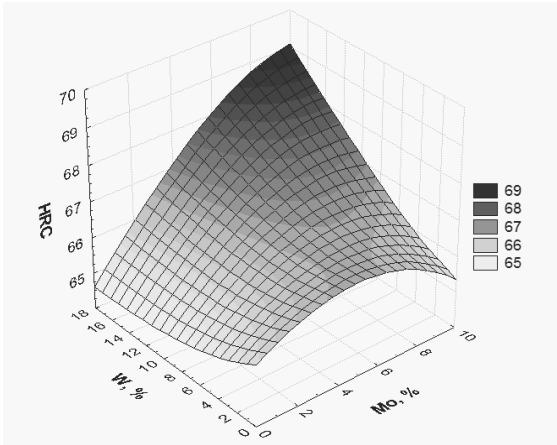


Fig. 67. Effect of tungsten and molybdenum on the high-speed steels hardness (Co=5.5%)

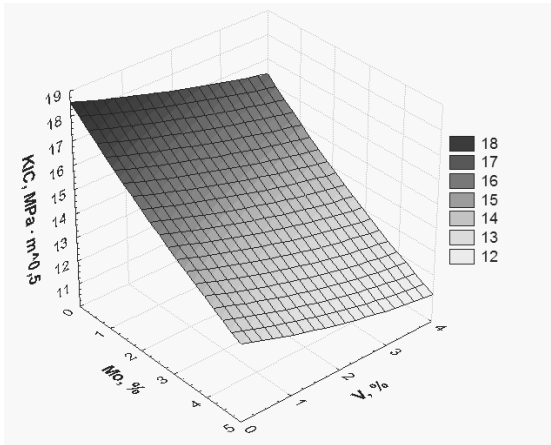


Fig. 70. Effect of vanadium and molybdenum on the high-speed steels fracture toughness K_{Ic}

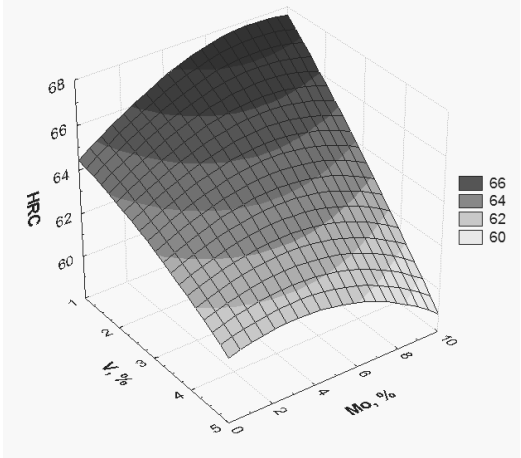


Fig. 68. Effect of vanadium and molybdenum on the high-speed steels hardness

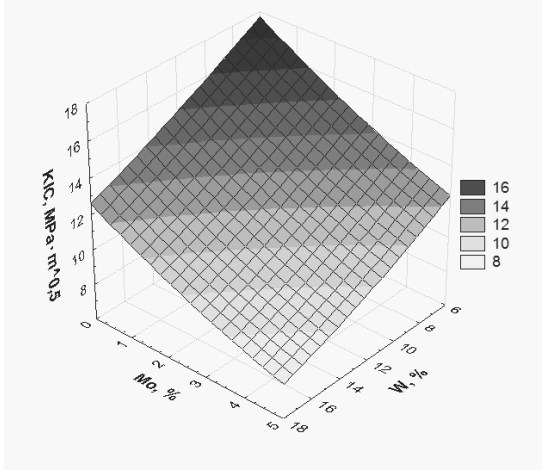


Fig. 71. Effect of tungsten and molybdenum on the high-speed steels fracture toughness K_{Ic}

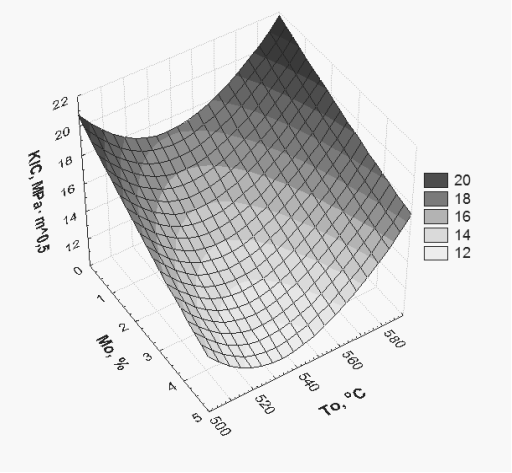


Fig. 72. Effect of molybdenum and tempering temperature on the steel s fracture toughness K_{Ic}

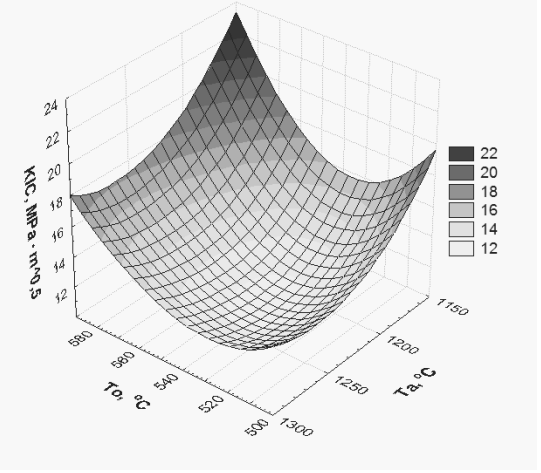


Fig. 75. Effect of austenitizing- and tempering temperatures on the steels fracture toughness K_{Ic}

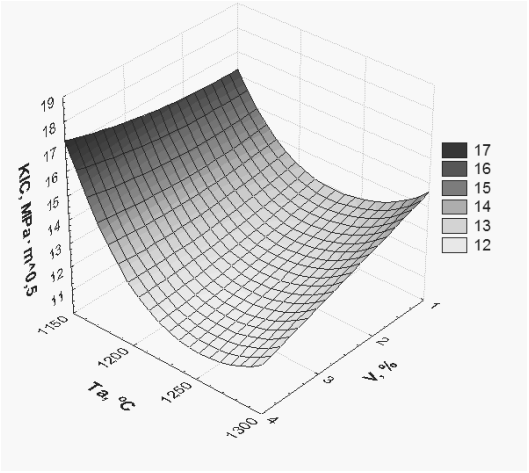


Fig. 73. Effect of vanadium and austenitizing temperature on the steels fracture toughness K_{Ic}

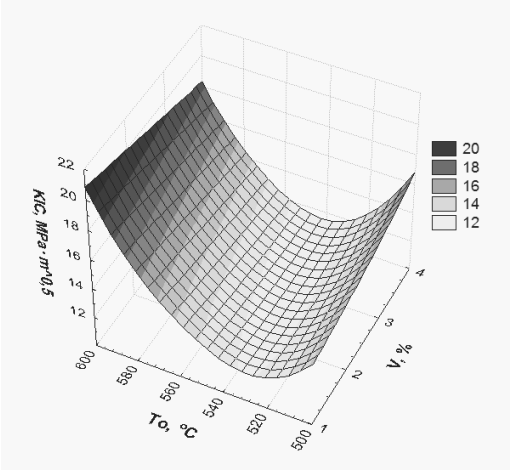


Fig. 74. Effect of vanadium and tempering temperature on the steels fracture toughness K_{Ic}

8. Summary

The main goal of the research carried out was developing the design methodology for the new high-speed steels with the required properties, including hardness and fracture toughness, as the main properties guaranteeing the high durability and quality of tools made from them. It was decided that hardness and fracture toughness K_{Ic} are the criteria used during the high-speed steels design. To this end the relevant models were developed - for hardness and for fracture toughness expressed with the K_{Ic} coefficient.

In case of hardness, two models were developed making computation possible of the high-speed steel hardness based solely on the steel chemical composition and its heat treatment parameters, i.e., austenitizing- and tempering temperatures. The first model, the statistical one, was developed using multiple regression. The other one is the neural network model. In both cases results of own work on the effect of alloy elements on the secondary hardness effect were used, as well as data contained in catalogues and pertinent standards regarding the high-speed steels [62, 63, 110, 114, 134, 174, 216]. Results of the research carried out confirmed the assumption that using the data from catalogues and from standards is possible, which - would supplement the set of data indispensable to develop the assumed model - improving in this way its adequacy and versatility.

The developed models were subjected to experimental verification, which is described in Chapter 5.1 (Table 15, Figures 28-30).

In the second case - high-speed steels fracture toughness, the neural network model was developed, making it possible to calculate the fracture toughness K_{Ic} based on the steel chemical composition and its heat treatment parameters without the need to carry out the metallographic examinations. The model verification results are presented in Chapter 5.2 (Table 16, Figures 34-44).

The developed material models were used for designing the chemical compositions if the new high-speed steel, demonstrating the desired properties, i.e., hardness and fracture toughness.

Methodology was developed to this end, employing the evolutionary algorithms, multicriteria optimisation of the high-speed steels chemical composition. The form of the object function used (eq. 11) and optimisation limitations (Tables 17 and 18) are presented in Chapter 6.

The developed own computer program makes investigations possible pertaining to designing the chemical composition of steel with the required hardness and fracture toughness. Arbitrary defining is possible, within the optimisation limits, of the search space of the optimum chemical composition of the high-speed steel. Moreover, provision is made in the program for adjustment of the optimisation parameters, which can also affect the calculations results, i.e., the arbitrary selection of the set of parameters connected with managing the population. One should clearly stress that computations yield different results each time which results from drawing the initial population. Therefore the results obtained are unique in the entire search space of the optimum chemical composition. On the other hand one should mention that the relationship - chemical composition/treatment parameters ⇔ properties, featuring the materials engineering paradigm holds one-sidedly only. This is because the material with the particular chemical composition at the particular treatment state demonstrated precisely defined properties. There are, however, many different materials with varying chemical compositions, which display the same properties at various treatment states.

Solutions presented in the work, based on using the adequate material models may feature an interesting alternative in designing of the new materials with the required properties. The practical aspect has to be noted, resulting form the developed models, which may successfully replace the above mentioned technological investigations, consisting in one time selection of the chemical composition and heat treatment parameters and experimental verification of the newly developed materials to check of its properties meet the requirements. One should also indicate the possibility of employing the developed models for simulation of the alloy elements effect on the high-steels properties, including analysis of the synergy of interactions of the particular alloy elements (Figs. 55-75) which features and interesting investigation- and didactic tool.

Moreover, it was demonstrated that employment of computer tools makes especially efficient use possible of the existing materials data resources contained in publications, standards, catalogues, and data bases, and their integration in the material models form. There is no denying nowadays the benefits resulting from computer assisted methods in design and manufacturing. The time factor deciding currently success of many projects, and also the economic aspect in design of new products indicates unambiguously to the need for developing and implementing the computer assisted methods also in the materials engineering area, and investigations carried out meet these expectations.

Progress in the area of materials engineering is connected inseparably with employment and development of mathematical modelling, numerical methods, computational intelligence methods, and artificial intelligence. Computer modelling and simulation make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application. Modelling becomes, therefore, the indispensable tool in materials science and in materials engineering.

The presented approach to new materials design, being the new materials design philosophy, assumes the maximum possible limitation of carrying out the indispensable experiments, to take advantage of the existing experimental knowledge resources in the form of databases and most effective computer science tools, including neural networks and evolutionary algorithms. It should be indicated that the materials science knowledge, pertaining oftentimes to the multi-aspect classic problems and described, or - rather - saved in the existing, broadly speaking, databases, features the invaluable source of information which may be used for discovery of the unknown so far relationships describing the material structure - properties relations. The main task is integration of the materials science knowledge and computer science tools to find the new, undiscovered yet relationships and development of materials models based on the knowledge, which was acquired in experimental research over many years. Using the adequate material models makes carrying computer simulations out, which let forecasting possible of materials properties in various configurations of, say, chemical composition, processing stage (e.g., heat treatment) or product type.

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