Journal of Achievements in Materials and Manufacturing Engineering
VOLUME 20
ISSUES 1-2
January-February
2007

Modelling of heterogenous structure materials – important contribution to the optimalisation of forming and heat treatment of structural steels

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Received 07.11.2006; accepted in revised form 15.11.2006

Analysis and modelling

ABSTRACT

Purpose: New laboratory equipped for modelling of technological processes.Methods of modelling.
Design/methodology/approach: Laboratory equipped by two Silicon Graphic Indigo R 5000 stations,by one 500 an DEC OSF/1 station and by Forge 2D and 3D,Hypermesh,Systus and Sysweld software systems was built up in the Department of Material Science and Technology at WBU Plzeň.
Findings: Some research programmes solving modeling of optimalization of technological processes like simulation of cold deformation influence on the structure of P900 steel,or simulation of free forging of shafts manufactured from CrMo steel were carried out.
Research limitations/implications: Partial results give a good agreement between experimental results and simulation methods.It is suitable to extent the experiments on futher forged components.
Practical implications: Results can be successfully used for efficient technology of components forging.
Originality/value: Published results are original informations about contribution of modelling to specifying of technological parameters.
Keywords: Modelling of technological processes; Computer simulation; Modeling programmes

1. Introduction

Recently the influence of external effect of enviroment on materials properties changes - influence of thermal exposition, stress, chemical effect, magnetic field, etc. - was solved almost exclusively by the manner indicated in fig. 1.

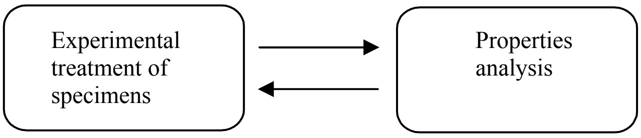

Fig. 1

Laboratory experiments save costs of real technological processes without any doubts but the verification of correct technology by the experimental tests and analyses which follows, is financially, timely and personally very exacting. From this reason and with together the development of computer technic possibilities, simulation programmes - relatively not long ago – quantitatively and qualitatively describing the graphically indicating processes passing in solid, liquid and gaseous systems, appeared recently. If the system, in which the process shall pass through simulation programme, is satisfactory exactly afflicted, it is possible to reach the values experimentally found before by calculation. That is the way of considerable efficiency of searching of optimum technology.

Modelling inclusion in the process of development of optimum technology can be demonstrated as follows. In the case of good agreement of calculated and tested properties, a great portion of tested technological processes can be carried out by the way of modelling and the number of real tests can be rapidly decreased.

Every process in the system of solids is influenced by many factors and it is not possible to describe it quantitatively from all points of view contemporaly.

Existing programmes are usually following only some selected parameters and from external influences on these parameters the most important ones are only considered. If the system is influenced by more indenpendant factors, more programmes must be used for finding out of values. The combination of two, or more programmes gives the possibility to approach to real changes in material and to necessities of technological practice.

2. Modelling of heterogenous systems

Most of real solid subjects are not consisted of homogeneous matter having the same properties and same structure in any place. Materials of objects created by human and natural production often include many different phases mutually different in chemical composition, crystallic structure and properties. To study heterogeneous systems, it is necessary to know the properties of each present phase as well as structure and behavior of their mutual interphases; these specific places can be limited localities from the point of view of limited properties. The behavior of material in these places can be different in comparison with inside individual monophase areas.

Modelling of heterogeneous systems represents new dimensions and enormous amount of unsolved tasks: Combination of two different approaches is necessary - modelling of continuum and discrete modelling of atomic structures.

2.1. Discrete and continous model

Atomic structure of real bodies is respected in discrete model. Individual atoms are substituted by mass points called particles, each of them being the carrier of definite attributes. The target of mathematical formulation of discrete model - to add to the particles their properties values: to perform the transformation from the set of particles into the set of attributes values. Each tranformation is generally the time function.

Mechanics apparatus of the system of massive points can be applied on discrete model of body.

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

Mechanical continuum - it is the model of body that abstracts from individual particles through their joint spreading and substitutes them by infinite infinitesimal particles. Such substitution is an adequate turn in macrovolumes significantly exceeding the dimensions and distances of particles; but in microvolumes is unacceptable. Individual processes are described by partial differential equations where constants and margin conditions are determined on the base of macroscopic watching of the process.

Two basic types of correspondence between discrete model and continuum exist:

- Correspondence of intensive (nonadditive) properties (attribute) - the set of discrete model particles can be transformated into the set of ”subareas” of continuous model so that the nearest ”subarea” of continuous model can be arranged to each particle of discrete model. This arrangement is called K. The position of particles of 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 discrete particle. Correspondences of intensive properties of continuous area, not having model in discrete model are not defined (3).
- Correspondence of extensive (additive) properties (attributes) - to the value of a given global property (relating to the whole system or to its substantional part) in discrete model corresponds to its value in continuous model. The requirement must be valid for any part of the body. Let us eliminate a part of body in continuous model as a subset of whole body. Subset of all particles of discrete model (transformation K arranges to this area). Additive local properties are constructed in continuum model from global properties as their intensity (3).

3. Programmesfor modeling on continuum base

Continuum base programmes offer for public use increased significantly in last years. Simulation programmes interfere now in many activities of engineering practice. The calculation analysis is solved by help of programme sets of finite elements method, joined in one integrated unity. Special tasks are fullfilled by individual members of this unity and they are mutually connected, using the same equipments (graphic labor stations), using the same language with user (interactive pre/post processors, connection with CAD). The tasks till up to 3D are solved by these programmes sets. Sysweld, Systus and Forge Programmes sets are especially favorized in our applications.

3.1. Sysweld programme set

Modelling of technological operation of volume and surface heat treatment, welding, tipping and some futher surface treatment by help of numeric methods of finite elements is possible by Sysweld programme set.

Thermal deformation and diffusion fields with the possibility of including phase transformations as well as materials structure can be solved (4, 5).

Simulation programme expresses mainly following properties an system parameters:

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

3.2. Sysweld programme set

This software is generally orientated system of finite elements making possible to solve tasks of continuum mechanics, thermal tasks and electromagnetic fields tasks. In its nonlinear modulus material models making possible to describe the behaviour of material with porosity (Gursan-Tvergaard model) are included. This programme set was recently elaborated in IRSID laboratories (France).

3.3. Forge 3 programme set

3D tasks dealing with calculations of all thermodynamic parameters at cold and warm formation can be solved by Forge 3 programme set. It includes numeric analysis of cold and warm formation of flexible body by the method of finite elements, futher functions of pre and postprocessing. The programme is autogenerative and during calculation the net of finite elements can be adapted by the subprogramme Mesh, capable to change interactively density of knots in necessary places during own simulation.

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

$$s_{ij} = 2K\left(\sqrt{3}\bar{\varepsilon}\right)^{m-1} \varepsilon_{ij} \qquad (1)$$

where s - deviator of stress tensor, ε - deformation velocity tensor, $\bar{\varepsilon}$ - equivalent deformation velocity. K - material constant, m - coefficient depending on deformation velocity.

Friction of tool during formation brings the necessity of including of shear stress τ - on interface tool - formed body. Its value is dependent on yield velocity of material on tool:

$$\tau = -\alpha K \Delta v \qquad (2)$$

where α - and K - variable coefficients depending on place of contact of tool with semi finished product.

The deformation process is solved by help of equilibrium forces equations system; forces including the behaviour of material according equation (1), its incompressibility and friction of deformed body with tool.

Thermo-viscoplastic analysis is carried out by current solution of continuum mechanics and thermal problems.

3.4. Task of experimental activity at modelling

Three basis partial parts must be fullfilled at modelling of any system:

a) Pre-processing-getting informations dealing with modelled system, its ordering in programme, ordering of environment influence on system.

b) Processing-treatment of introductory informations and own calculations of system parametres - changes of material properties, intensity of forces fields, energies, etc.

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

4. Application of real modeling systems

Thanks to the project of Czech Ministry of Education, Youth and Gymnastics, called ”250”, in our Department Materials Science and Technology, a new modern laboratory of processes simulation, equipped by two Silicon Graphic Indico R5000 stations by one 500 an 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 on the structure of P900 steel

Austenitic CrMn steels with N are characterized by high strength, high R_E/R_M value, high toughness, stability of austenitic structure and excellent stress-corrosion resistance. They are used for the components extremely loaded by mechanical stress and corrosion; contemporarely paramagnetic behaviour of material must be guarantied [8, 9, 10].

Increase of the strength of this type of steel can be reached by different manner. It is possible either to change the chemical composition of alloy steel (to achieve the maximum N concentration) or to optimalize technology of following treatment (formation and heat treatment) of cast semi-product.

Experimental programmes orientated to the optimalization process of cold deformation and treatment are carried out on P900 - Cr18Mn18N steel. During material treatment, stress and deformation tensors in any place of forged piece, resp. of model specimen, are under determination. These parameters are influenced directly by very fine substructure of slip bands of dislocations and deformation twins inside austenitic grains.

If more systems (inside dislocations are in motion) are activated and if deformation twins appear on different planes of type (111), their mutual crossing follow. Places of two slip bands intersection and mainly deformation twins intersections create areas of effective blocking of dislocation movement [7]. With respect to the dimensions and mutual distances of deformation twins, ten thousends of such intersections (in volume of cca 0,2 mm^2) may appear. Along with futher strengthing mechanisms high strength values of these austenitic types can appear. One of the main targets of this research programme is to reach the optimalized distribution of deformation twins (uniform and of highest density).

The tool of influencing of the structure by controlled deformation combined with heat treatment - it is functionally structuring of treated material. There is presented partial study from extent programme, where computer simulation by help of Forge 2 (based on the method of finite elements) utilizing tensile and pressure tests was carried out.

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

Stress-deformation curves, were the product of all types of tests, giving the possibility of materials behaviour for computer simulation.

Because of strong influencing of tests by friction, some modifications of pressure tests were carried out to evaluate the possibility of decrease of friction. By friction influence (comparing individual modifications of pressure tests) the curves are shifted to the higher values of deformation stress with increasing friction (fig. 2). Evident shift of the curves follows to lower stress depending on the method of friction elimination pressure-specimen No. 4 - flat specimen without lubricant, pressure-specimen No. 9 - Rastragaev method, pressure - specimen No. 14 - grooving face with lubricant use, Larke method of extrapolation. Curves of grooving faces specimens are the similar curves as flat faces specimens ones; this way of removing of friction influence on pressure tests is not suitable for tests at given conditions. Curves from Rastragaev specimens give lower values of deformation stresses comparing with former tests modifications.

The elimination of friction by help of Larke method brought futher decreasing of deformation stresses in dependance on deformation.

Comparing individual modifications of pressure tests with tensile ones, it is found that pressure tests curves approach to the tensile one with decreasing influence of friction (fig. 2). After tests results analysis describing deformation behaviour of the curve of tensile test of undeformed material rheological parameters for computer simulation were chosen for evaluation. A part of curve representing elastic behaviour was removed first and afterwards the part from the beginning of neck formation was removed too. Constructing graph in coordinates real stress - real deformation, the curve describing deformation behaviour of steel for computer simulation was obtained. The resulting curve approaches to the straight line (by shape) - fig. 4. In Forge 2 programme some material models are implemented for material behaviour description, equation describing material with linear strengthening complies in this case. To get parameters for this equation regresive analysis of limited (cut) curve in the Microsoft Excell programme was made. The parameters of regresive 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, MFE simulation of pressure and tensile tests was made to compare tested values with calculated ones.

Simulation of pressure test

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

First, geometric model of testing body - small cylinder was formed. With respect to that task, it was symmetric, half of the specimen, followly meshed, was sufficient. The calculation net was formed by triangles, with nine integral points. The formation of geometry of pressured plates followed, modelled as assymetric and perfectly rigid ones. Top plate was firm and bottom one mobile as in the case of deformation on the MTS 500 kN machine. Deformation velocity was identical with one during pressure tests. After first calculation the values of deformation stress in dependence on deformation obtained by simulation and experimentally examined were compared. After comparing of dependency strength-deformation calculated model of material proved to be ”soft”. To achieve the maximum agreement of simulation and experimental results some calculations at gradual increasing of parameter a were carried out. Minimum difference between experimentally measured and calculated curves was reached at a = 3,57 - fig. 4.

Simulation of tensile test

FE 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.The task was calculated as the symmetric case and jaws were mentioned to be perfectly rigid.

The stress in dependence on specimen deformation was evaluated, again after calculation; the curve after simulation is almost identical with the measured one - fig. 3.

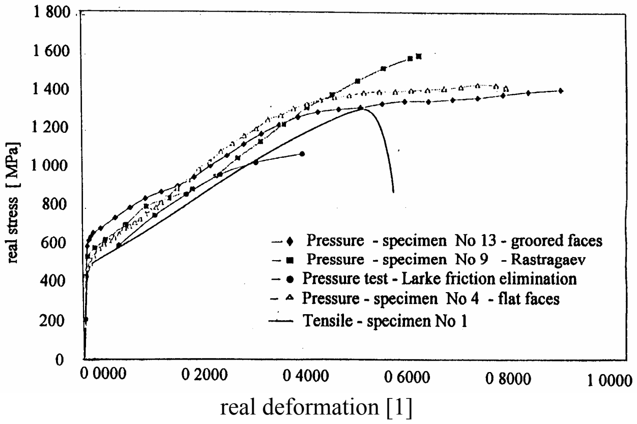

Fig. 2. Comparison of individual methods of pressure tests with tensile one

Computer simulation evaluation

Computer simulation gave informations of loading during specimen deformation, of geometry of deformed bodies and distribution across the section of component after deformation. Courses of loading in dependence on deformation were exported from the Forge 2 programme into Microsoft Excell one, where they were evaluated.

Dependences obtained by simulation were recounted to the real stress and deformation values, such prepared curves were compared. Curves obtained after ”tuning” of deformation strengthening coefficient are in good agreement with experimentally found values.

Some deviation from the experimental curve is visible in the 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 friction coefficient value should prove the growth of deformation stress, then the curve from simulation should approach to the measured one.

4.2. Simulation of free forging of CrMo steel shafts

42CrMo4 steel is used for manufacture of bulky crankshafts in inland as well as abroad.

CrMn steel is relatively well warm formed, in softannealed state is also well machinable. It is suitable for quenching in oil, reaching comfortable value of notch toughness at high strength. It posseses increased resistance against tempering, it is suitable for application at increased temperatures up to 500 °C. Heat treated to the strength over 1050 MPa proves increased friction resistance. It is suitable for surface quenching and is not sensitive to the temper brittleness.

Experimental verification of structure, resp. of properties in the whole volume of forging is timely financially and technically very exactive. One of the possibilities of this problem solution is modelling of processes passing during the own manufacture; it could substitute large part of experiments. Forming and heat treatment are simulated by Forge 3D and Sysweld programmes; their combination makes possible to model warm deformation, quenching and tempering. Simulation is directed to the final structure, hardness, strength and notch toughness.

Presented partial study demonstrates the application of Sysweldprogrammeforestimation ofstructurecomponents portions during cooling of 16 343 steel from quenching temperature.

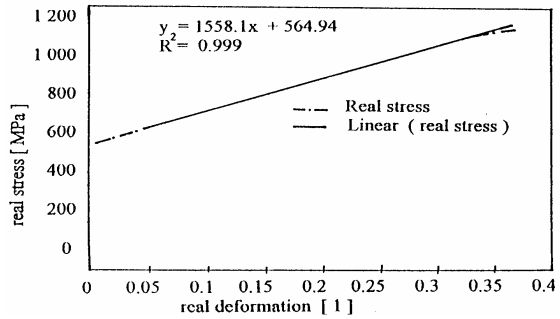

Fig. 3. Determination of deformation strengthening coefficient

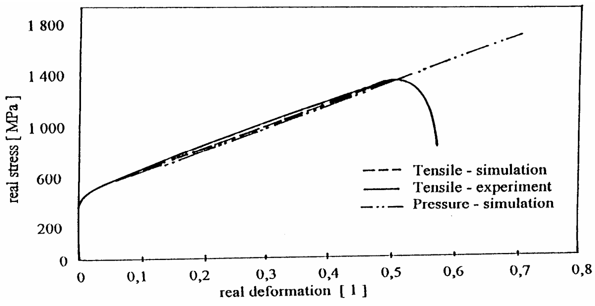

Fig. 4. Comparison of MFE simulation results with experimental values

The values got by dilatometric measurement and values from quantitative image analysis are well comparable. Dilatometric analysis gives systematically higher amount of bainite (4 - 5% more) than picture analysis measurement for all five investigated specimens (fig. 5). The values obtained by calculation in Sysweld programme are dependent on accuracy of assigning of ARA diagrams into programme. ARA diagram accuracy is wound off corectness of thermophysical material values, measured transformation temperatures and qualitative evaluation of phase portions. More precise description of individual phase tranformation gives more precise results of phase portions for applied cooling of experimental material.

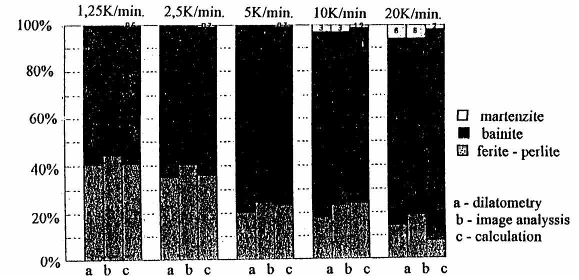

Fig. 5. Comparison of final phase portions determined by method of evaluation of dilatometric curves, by image analysis and numerical calculation

5. Conclusions

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

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