1. Introduction

Recently the influence of external effect of the environment on material properties - influence of thermal exposition, stress, chemical effect, magnetic field, etc. - was solved above all by the manner indicated in Fig. 1.

Fig. 1

Without any doubts laboratory experiments save costs of real technological processes but the verification of correct technology by experimental tests and analyses which follow, spends time, money and human capacity. That's a reason why simulation programmes, appearing in the last decades, which allow quantitative and qualitative description and graphical monitoring of processes passing in solid, liquid and gaseous systems, have found a broad application. If a simulation programme reflects the system in which the process occurs with sufficient accuracy, calculated values approach to those determined by experiments. This is the way how to make the optimization of technology more efficient.

The modelling of optimum technology development can be demonstrated as follows. In the case of good agreement between calculated and tested properties, a great part of experimentally verified technological processes can be modelled and thus the number of real tests rapidly decreased.

Each process in system of solids is influenced by numerous factors and it is not possible to describe it quantitatively from all points of view simultaneously. The existing programmes usually deal with several selected parameters and only the effect of the most important external factors is considered. If the system is influenced by more independent factors, more programmes must be used for finding out the values. The combination of two, or more programmes gives the possibility to approach to the real changes in material and to the needs of technological practice.

2. Modelling of heterogenous systems

Most of real solid subjects do not consist of homogeneous matter having the same properties and same structure in any place. Materials of objects created by human and natural activity often include many different phases mutually different in chemical composition, crystallic structure and properties. To study heterogenous systems, it is necessary to know the properties of each present phase as well as the structure and behaviour of their boundaries because such specific places can be limiting localities from the view of point of limited properties. The behaviour of material in these places can be different in comparison with the inside of individual monophase areas.

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The modelling of heterogeneous systems represents new dimensions and enormous amount of unsolved tasks, and for their solution, a combination of two different approaches is necessary, i.e. modelling of continuum and discrete modelling of atomic structures.

2.1 Discrete and continuous model

The atomic structure of real bodies is respected in a discrete model. Individual atoms are substituted by mass particles, each of them being the carrier of definite attributes. The target of mathematical formulation of a discrete model is to add to the particles their properties values; i.e. to perform the transformation from the set of particles into the set of attributed values. Each transformation is generally a function of time.

Methods of mechanics of the system of mass particles can be applied on a discrete model of a flexible body.

The number of particles in the bodies of usual dimensions is so large that the applications of discrete models are practically limited to the description of processes in very small material volumes. A physically correct description of material degradation at cyclic load (1, 2), a description of phases boundaries, calculations connected with crystal lattice defects (dislocations, stacking faults, cracks), etc. are the targets of those research activities.

The mechanical continuum - is the model of a body that abstracts from individual particles and substitutes them by infinite infinitesimal particles. Such substitution is an adequate step in macrovolumes which significantly exceed the dimensions and distances between particles; but which is unacceptable in microvolumes. Individual processes are described by partial differential equations where constants and boundary conditions are determined by macroscopic observation of the process.

There are two basic types of correspondence between the discrete model and continuum:

• The correspondence of intensive (nonadditive) properties (attributes) - the set of discrete model particles can be transformed into the set of "subareas" of continuous model so that the nearest "subarea" of the continuous model can be arranged to each particle of a discrete model. This arrangement is called K. The position of particles of a discrete and continuous model is expressed in the same vector area. The attribute value in the given particle of continuum corresponds to the attribute value in a discrete particle. The correspondence of intensive properties values in continuum, which have not its pattern in a discrete model is not defined.

• The correspondence of extensive (additive) properties (attributes) - to the value of a given global property (relating to the whole system or to its substantial part) in a discrete model corresponds its value in the continuous model. The requirement must be valid for any part of the body. Let is chosen a part of the body in the continuous model as a subset of the whole body. This subset corresponds with the subset of all particles in a discrete model to which K arrangement allocates subareas of the continuum in the given area. Additive local properties in the continuum model are designed from global properties as their intensities [3].

3. Programmes for modelling on a continuum base

The number of continuum based programmes offered for the use has significantly increased in the last years. Simulation programme interfere now with many activities of engineering practice. The calculation analysis is solved with the help of FEM programme packages. Special tasks are fulfilled by individual programmes which are mutually connected, using the same equipment (graphic labor stations), using the same language with user (interactive pre/post processors, connection with CAD). The tasks up to 3D are solved by these programme sets. Sysweld, Systus and Forge Programmes packages are especially preferred in our applications.

3.1 Sysweld programme package

The modelling of technological operation of the volume and surface heat treatment, welding, tipping and some further surface treatments is carried out by Sysweld programme package.

Thermal deformation and diffusion fields with the possibility to include phase transformations as well as materials structure can be solved [4, 5].

The simulation programme follows above all from the following parameters of the system:

• Phase composition and phase transformations
• Material structure
• Temperature distribution in system
• Concentration distribution of some elements
• Stress and deformation distribution

3.2 Systus programme package

This software is a general system of finite elements enabling to solve the tasks of continuum mechanics, thermal and electromagnetic field tasks. Its nonlinear modulus includes material models which enable to describe the behaviour of material with porosity (Gursan-Tvergaard model). This programme package was recently elaborated in IRSID laboratories (France).

3.3 Forge 3 programme package

3D tasks dealing with calculations of all thermodynamic parameters for cold and hot forming can be solved by Forge 3 programme. It includes a numerical analysis of cold and hot forming of a flexible body by the method of finite elements, further functions of pre- and post-processing. The programme is autogenerative
and during calculation the net of finite elements can be adapted by the subprogramme Mesh, capable to change interactively the density of knots in localities where it is necessary for simulation.

It is supposed that the material model of an investigated body is homogeneous and incompressible in all places. Its behaviour at deformation is described by Norton-Hoff constitutional law:

\[ s_g = 2K(\sqrt{3})^{m-1}e^{\epsilon} \]  \hspace{1cm} (1)

where \( s \) - deviator of stress tensor,  
\( e \) - deformation velocity tensor,  
\( K \) - material constant,  
\( m \) - coefficient depending on deformation velocity.

The friction of tool during forming brings the necessity to include shear stress \( \tau \) on the interface tool/formed body. Its value depends on the slip rate of deformed material on the tool:

\[ \tau = -aK\Delta\nu \]  \hspace{1cm} (2)

where \( \alpha \) and \( K \) - variable coefficients depending on the place of contact of a tool with a semi-finished product.

Deformation process is solved by auxiliary system of equations of equilibrium forces. The forces include the behaviour of material according to equation (1), its incompressibility and friction of a deformed body with a tool.

The thermo-viscoplastic analysis is carried out by simultaneous solution of continuum mechanics and thermal problem.

3.4 Task of experimental activity at modelling

Three basic partial parts must be fulfilled at modelling of any system:

a) Pre-processing - getting data dealing with the system to be modelled, data entry into the programme, the entry of the environment influence on the system.

b) Processing - treatment of input data and own calculations of the system parameters - changes of material properties, intensity of force fields, energies, etc.

c) Post-processing - treatment of calculated values, their comparison with experiments.

4. Application of real modelling systems

Thanks to the project of the Czech Ministry of Education, called "250", at our Department of Materials Science and Technology, a new modern laboratory of processes simulation, equipped with two Silicon Graphic Indigo R5000 stations, one 500au DEC OSF/1 graphic station, and Forge 2D and 3D, Hypermesh, Systus and Sysweld software systems was built up and some research programmes were initiated.

4.1 Simulation of cold deformation effect on the structure of P900 steel

Austenitic CrMn steels with N are characterized by high strength, high \( R_m/R_m \) value, high toughness, stability of austenitic structure and by excellent stress-corrosion resistance. They are used for the components with extreme mechanical and corrosion load. At the same time paramagnetic behaviour of material must be guaranteed.

The increase of the strength of this type of steel can be reached by different ways. It is possible either to change chemical composition of the steel (to achieve the maximum N concentration) or to optimize technology of the following treatment (i.e. cold forming and heat treatment) of cast semi-product.

Experimental programmes aimed at the optimization process of cold deformation and subsequent treatment are carried out on P900 - Cr18Mn18N steel. During material treatment, stress and deformation tensors in any place of a forged piece, or of a model specimen, are determined. These parameters have a direct effect on the creation of very fine substructure of slip band dislocations and deformation twins inside austenitic grains.

If more slip systems (with moving dislocations inside) are activated and if deformation twins appear on different planes of the type (111), their mutual crossing occurs. Slip bands intersection and above all the intersections of deformation twins create areas of effective blocking of dislocation movement [7]. With respect to the dimensions and mutual distances of deformation twins, ten thousands of such intersections (in volume of approx. 0.2 mm³) may appear. This effect and further strengthening mechanisms lead to high strength values of these austenitic types. One of the main targets of this research programme is to reach optimum distribution of deformation twins (uniform with the highest density).

The tool to influence the structure by a controlled deformation combined with heat treatment - it is functionally structuring of treated material.

A partial study from a broad program is presented, where computer simulation with the help of Forge 2 (based on FEM) using tensile and pressure tests was carried out.

For the measuring of P900 steel deformation characteristics, tensile tests and some modifications of pressure and torsion tests were used.

The obtained stress-deformation curves allow to assess material behaviour for a computer simulation.

As the tests were strongly influenced by friction some modifications of pressure tests were carried out in order to evaluate the possibility how to decrease the friction. From comparison of individual modifications of pressure test, it is clear, that the effect of increased friction shifts the curves to higher values of deformation stress (Fig. 2). The evident shift of the curves to lower stresses depends on the method used for the elimination of friction; pressure-specimen No. 4 - flat specimen without lubricant, pressure-
specimen No. 9 - Rastragaev method, pressure - specimen No. 14 - grooved face with lubricant use, Larke method of extrapolation.

The curves of grooved face specimens are similar to those of flat face; this way to reduce friction on pressure tests is not suitable for the tests at the given conditions. The curves from Rastragaev specimens give lower values of deformation stresses comparing with the former tests modifications.

Depending on deformation the elimination of friction with the help of Larke method brought a futher decrease of deformation stresses.

Comparing individual modifications of pressure tests with tensile ones, it is found that pressure tests curves approach to the tensile one with the decreasing influence of friction (Fig. 2). Based on the analysis of test results describing deformation behaviour, tensile test curve for underformed material was chosen for the evaluation of rheological parameters for computer simulation. In order to obtain relevant coefficients, a part of the curve representing elastic behaviour was removed at first and the part from the beginning of neck formation was removed afterwards. The curve in coordinates real stress - real deformation, describes deformation behaviour of the steel for computer simulation. It approaches to the straight line (by shape) - Fig. 3. In Forge 2 programme some material models are implemented for the description of material behaviour, equation describing material with linear strengthening complies for this case. To get parameters for this equation regressive analysis of cut curve in the Microsoft Excell programme was made. The parameters of regressive straight line are in Fig. 3: $K_o = 565$ MPa and $a = 3.38$. Friction coefficient value was taken from ring specimen test $\mu = 0.15$. Using these parameters, FEM simulation of pressure and tensile tests was made to compare experimental and calculated values.

4.1.1 Simulation of pressure test

Simulation of pressure test represents the solution of rotationally symmetric task at normal temperature in material with linear strengthening.

At first, the geometric model of testing body (small cylinder) was formed. With respect to the symmetry, one half of the specimen, suffices for simulation. This half was subsequently meshed and calculation net formed by triangles, with nine integral points. Then the geometry of pressing plates was created, modelled as asymmetric and perfectly rigid body. Top plate was firm and bottom mobile as in the case of loading on the MTS 500 kN machine. Deformation velocity was identical with that during pressure tests. After first calculation, stress/deformation relationships obtained by simulation and experiment were compared. Based on this comparison, calculated model of material proved to be "too soft". To achieve maximum agreement between simulation and experiment some calculations with gradually increased parameter $a$ were carried out. Minimum difference between experimental and calculated curves was reached for $a = 3.57$ - Fig. 4.

4.1.2 Simulation of tensile test

FEM simulation of tensile test was made to evaluate proposed rheological parameters for P900 steel. Similar simplifications as in the previous case were used - Fig. 3. Problem was calculated as a symmetric task and jaws were mentioned to be perfectly rigid. After calculation, the stress curve deformation relationship was evaluated again and simulated was almost identical with the measured one - Fig. 3.

4.1.3 Computer simulation evaluation

Computer simulation gave informations about loading during specimen deformation, geometry of deformed bodies and stress distribution in cross-section of the component after deformation. The course of loading related to deformation was trasferred from Forge 2 into Microsoft Excell and evaluated.

Relationship obtained by simulation were recalculated to the values of real stress and deformation, and such prepared curves compared. Curves obtained after deformation strengthening coefficient "tuning" are in a good agreement with experimentally found values.
Some deviation from the experimental curve is visible in case of pressure test. The deviation may be caused by inaccuracy in determination of friction coefficient. Friction coefficient value determined by ring specimen tests is probably lower than the real value.

Higher value of friction coefficient should result in the growth of deformation stress and simulated curve should approach to the measured one.

4.2 Simulation of free forging of CrMo steel shafts

The 42CrMo4 steel is used for the manufacture of large crankshafts in inland and abroad. This CrMo steel possesses relatively good hot formability and, in soft annealed state also good machinability. It is suitable for quenching in oil, reaching comfortable value of notch toughness at high strength. It possesses increased resistance against tempering and is suitable for application at increased temperatures up to 500 °C. Heat treated at strength over 1050 MPa it proves also an increased wear resistance. It is suitable for surface quenching and is not sensitive to the temper brittleness.

Experimental verification of structure, and properties in the whole volume of forging spends time and money and puts high demands on technical realization. One possibility how to solve this problem is modelling of processes passing during the own manufacture. This could substitute a large part of experiments. Forming and heat treatment are simulated by Forge 3D and Sysweld programmes; their combination allows to model hot forming, quenching and tempering. Simulation is aimed at final structure, hardness, strength and notch toughness.

Presented partial study demonstrates the application of Sysweld programme for the estimation individual structural components fraction during cooling of 16 343 steel from quenching temperature. Experimental values were obtained by dilatometric measurement and quantitative image analysis.

Procedure to determine parameters for Leblond model is included in Sysweld +. Coefficients necessary for calculations; are determined from ARA diagram, the beginning and end of transformation and final fraction of each phase according to the cooling rate. On the basis of these coefficients, the set representing metallurgical transformations in material is formed. Sysweld + programme includes the tool for drawing of ARA diagram too.

5. Conclusion

Simulation methods prove important qualitative as well as quantitative contribution to the optimization of technological processes and properties of products.

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Literatura - References


